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Guidance on the Biocidal Products Regulation

Volume IV Environment - Assessment and Evaluation (Parts B + C)

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European Chemicals Agency

Mailing address: P.O. Box 400, FI-00121 Helsinki, Finland
Visiting address: Annankatu 18, Helsinki, Finland

DOCUMENT HISTORY

Version	Changes	
Version 1.0	First edition (active substances only)	April 2015

Version 2.0	Update to:
	• address Part C Evaluation: The text has been revised as follows:
	  ○ Preface: updated to be in line with the general information in the Part A;
	  ○ General Introduction: a new paragraph to explain the association of the evaluation and assessment processes.
	• add text and links on "Applicability of Guidance" in the Preface;
	• add guidance on Biocidal Products and incorporating the published Transitional Guidance on Mixtures;
	• add guidance on Substances of Concern
	• Deletion of Appendix 5 (Information on the difference in diversity between seawater and freshwater);
		October 2017

PREFACE

The Guidance on the Biocidal Products Regulation (BPR) is to be applied to applications for active substance approval and product authorisation as submitted from 1 September 2013, the date of application (DoA) of the Biocidal Product Regulation (the BPR).

This document describes the requirements under the BPR and how to fulfil them.

The scientific guidance provides technical scientific advice on how to fulfil the information requirements set by the BPR (Part A), how to perform the risk assessment and the exposure assessment for the evaluation of the human health and environmental aspects and how to asses and evaluate the efficacy to establish the benefit arising from the use of biocidal products and that it is sufficiently effective (Parts B & C).

In addition to the BPR guidance, the Biocidal Products Directive (BPD) guidance and other related documents are still considered applicable for new submissions under the BPR in the areas where the BPR guidance is under preparation. Furthermore these documents are still valid in relation to the evaluation of applications for active substance approval or applications for product authorisation submitted for the purposes of Directive 98/8/EC (BPD) which may still be under the Biocidal Products Regulation (BPR). Also the Commission has addressed some of the obligations in further detail in the Biocides competent authorities meetings documents which applicants are advised to consult. Please see ECHA Biocides Guidance website for links to these documents: [https://echa.europa.eu/guidance-documents/guidance-on-biocides-legislation].

The basis of this guidance is the EU-TGD of 2003, which was adapted with regard to references and content of the BPR. In addition any text from existing other guidance under the BPD was merged in case it was not covered by the TGD (e.g. text from the TNsG on BPR Annex I inclusion and TNsG on product evaluation but also existing specific guidance on e.g. rapidly degrading substances). This was done to concentrate environmental risk assessment related text in single document to have one common basis for future revisions.

The former Appendix I of the TGD (containing emission factors for the tonnage-based approach for emission estimation including the A and B tables) is in **Appendix 6** of this guidance.

The former Appendix II of the TGD (containing tables to estimate the distribution in the STP) has not been includedbecause the distribution in the STP should be calculated with EUSES or Simple Treat (decision of TM I 2011) owing to the calculations being more accurate.

New developments in the exposure, effect and risk assessment described in the Manual of Technical Agreements (MOTA), version 6 and the Evaluation Manual (prepared by NL) have been included in this document mainly in the form of "Info-boxes". The MOTA will continue to exist (as TAB: Technical agreements for Biocides[1]) and those parts of MOTA v.6 that did not fit in to the guidance have been carried forward to the TAB, prepared by ECHA.

[1] Avaliable on ECHA website: https://www.echa.europa.eu/web/guest/about-us/who-we-are/biocidal-products-committee/working-groups

Applicability of Guidance

Guidance on applicability of new guidance or guidance related documents for active substance approval is given in the published document "*Applicability time of new guidance and guidance-related documents in active substance approval*" available on the BPC Webpage[2] [https://echa.europa.eu/about-us/who-we-are/biocidal-products-committee] and for applicability of guidance for product authorisation, please see the CA-document CA-july2012-doc6.2d (final), available on the ECHA Guidance page [https://echa.europa.eu/documents/10162/23036409/ca-july12-doc_6_2d_final_en.pdf].

[2] Link available under Working Procedures (right column) [https://echa.europa.eu/about-us/who-we-are/biocidal-products-committee]

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NOTES to the reader:

In this document text cited from the Biocidal Products Regulation (EU) No 528/2012 is indicated in green boxes.

This symbol highlights text to be noted.

List of Abbreviations

Standard term / Abbreviation	Explanation
AA-EQS	Annual average environmental quality standards
ACR	Acute to chronic ratio
AF	Assessment factor
AOPWIN	EPI Suite software to estimate the atmospheric oxidation rates (US EPA)
AV	Avoidance factor
AVS (-concept)	Acid Volatile Sulphide
BCF	Bioconcentration factor
BMF	Biomagnification factor
BPD	Directive 98/8/EC of the European Parliament and of the Council of 16 February 1998 concerning the placing of biocidal products on the market
BOD	Biological oxygen demand
BW	Body weight [g or kg]
CA	Concentration addition
CAR	Competent Authority report
CBA	Component-based approaches
CBB	Critical body burden
CDS	Core data set
CHARM	Chemical Hazard Assessment and Risk Management (model)
ChemUSES	Chemical Use Standard Encoding System
CLASSIC	Community Level Aquatic System Studies Interpretation Criteria (PPP)

Standard term / Abbreviation	Explanation
CLP	Regulation (EC) No 1272/2008 of the European Parliament and of the Council of 16 December 2008 on classification, labelling and packaging of substances and mixtures, amending and repealing Directives 67/548/EEC and 1999/45/EC, and amending Regulation (EC) No 1907/2006
COD	Chemical oxygen demand
CONCAWE	The Oil Companies' European Organisation for Environmental and Health Protection
CONV	Conversion factor from NOAEL to NOEC ($CONV_{mammal}$ or $CONV_{bird}$.) [$kg_{bw} \cdot d \cdot kg_{food}^{-1}$]
DFI	Daily food intake [$g \cdot day^{-1}$]
DRANC	Dutch Risk Assessment System for New Chemicals
DT_{50}	Period required for 50% degradation (define method of estimation)
DWI	Daily water intake [$mg \cdot l^{-1} \cdot day^{-1}$]
DWI/DFI	Conversion factor from $mg \cdot l^{-1} \cdot day^{-1}$ to $mg \cdot kg\ food^{-1}$
EBI	Ergosterolbiosynthesis-inhibting
EC	Effect Concentration
EC_{50}	Median effective concentration
ECB	European Chemicals Bureau
ECETOC	European Centre for Ecotoxicology and Toxicology of Chemicals
EDTA	Ethylenediaminetetraacetic acid
EEA	European Economic Area
EF	Emission factor
EFSA	European Food Safety Agency
EIFAC	European Inland Fisheries Advisory Commission
EINECS	European Inventory of Existing Commercial Chemical Substances
ELINK	Linking aquatic exposure and effects in the registration procedure of plant protection products
EPA (DK, US)	Environmental Protection Agency (of Denmark, or the United States of America)
EPM	Equilibrium Partitioning Method
E-PRTR	European Pollutant Release and Transfer Register
EQS	Environmental Quality Standard
ERA	Environmental risk assessment
ERC	Ecotoxicologically relevant concentration (ERC)

Standard term / Abbreviation	Explanation
ESD	Emission Scenario Document
ETO	Ecological threshold option
EU	European Union
EUBEES	"Gathering, review and development of environmental emission scenarios for biocides" (EU project)
EUSES	European Union System for the Evaluation of Substances
FAO	Food and Agriculture Organization
FOCUS	Forum for the Coordination of Pesticide Fate Models and their Use (European pesticide project for risk assessment)
HARAP	Higher-Tier Aquatic Risk Assessment for Pesticides
HBM	Hydrocarbon Block Method
HEDSET	Harmonised Electronic Data Set (EC/OECD)
HELCOM	The Baltic Marine Environment Protection Commission
HPVC	High production volume chemicals
IA	Independent action
IC	Industrial category
IR	Infrared
IFEN	Institut Français de l'Environnement
ISO/DIN	International Standards Organisation/ German Institute for Standardization
IUCLID	International Uniform Chemical Information Database
JRC	Joint Research Centre
K_{OC}	Organic carbon adsorption coefficient
K_{OM}	Partition coefficient normalized to organic matter [L kg^{-1}]
K_{OW}	Octanol-water partition coefficient
K_P	Solids-water partition coefficient [L · kg^{-1}]
LC_{50}	Median lethal concentration
L(E)CX	Lethal (effective) concentration at a specific mortality rate [X %]
LEMTOX	Ecological models in support of regulatory risk assessments of pesticides Developing a Strategy for the Future
LOD	Limit of quantification
LOEC	Lowest observed effect concentration

Standard term / Abbreviation	Explanation
LOQ	Limit of quantification
MAF	Mixture assessment factor
MAMPEC	Marine antifoulant model to predict environmental concentrations
MATC	Maximal acceptable toxicant concentration
MC	Main Category
MCR	Maximum cumulative ration
MDD	Minimal detectable difference
MITI	Ministry of International Trade and Industry (Japan)
MoA	Mode of action
MOTA	Manual of Technical Agreements of the Biocides Technical Meeting
MS/MSCA	Member State/Member State Competent Authority
NOAEL	No observed adverse effect level
NOEAEC	No observed ecologically adverse effect concentration
NOEC	No observed effect concentration
NTA	Non-target arthropods
OECD	Organisation for Economic Cooperation and Development
OPPTS	Office of Prevention, Pesticides, and Toxic Substances (U.S.-EPA)
OPS	Operational Priority Substances (model)
OSPAR	Oslo and Paris Conventions
PBT/vPvB	Persistent Bioaccumulative and Toxic/ very Persistent very Bioaccumulative
PEARL	Pesticide Emission At Regional and Local Scales
PEC	predicted environmental concentration
PELMO	Pesticide Leaching Model
PD	Fraction of food type in diet
pH	pH-value, negative decadic logarithm of the hydrogen ion concentration
PNEC	Predicted no effect concentration
POP	Persistent organic pollutant
PPP	Plant Protection Products
PRISEC	PRIority Setting system for Existing Chemicals
PT	Product-type

Standard term / Abbreviation	Explanation
PT	Fraction of diet obtained in treated area
QSAR	Quantitative structure-activity relationship
RA	Risk assessment
RAC	Regulatory acceptable concentrations
RBT	Ready biodegradability test
REACH	Regulation (EC) No 1907/2006 of the European Parliament and of the Council of 18 December 2006 concerning the Registration, Evaluation, Authorisation and Restriction of Chemicals (REACH), establishing a European Chemicals Agency, amending Directive 1999/45/EC and repealing Council Regulation (EEC) No 793/93 and Commission Regulation (EC) No 1488/94 as well as Council Directive 76/769/EEC and Commission Directives 91/155/EEC, 93/67/EEC, 93/105/EC and 2000/21/EC
RIVM	Rijksinstituut voor Volksgezondheid en Milieu (Dutch National Institute of Public Health and the Environment)
RMM	Risk Mitigation Measure
RQ	Risk quotient
$RQ_{Product}$	Risk Quotient of the Product
SCB	Statistiska centralbyrån (Official Statistics of Sweden)
SoC	Substance of concern
SOP	Standard operating procedure
SRT	Sludge retention time
SSD	Species sensitivity distribution
STP	Sewage treatment plant
STU	Sum of Toxic Units
TGD	Technical guidance document (EU, 2003)
TM	Technical meeting
TNO	Nederlandse Organisatie voor Toegepast Natuurwetenschappelijk Onderzoek (Netherlands Organisation for Applied Scientific Research)
TNsG	Technical Notes for Guidance
TU	Toxic Unit
TUS	Toxic unit summation
TWA	Time-weighted average
UBA	Umwelt Bundesamt (Federal Environment Agency of Germany)
UC	Use category

Standard term / Abbreviation	Explanation
UNEP	United Nations Environment Programme
UVCB	Undefined or variable composition, complex reaction products or biological material
UWWTD	Urban Waste Water Treatment Directive (UWWTD, 91/271/EEC)
WAF	Water accommodated fraction
WWTP	Waste water treatment plant

PART I ACTIVE SUBSTANCES

1. Introduction

Evaluation

The process of evaluation of active substance applications is given in Article 8 (BPR) and the common principles for the evaluation of dossiers for biocidal products (including the representative biocidal product in the context of active substance approval) is given in Annex VI (BPR).

The evaluating or receiving CA uses the data submitted in support of an application for active substance approval or authorisation of a biocidal product to make a risk assessment based on the proposed use of the (representative) biocidal product. The general principles of assessment are given in Annex VI (BPR) and the evaluation is carried out according to these general principles. The evaluating body will base its conclusions on the outcome of the evaluation and decide whether or not the (representative) biocidal product complies with the criteria for authorisation set down in Article 19(1)(b) and/or whether the active substance may be approved.

Thus the risk assessment is the principle part of the evaluation process and this guidance explains how to perform the risk assessment and the exposure assessments for the evaluation of the environmental aspects.

Assessment

Regulation (EU) 528/2012 in the following referred to as "BPR" requires that an environmental risk assessment on the active substance present in the biocidal product must always be carried out. If there are, in addition, any substances of concern present in the biocidal product then a risk assessment must be carried out for each of these. The risk assessment must cover the proposed normal use of the biocidal product, together with a realistic worst-case scenario including any relevant production and disposal issue. The assessment must also take account of how any "treated articles" treated with or containing the product may be used and disposed of. As the provisions for treated articles are new for biocides, specific descriptions on treated articles were added (**section 2.3.3.2** of this guidance). Active substances that are generated in-situ and the associated precursors must also be considered. The risk assessment must entail:

- **Hazard identification**: the identification of the adverse effects which a substance has an inherent capacity to cause
- **Dose (concentration) - response (effect) assessment** (as appropriate): the estimate of the relationship between the dose, or level of exposure, of an active substance or a substance of concern in a biocidal product and the incidence and severity of an effect
- **Exposure assessment**: the determination of the emissions, pathways and rates of movement of an active substance or a substance of concern in a biocidal product and its transformation or degradation in order to estimate the concentration/doses to which environmental compartments are or may be exposed
- **Risk characterisation**: the estimation of the incidence and severity of the adverse effects likely to occur in environmental compartments due to actual or predicted exposure to any active substance or substance of concern in a biocidal product. This may include "risk estimation" i.e. the quantification of that likelihood.

The risk assessment must take account of any adverse effects arising in any of the environmental compartments sewage treatment plant (STP), air, soil (including groundwater) and water (freshwater and marine, including sediment). Where quantitative results are not available the results of the qualitative assessments must be integrated in a similar manner.

The present document is intended to assist applicants and competent authorities to carry out the environmental risk assessment of active substances, their metabolites (if relevant) and substances of concern in a biocidal product or in a treated article (in the following, these are subsumed under the term "substance").

This guidance document includes advice on the following issues:

- how to calculate Predicted Environmental Concentrations (PECs) (**sections 2** and **4.2** of this guidance)
- how to calculate Predicted No-Effect-Concentrations (PNECs) (**section 3** of this guidance) and,
- where the calculation of PECs and PNECs is not possible, how to make qualitative estimates of environmental concentrations and effect/no effect concentrations
- how to calculate the PEC/PNEC ratio (**section 4** of this guidance)
- how to assess exclusion criteria, including how to conduct a PBT/vPvB assessment and how to assess endocrine disrupting properties assess (**section 3.11** of this guidance)
- how to assess aggregated exposure (**section 4.7** of this guidance);

To ensure that the predicted environmental concentrations are realistic, all available exposure-related information on the substance should be used. When detailed information on the use patterns, release into the environment and elimination is provided, the exposure assessment will be more realistic. A general rule for predicting the environmental concentration is that the best and most realistic information available should be given preference. However, it may often be useful to initially conduct an exposure assessment based on worst-case assumptions, and using default values when model calculations are applied. Such an approach can also be used in the absence of sufficiently detailed data. If the outcome of the risk characterisation based on worst-case assumptions for the exposure is that the substance is not "of concern", the risk assessment for that substance can be stopped with regard to the compartment considered. If, in contrast, the outcome is that a substance is "of concern", the assessment must, if possible, be refined using a more realistic exposure prediction. The guidance has been developed mainly from the experience gained on individual organic substances. This implies that the risk assessment procedures described cannot always be applied without modifications to certain groups of substances, such as inorganic substances and metals. The methodologies that may be applied to assess the risks of metals and metal compounds, petroleum substances and ionisable substances are specifically addressed in **section 4.5** of this guidance.

The risk assessments that have to be carried out according to the BPR are in principle valid for all countries in the European Union. Therefore, in the first stage of the exposure assessment, where exposure models are used, so-called generic exposure scenarios are applied in this document. These assume that substances are emitted into a model environment with predefined agreed environmental characteristics. These environmental characteristics can be average values or reasonable worst-case values depending on the parameter in question. Generic exposure scenarios have been defined for local emissions from a point source and for emissions into a larger region. It is recognised, however, that exposure estimation, for example, is subject to variation due to topographical and climatological variability. When more specific information on the emission of a substance is available, it may well be possible to refine the generic or site-specific assessment.

While comprehensive risk assessment schemes are presented for the aquatic and the terrestrial compartment and for secondary poisoning, allowing a quantitative evaluation of the risk for these compartments, the risk assessment for the air compartment can normally only be carried out qualitatively because no standardised biotic testing systems are available at present.

For some substances the information on the environmental release from certain stages of the life-cycle, which may include the presence of the substance in mixtures, is so scarce

that the PEC is quite uncertain or even not possible to estimate quantitatively. In the latter case a qualitative risk assessment is conducted (see **section 4.4** of this guidance). For further guidance on the exposure, effect or risk assessment for a biocidal active substance please consult **section 2.3.3.8** where additional guidance documents from other legislations are listed.

1.1 General principles of assessing environmental risks

The environmental risk assessment (BPR Annex VI) attempts to address the concern for the potential impact of individual substances on the environment by examining both exposures resulting from discharges and/or releases of biocides and the effects of such emissions on the structure and function of the ecosystem. Three approaches are used for this examination:

- quantitative PEC/PNEC estimation for environmental risk assessment of a substance comparing compartmental concentrations (PEC) with the concentration below which unacceptable effects on organisms will most likely not occur (PNEC). This includes also an assessment of food chain accumulation and secondary poisoning;
- the qualitative procedure for the environmental risk assessment of a substance for those cases where a quantitative assessment of the exposure and/or effects is not possible;
- the PBT (hazard) assessment of a substance consisting of an identification of the potential of a substance to persist in the environment, accumulate in biota and be toxic combined with an evaluation of sources and major emissions.

At present, the environmental risk assessment methodology has been developed for the following compartments:

For inland risk assessment:

- aquatic ecosystem (including sediment);
- terrestrial ecosystem (including groundwater);
- top predators;
- microorganisms in sewage treatment systems;
- atmosphere.

For marine risk assessment:

- aquatic ecosystem (including sediment);
- top predators.

The methodologies implemented have as aim the identification of acceptable or unacceptable risks. This identification provides the basis for the regulatory decisions, which follow from the risk assessment.

If it is not possible to conduct a quantitative risk assessment, either because the PEC or the PNEC or both cannot be derived, a qualitative evaluation is carried out of the risk that an adverse effect may occur.

In some cases, the current quantitative risk assessment approach does not provide sufficient confidence that the environmental compartments considered are sufficiently protected. The PBT assessment, to which is referred to in **section 3.11** of this guidance, has been developed with the aim of identifying these cases. **Table 1** shows a summary of the different protection targets of the risk characterisation and the exposure scenarios to which they apply for inland and marine risk assessment. In addition to the PECs mentioned in Table 1, several other exposure levels are derived in **section 2** of this guidance. These are used for the assessment of indirect human exposure through the environment, which is described in Volume III, Part B (Risk Assessment for Human Health). The PECs that are specifically derived for this indirect exposure assessment are summarised in

Table 2.
Table 1: Environmental protection targets

Protection target		Related compartment	Section	PNEC	Section
Biological sewage treatment plant	Microorganisms	STP aeration tank	**2.3.7.1**	$PNEC_{micro-organisms}$	**3.4**
Freshwater ecosystem	Freshwater organisms	Freshwater	**2.3.7.3**	$PNEC_{water}$ (freshwater)	**3.3**
	Sediment organisms	Freshwater sediments	**2.3.7.4**	$PNEC_{sed}$ (freshwater)	**0**
	Fish-eating Predators[3]	Fish	**3.8**	$PNEC_{oral}$	**3.8**
Marine ecosystem	Marine water organisms	Marine water	**2.6.5.2**	$PNEC_{saltwater}$	**3.9.1.3**
	Sediment organisms	Marine sediments	**2.6.5.3**	$PNEC_{sed,marine}$	**3.9.2.4**
	(Fish eating) predators[4]	Marine fish	**3.9.3**	$PNEC_{oral}$	**3.9.3**
	Top predators[4]	Marine predators	**3.9.3**	$PNEC_{oral}$	**3.9.3**
Terrestrial ecosystem[4]	(Agricultural) Soil organisms	(Agricultural) Soil	**2.3.7.5**	$PNEC_{soil}$	**3.6**
	(Worm-eating) Predators[4]	Earthworm	**3.8**	$PNEC_{oral}$	**3.8**
Air	Atmosphere	Air	**2.3.7.2**	$PNEC_{air}$[5]	**3.7**

Table 2: Exposure levels used for indirect human exposure

Target	Exposure scenario	Section
Drinking water production	Surface water (annual average) Groundwater	**2.3.7.3** & **2.3.7.7** **2.3.7.6** & **2.3.7.7**
Inhalation of air	Air (annual average)	**2.3.7.2**
Production of crops	Agricultural soil (averaged over 180 days)	**2.3.7.5** & **2.3.7.7**
Production of meat and milk	Grassland (averaged over180 days)	**2.3.7.5** & **2.3.7.7**
Fish for human consumption	Surface water (annual average)	**2.3.7.3**

[3] Exposure of predators and top predators is also referred to as "secondary poisoning".

[4] Non-target arthropods, bees and other non-target organisms are currently not covered in this guidance. The development of assessment methods for these species groups is currently under discussion.

[5] Usually a $PNEC_{air}$ is not available and a qualitative assessment is to be carried out if some hazard is identified such as ozone depletion. A $PNEC_{air}$ may be derived corresponding to the effect on plants exposed via the air and as such not protecting the atmosphere but the terrestrial ecosystem.

2. Exposure assessment

2.1 Introduction

According to the BPR Annex VI, exposure assessment comprises of the determination of the emissions, pathways and rates of movement of an active substance or a substance of concern, in a biocidal product or in a treated article, and its transformation or degradation in order to predict their likely concentration in the environment, which is known as predicted environmental concentration (PEC). However, in some cases it may not be possible to establish a PEC and a qualitative estimate of exposure has then to be made.

A PEC, or where necessary a qualitative estimate of exposure, need only be determined for the environmental compartments to which emissions, discharges, disposal or distributions (including any relevant contribution from articles treated with biocidal products) are known or are reasonably foreseeable.

The PEC, or the qualitative estimation of exposure, must be determined taking account of, in particular and where appropriate:

- adequately measured exposure data;
- the form in which the product is marketed;
- the type of biocidal product/treated article;
- the application method and application rate;
- the physico-chemical properties;
- breakdown/transformation products;
- likely pathways to environmental compartments and potential for adsorption/desorption and degradation;
- the frequency and duration of exposure;
- the size of the receiving compartment;
- long range environmental transportation.

When conducting the exposure assessment, special consideration should be given to adequately measured, representative exposure data where such data are available. Where calculation methods are used for the estimation of exposure levels, adequate models should be applied. Where appropriate, on a case-by-case basis, relevant monitoring data from substances with analogous use and exposure patterns or analogous properties should also be considered.

The assessment of environmental exposure consists in more detail of:

- the estimation of emissions into the different environmental compartments: air, water (fresh- and seawater), sediment (fresh- and seawater), soil (including groundwater) and sewage treatment plant;
- the assessment of the degradation and transformation processes;
- the assessment of distribution over the different compartments;
- the exposure of organisms within those compartments, either directly or indirectly via the food chain.

The environment may be exposed to biocides during all stages of their life-cycle from production to disposal or recovery. However, for biocides only certain life-cycle stages are assessed in line with Article 2 of the BPR since it is assumed that the other stages are covered by other legislations. The life-cycle stages for biocides to be covered by a quantitative risk assessment are highlighted in the following list **in bold letters**. The life-cycle stage for biocides (see also **Figure 2**) for which no quantitative assessment is needed

(in particular production and waste disposal) should nevertheless be covered at least by a qualitative assessment:

- production (of an active substance);
- **formulation** (of an active substance in a biocidal product)[6];
- **application/use**:
  - **industrial/professional** (large scale use including processing (e.g. industry) and/or small scale use (e.g. trade or trained experts));
  - **private or consumer**;
- **service life**;
- waste disposal (including waste treatment, landfill and recovery)[7].

For each environmental compartment potentially exposed, the exposure concentrations should be derived.

Exposure may also occur from sources not directly related to the life-cycle of the substance being assessed. Examples of such sources are substances of natural origin, substances formed in combustion processes and other indirect emissions of the substance (e.g. as by-product, contaminant or degradation product of another substance). These kinds of sources have been referred to as "unintentional sources". Guidance on how to deal with emissions not covered by the life-cycle of a substance related to the use of a biocidal product is given in **section 4.6** of this guidance.

In view of uncertainty in the assessment of exposure of the environment, the exposure levels should be derived on the basis of both model calculations and measured data, if available. Relevant measured data from substances with analogous use and exposure patterns or analogous properties, if available, should also be considered when applying model calculations. Preference should be given to adequately measured, representative exposure data where these are available (**sections 2.2.2** and **2.4**).

Consideration should be given to whether the substance being assessed can be degraded, biotically or abiotically, to give stable and/or toxic degradation products. Where such degradation can occur, the assessment should give due consideration to the properties (including toxic effects and mobility) of the products that might arise. Relevant degradation products should also be subject to risk assessment. Where no information is available, a qualitative description of the degradation pathways can be made. A summary of some of these is presented in **Appendix 3**. Furthermore it should be noted that guidance on how to assess and test relevant metabolites and transformation products is available for plant protection products and can be used also for biocides (see **Appendix 5**).

[6] Relevant for active substances used in treated articles, formulation of disinfectants, preservatives, repellents and insecticides into the end-product to be preserved.

[7] This step is considered quantitatively only in the exposure assessment for Product-type 13.

Info-box 1: Metabolites

A difference is made between:

Major metabolite: In Part 1 of the *Guidance on the Biocidal Product Regularion: Volume IV Environment, Part A Information Requirements* it is stated that major metabolites (formed ≥ 10% on a molar basis, of the active substance in any relevant environmental compartment or appearing at two consecutive sampling points at amounts ≥ 5% on a molar basis, or if at the end of the study the maximum of formation is not yet reached but accounts for ≥ 5% on a molar basis, of the active substance at the final time point), should be identified and their behaviour and toxicity should be assessed. In general, an environmental risk assessment for the relevant compartments needs to be performed for all major metabolites. However, as a first step a qualitative or semi-quantitative assessment of these metabolites using the available data and expert judgement to fill data gaps may be sufficient. If the assessment indicates a potential risk, a quantitative assessment should be performed. Fate and ecotoxicological information are required for all major metabolites and a risk assessment should be performed.

Minor metabolite: metabolites that are not major metabolites.

Ecotoxicologically relevant metabolite: a metabolite which poses a higher or comparable hazard to any organism as the active substance. In general, an environmental risk assessment for the relevant compartments need to be performed for all ecotoxicologigally relevant metabolites (minor and major).

For many substances available biodegradation data is restricted to aerobic conditions. However, for some compartments, e.g. sediment or ground water, anaerobic conditions should also be considered. The same applies to anaerobic conditions in e.g. manure and treatment of sewage sludge. Salinity and pH are examples of other environmental conditions that may influence the degradation.

In the risk assessment a proper functioning of waste treatment is assumed. However, if thermal treatment of waste is operated at insufficient technical conditions, organic substances may be formed having a PBT or POP profile[8]. This may be the case in particular in the presence of halogens (Cl and Br) and catalysing metals (e.g. copper). If the formation of PBT or POP substances is identified as a special concern, this should be noted in the risk assessment. In that case it could be considered to add an appendix to the risk assessment report with further information on the possible formation of substances with a PBT or POP profile.

2.2 Exposure assessment principles

2.2.1 Assessment scale

The exposure to the environment is in principle assessed for biocides only on the local scale, i.e. in the vicinity of point sources of release to the environment.

The regional scale covers a larger area that includes all point sources and wide dispersive sources in that area. Releases at the continental scale are considered to provide inflow concentrations for the regional environment. However, regional (and continental concentrations) are used as endpoints in the exposure assessment of biocides only case by case, for example for treated articles.

For the local assessment, concentrations of substances released from a single point source are assessed for a generic local environment. This is not an actual site, but a hypothetical site with predefined, agreed environmental characteristics, the so-called "standard

[8] Substances being persistent, bioaccumulative and toxic (PBT) or substances classified as a persistent organic pollutant under the UN Stockholm Convention on Persistent Organic Pollutants (POPs).

environment" and a standard town of 10,000 inhabitants (including a standard sewage treatment plant). The exposure targets are assumed to be exposed in, or at the border of the site. In general, concentrations during an emission episode are measured or calculated. This means that local concentrations (PEClocal) are calculated on the basis of a daily release rate, regardless of whether the discharge is intermittent or continuous. They represent the concentrations expected at a certain distance from the source on a day when discharge occurs.

Only for the soil compartment (being a less dynamic environment than air or surface water) longer-term average is used instead of daily release rates. This is because exposure is assumed not to be influenced by temporal fluctuation in release rates. However, in some cases time related concentrations may be obtained, for instance in situations where intermittent releases occur.

In principle, degradation and distribution processes are taken into consideration for the calculation of the PEClocal. However, because of the relatively short time between release and exposure, concentrations at local scales are mainly controlled by initial mixing (dilution into environmental compartment) and adsorption on suspended matter.

A fixed dilution factor of 10 is applied to the effluent concentration of an STP (by default assumed to be present). For further iterations, more specific assessments may be appropriate. The actual dilution factor after complete mixing can be calculated from the flow rate of the river and the effluent discharge rate of the STP. This approach should be used for rivers only and not for estuaries or lakes. In other cases, the calculation of the PEClocal can be carried out using actual environmental conditions around the point source.

Release to the environment at the local scale can be from private settings (e.g. painted houses), industrial settings or from wide dispersive uses:

- Releases from uses in **private** and **industrial settings** are assessed as independent point source releases; it means that each identified use of the substance is assumed to occur at a different site. However, in some cases those assessments are combined (e.g. for Product-type 6: Preservatives for products during storage, or for Product-type 18: Insecticides, acaricides and products to control other arthropods and for certain treated articles). Releases to water can be treated in an on-site industrial waste water treatment plant (WWTP) or in a municipal sewage treatment plant (STP). For industrial or municipal biological treatment plants, a standard model is available to calculate the releases after treatment (**section 2.3.6.7** of this guidance). Indirect releases to air via the STP, as a result of water treatment in the STP, are also considered. Release to soil at the local scale will occur via application of sludge from an STP to agricultural soil[9] and via atmospheric deposition of substances released to air. Direct releases to soil or surface water from private settings are only relevant for specific uses of certain product types (PT), for example direct release during painting a house with a wood preservative (PT 8). Guidance on how to perform the assessment of direct releases is provided in the PT-specific emission scenario documents (ESDs), see also **section 2.3.3.3.1** of this guidance.

[9] It should be noted that sewage sludge is not applied as a soil fertiliser in many European countries, but fermented and eventually burned as hazardous waste. Exposure to soils via sewage sludge is therefore not relevant in many European countries.

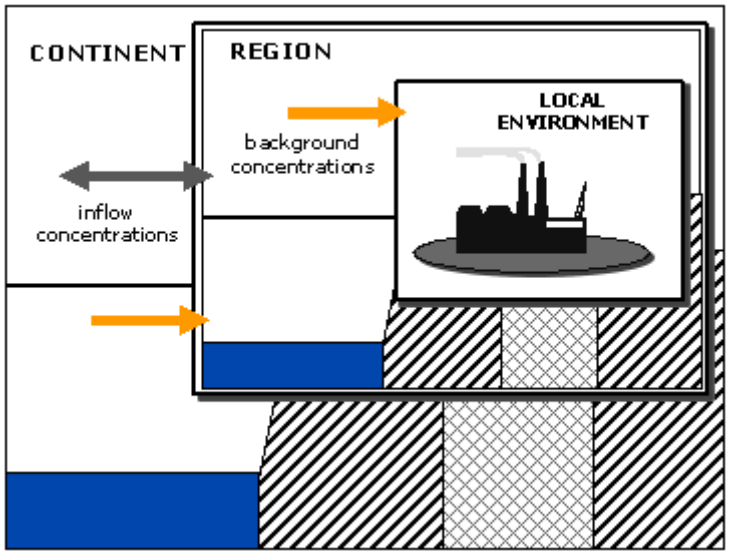

Figure 1: The relationship between the continental, regional, and local scale exposure assessments

- A **wide disperse use** of a substance is characterised by the assumption that the substance is used by consumers or by many users in the public domain, including small, non-industrial companies. A wide dispersive use of a substance is by default associated with a point source release of a local municipal STP of a standard 10,000-inhabitant town that collects the releases to water from that use. This is not the case for direct releases to air and soil from wide dispersive uses.

On the **regional scale**, concentrations of substances released from point and diffuse sources over a wider area are assessed for a generic regional environment. The PECregional takes into account the further distribution and fate of the chemical upon release. It also provides a background concentration to be incorporated in the calculation of the PEClocal. As with the local models, a generic standard environment is defined. The PECregional is assumed to be a steady-state concentration of the substance.

Concentrations in air and water are also estimated at a continental scale (Europe) to provide inflow concentrations for the regional environment. These concentrations are not used as endpoints for exposure in the risk characterisation.

Figure 1 above illustrates the relationships between the three spatial scales. The local scale receives the background concentration from the regional scale; the regional scale receives the inflowing air and water from the continental scale.

This implies that the continental, regional, and local calculations must be done sequentially. It should be noted that the use of regional data as background for the local situation may not always be appropriate. If there is only one source of the substance, this emission is counted twice at the local scale: not only due to the local emission, but the same emission is also responsible for the background concentration of the region.

2.2.2 Measured/calculated environmental concentration

No measured environmental concentrations will normally be available for new active substances. Therefore, concentrations of a substance in the environment must be estimated. In contrast, the exposure assessment of existing active substances does not always depend upon modelling. Data on measured levels in various environmental compartments have been gathered for a number of existing substances. They can provide the potential for greater insight into specific steps of the exposure assessment procedure (e.g. concentration in industrial emissions, "background" concentrations in specific compartments, characterisation of distribution behaviour).

In many cases, a range of concentrations from measured data or modelling will be obtained. This range can reflect different conditions during use or service life of the substance, or may be due to assumptions in or limitations of the modelling or measurement procedures. It may seem that measurements always give more reliable results than model estimations. However, measured concentrations can have a considerable uncertainty associated with them, due to temporal and spatial variations. Both approaches complement each other in the complex interpretation and integration of the data. Therefore, the availability of adequate measured data does not imply that PEC calculations are unnecessary.

Initially, a generic "reasonable worst-case" exposure assessment based on modelling should be performed, to derive an environmental concentration. Measured data, i.e., site-specific or monitoring information, can then be used to revise the calculated concentrations. Other site-specific information such as e.g. effluent volumes, size of STP, river flow may also be useful. In carrying out this revision, it is recommended to include in the exposure assessment of active substances, a table containing availability of site-specific information for industrial sites (if limited in number) or group of industrial sites (if numerous), as far as confidentiality issues allow. The "site-specific" concentrations estimated may involve the use of actual site-specific information and more generic values (and possibly extrapolated values as described below). It should then be considered in which cases extrapolation is possible from sites with site-specific information to a site without information. Aspects to consider here include the proportion of the industry covered by specific information, the nature of the industry and information about its distribution, the comparative size of sites, the types of process used etc. The grounds on which the extrapolation has been done should be justified in the risk assessment. It may be possible to extrapolate some aspects but not others, for example emission factors (on the basis of similar processes) but not effluent flows (on the basis of differing sizes of site). If no such extrapolation can be justified, then the modelling approach described in this document should be followed for the (group of) site(s).

It should be noted that the site-specific risk assessment is not based on a detailed and complete description of the environmental conditions. The aim is to estimate environmental concentrations that are reasonably applicable for a risk assessment. Some site-specific data may be used to replace the default data characterising the standard scenario.

For measured data, the reliability of the available data has to be assessed as a first step. Subsequently, it must be established how representative the data are of the general emission situation. **Section 2.4** of this guidance provides guidance on how to perform this critical evaluation of measured data. For model calculations, the procedure to derive an exposure level should be made transparent. The parameters and default values used for the calculations must be documented. If different models are available to describe an exposure situation, the best model for the specific substance and scenario should be used and the choice should be explained. If a model is chosen which is not described in this document, that model should be explained and the choice justified. **Section 2.3** of this guidance discusses modelling in detail. **Section 2.5** of this guidance gives further advice on critical comparison between calculated and measured PECs.

2.3 Model calculations

2.3.1 Introduction

The first step in the calculation of the PEC is to evaluate the data set. The subsequent step is to estimate the substance's release rate based on its use pattern. All potential emission sources need to be analysed, and the releases and the receiving environmental compartment(s) identified. After assessing releases, the fate of the substance once released to the environment needs to be considered. This is estimated by considering likely routes of exposure and biotic and abiotic transformation processes. Furthermore, secondary data (e.g. partition coefficients) are derived from primary data. The quantification of distribution and degradation of the substance (as a function of time and space) leads to an estimate of PEC values in the receiving compartments. The PEC calculation is not restricted to the

primary compartments; surface water (**section 2.3.7.3**), soil (**section 2.3.7.5**) and air (**section 2.3.7.2**); but also includes secondary compartments such as sediments (**section 2.3.7.4**) and groundwater (**section 2.3.7.6**). Transport of the substance between the compartments must, where possible, be taken into account.

This section is arranged as follows:

- description of the minimum data set requirements for the distribution models described in the following sections;
- estimation of emissions to the environment;
- definition of the characteristics of the standard environment used in the estimation of PECs;
- derivation of secondary data: intermedia partition coefficients and degradation rates. These parameters might be part of the data set, otherwise, they are derived from primary data by estimation routines;
- fate of the substance in sewage treatment;
- distribution and fate in the environment, and estimation of PECs.

The structure of this section is shown schematically in **Figure 2**, including the flow of data between the separate steps of the calculations.

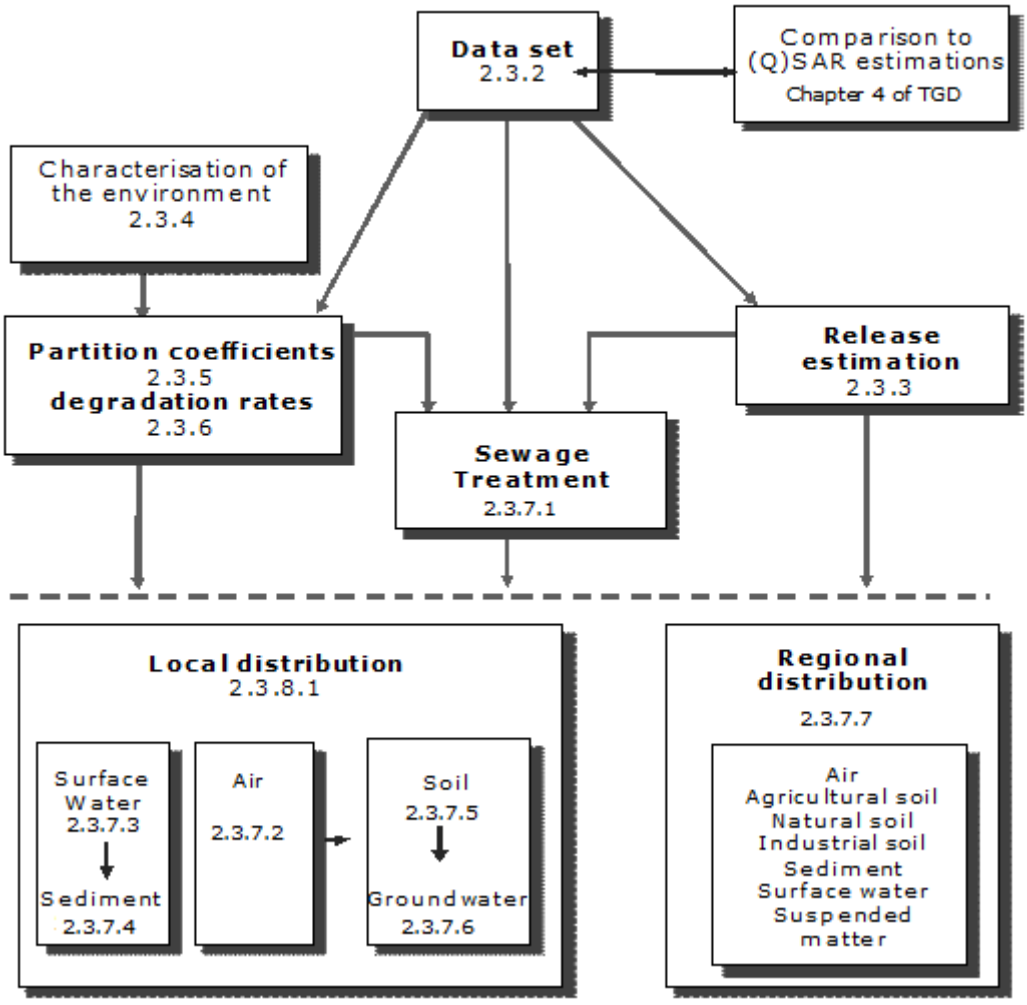

Figure 2: Layout of section 2.3, including the flow of data between the different sections

The model calculations are given in each section. The following table format is used for explaining the symbols used in an equation:

Explanation of symbols

[Symbol]	[Description of required parameter]	[Unit]	[Default value, equation number where this parameter is calculated, or reference to a table with defaults]
[Symbol]	[Description of resulting parameter]	[Unit]	

The following conventions are applied where possible for the symbols:

- parameters are mainly denoted in capitals;
- specification of the *parameter* is done in lower case;
- specification of the *compartment* for which the parameter is specified is shown in subscripts.

Some frequently occurring symbols

E	for emissions (direct and indirect)	[kg·d^{-1}]
F	for dimensionless fractions	[kg·kg^{-1}] or [m^3·m^{-3}]
C	for the concentration of a substance	[mg·l^{-1}], [mg·kg^{-1}] or [mg·m^{-3}]
RHO	for densities of compartments or phases	[kg·m^{-3}]
K	for intermedia partition coefficients	[various units apply]
k	for (pseudo) first-order rate constants	[d^{-1}]
T	for a period of time	[d]

As an example, the symbol $F_{oc, soil}$ means the fraction (*F*) of organic carbon (*oc*) in the soil compartment (*soil*). For other parameters, recognisable symbols are chosen. It should be noted that in several equations fixed factors (e.g. 1000 or 10^6) are applied for dimensional consistency.

Sensitivity analysis

In the case of conflicting data, great variation or uncertainty in data, a few carefully selected scenarios could be considered employing alternative input parameters for the fate-related properties in question. The fate-related properties may include data for bioaccumulation, sorption, degradation, volatilisation etc. The concept may also be useful for emissions if they are uncertain in relation to their size to certain environmental compartments.

However the most appropriate input parameter should be selected according to the "realistic worst case" scenario being assessed and should be used in the "core assessment". In most cases, the vulnerability of the realistic worst case scenario will be a result of the choices of realistic worst case default scenario assumptions. In such cases it will often be appropriate to use average, median or geometric mean substance specific input parameters rather than worst case values to avoid the overall assessment being overly conservative. The use of average input values will generally be appropriate when the full active substance or metabolite information requirements have been fulfilled. In all cases the selection of substance specific input parameters should be detailed and justified as part of the exposure assessment. Alternative input values should only be included in alternative estimations performed for investigation purposes. Alternative input parameters (e.g. worst case values) may be justified when the full information requirements have not been fulfilled to ensure an appropriately conservative assessment is performed.

It should be noted that fixing a parameter, which results in e.g. a higher PEC/PNEC ratio for sediment, soil, secondary poisoning and STP, will result in a lower PEC/PNEC ratio for pelagic organisms. Therefore, in such cases it is possible that one particular set of parameters will give rise to the highest risk for one compartment, and another set for another compartment; both might be valid extremes.

The approach described above should especially be considered in relation to multi-component substances / groups of substances where the intrinsic properties vary between the different components of the substance. It is important to know which components any measured values relate to. The concept may, however, also be useful for certain discrete substances, where there is special uncertainty about a fate related property or an emission that may be of key importance.

The outcome of the alternative exposure assessments should be presented in an illustrative appendix to the risk assessment report. If the analysis shows that the variation of the input parameter(s) is critical in relation to the result of the assessment (i.e. changes the conclusion), then further consideration is necessary of ways to improve the certainty of the input parameter(s) in question. If on the other hand the analysis shows that the results of the assessment are not changed, the confidence in the assessment has increased.

2.3.2 Data for exposure models

The following parameters from the core data set (CDS) are directly used in the exposure models as discussed in the following sections:

Physico-chemical properties

M	molecular weight	[g·mol^{-1}]
K_{ow}	octanol-water partition coefficient[10]	[-]
S	water solubility	[mg·l^{-1}]
VP	vapour pressure	[Pa]
BP	boiling point (only for some release estimations)	[°C]

Sections 2.3.5 and **2.3.6** describe how secondary data (partition coefficients and degradation rates) are derived from the minimum data requirements. When adequately measured data are known, these should be used instead of the estimations.

It should be noted that the data requirements for the exposure models, as listed above, are only valid for neutral, organic, non-ionised substances. Before proceeding with the modelling exercise due consideration should be given whether the substance can be classified as a neutral, organic, non-ionised substance. More specific information (e.g. partition coefficients or acid/base dissociation constant for ionising substances) may be required for other types of substances. For ionising substances, the pH-dependence of K_{ow} and water solubility should be known. Partition coefficients should be corrected according to the pH of the environment and the effect across a typical environmental range should be investigated (e.g. the influence on partitioning across pH 4 to 9).

The correction can be done by using the following correction factor (see also **section 4.5.3** of this guidance):

$$CORR = \frac{1}{1 + 10^{A(pH - pKa)}}$$ **Equation 1**

[10] The term K_{ow} is used in this document and is equivalent to P_{ow}.

Explanation of symbols

A	1 for acids, -1 for bases	
pH	pH value of the environment	
pKa	acid dissociation constant	data set

Equation 1 results in the fraction of undissociated compound for the proton donating (acidic) reactions for an acid:

$AH \rightarrow A^- + H^+$ with the value for A = +1;

or for a base:

$BH^+ \rightarrow B + H^+$, with the value of A = -1.

In both cases, the acid dissociation constant (pKa) should be used in Equation 1. This means that for a base B, the dissociation constant for the proton releasing reaction of its conjugated acid BH+ should be used.

This equation is only valid for monoprotic substances.

If the sorption behaviour has been investigated for a substance over a relevant pH range, the measured value should be used preferably over the use of the above equation. In this case, the most applicable (worst case) measured organic carbon normalised partition coefficient (K_{oc}) or organic matter normalised partition coefficient (K_{om}) for the compartment to be considered should be selected, which may result in the use of different K_{oc} or K_{om} values for respective compartments (e.g. the use of different values for groundwater and sediment).

For surface active substances specifically, and for substances for which adsorption and partition is not related to binding to organic matter in general, it may not be advisable to use estimated or measured K_{ow} values as a predictor for e.g. K_{oc} (soil, sediment, suspended organic matter and sludge) and bioconcentration factor - BCF (fish, worm) because the predictive value of log K_{ow} for such estimations may be too low. Instead, for surfactants it may be appropriate to obtain measured solids-water partition coefficient (K_p) and BCF values.

If experimentally determined physico-chemical data have been obtained at a temperature which for the substance under consideration would significantly change when extrapolated to the relevant temperature of the exposure models employed (e.g. 12 °C in the regional model or 9 °C for marine environments) then such an extrapolation should be considered. In other cases this will not be necessary. Particular care is also required for the interpretation of test results for thermolabile substances.

However, the vapour pressure may for some substances change considerably according to the temperature even within a temperature range of only 10 °C. In this case a general temperature correction should be applied according to the following equation:

$$VP(T_{env}) = VP(T_{test}) \cdot e^{\left(\frac{H_{0vapor}}{R} \cdot \left(\frac{1}{T_{test}} - \frac{1}{T_{env}} \right) \right)}$$ **Equation 2**

Explanation of symbols

$VP(T_{env})$	vapour pressure at the environmental temperature	[Pa]	
$VP(T_{test})$	vapour pressure as give in the data set	[Pa]	data set
T_{env}	environmental temperature (scale-dependent)	[K]	
T_{test}	temperature of the measured experimental VP	[K]	data set
H_{0vapor}	enthalpy of vapourisation	[J·mol^{-1}]	5·10^4
R	gas constant	[Pa·m^3· mol^{-1} · K^{-1}]	8.314

Care must be taken when the melting point is within the extrapolated temperature range. The vapour pressure of the liquid is always higher than of the solid ('fugacity ratio' see **Equation 20**). Extrapolation will therefore tend to overestimate the vapour pressure. There is no general solution to this problem. One approach to overcome the problem is to use K_{ow}, $K_{octanol-air}$, and $K_{air-water}$ instead of the 'three solubilities' (vapour pressure water solubility, solubility in octanol), as discussed in **Equation 20**.

The same approach can be followed for correcting the water solubility:

$$S(T_{env}) = S(T_{test}) \cdot e^{\left(\frac{H_{0solut.}}{R} \left(\frac{1}{T_{test}} - \frac{1}{T_{env}} \right) \right)}$$

Equation 3

Explanation of symbols

$S(T_{env})$	solubility at the environmental temperature	[mg L^{-1}]	
$S(T_{test})$	solubility as give in the data set	[mg L^{-1}]	data set
T_{env}	environmental temperature (scale-dependent)	[K]	
T_{test}	temperature of the measured experimental S	[K]	data set
H_{0solut}	enthalpy of solution	[J·mol^{-1}]	1·10^4
R	gas constant	[Pa·m^3·mol^{-1}·K^{-1}]	8.314

2.3.3 Release estimation

In this section the following parameters are derived:

- local emission, the rates to air and wastewater during an emission episode;
- regional emissions to air, wastewater, and soil (annual averages).

2.3.3.1 Life-cycle of substances

Releases into the environment can take place from processes at any stage of the life-cycle of a substance (see **Figure 3** on the next page). However, emissions from substance production, and product formulation are considered less relevant (since potentially covered by other legislations) compared to emissions from the application- and in service phase of the product. Therefore, production and formulation would generally not need to be assessed, with the exception of the formulation step of active substances used in treated articles, formulation of disinfectants, preservatives, repellents and insecticides into the end-product to be treated.

For the application- and in service phases, the emission routes should be identified and be assessed. The exposure assessment must cover the proposed normal use of the biocidal product or treated article together with a realistic worst-case scenario. Determination of the relevance of the emission routes and quantification of emissions are based on emission scenarios that have been drawn up for various product-types (see **section 2.3.3.3.1** of this guidance).

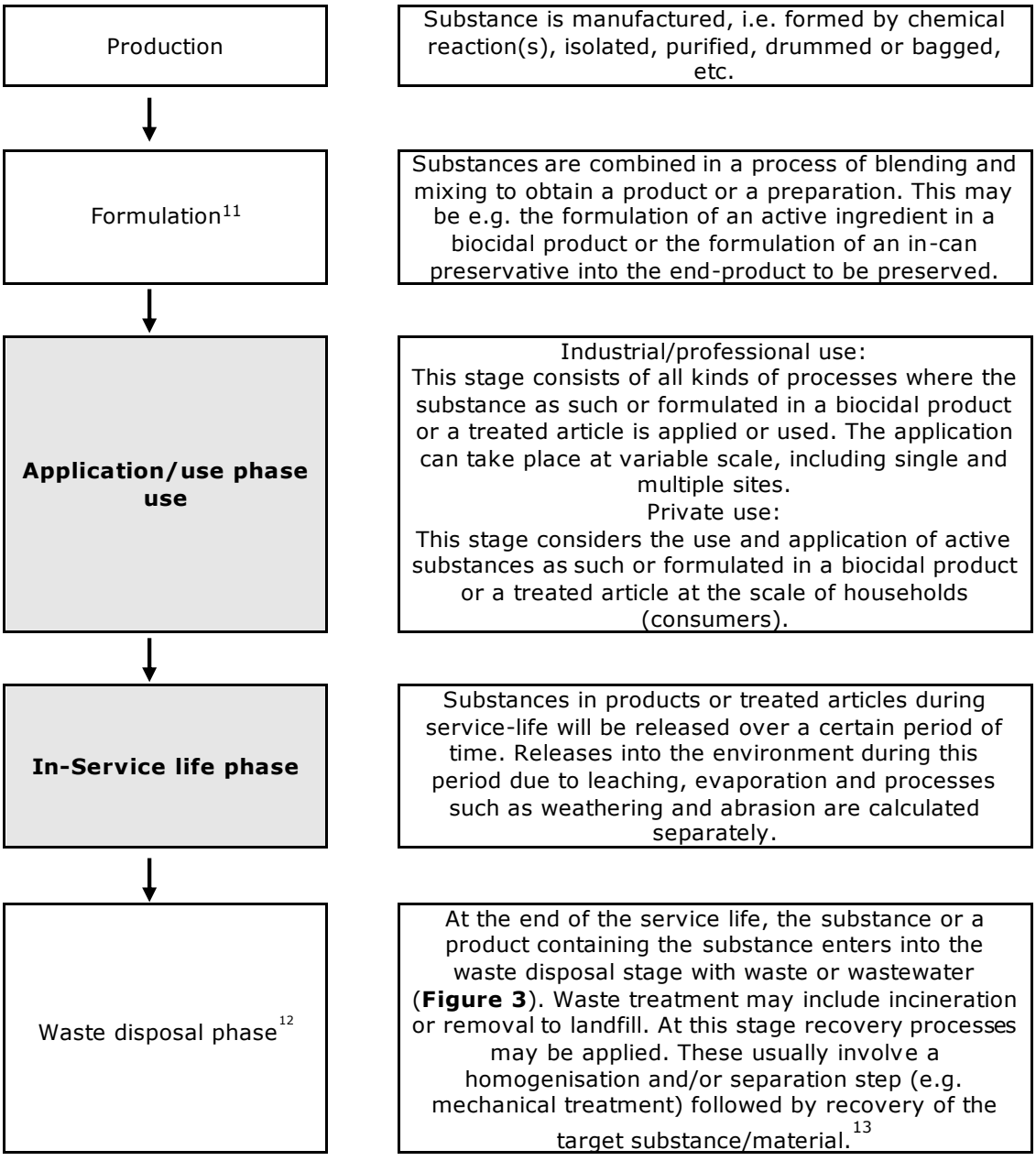

Figure 3: Schematic representation of the life cycle stages of a substance

[11] Relevant for active substances used in treated articles, formulation of disinfectants, preservatives, repellents and insecticides into the end-product to be treated.

[12] This step is considered quantitatively only in the exposure assessment for Product-type 13.

[13] The recovered substance or material may be:

1. reprocessed for the original type of product (recycling) - the substance returns into life-cycle stages already assessed before;

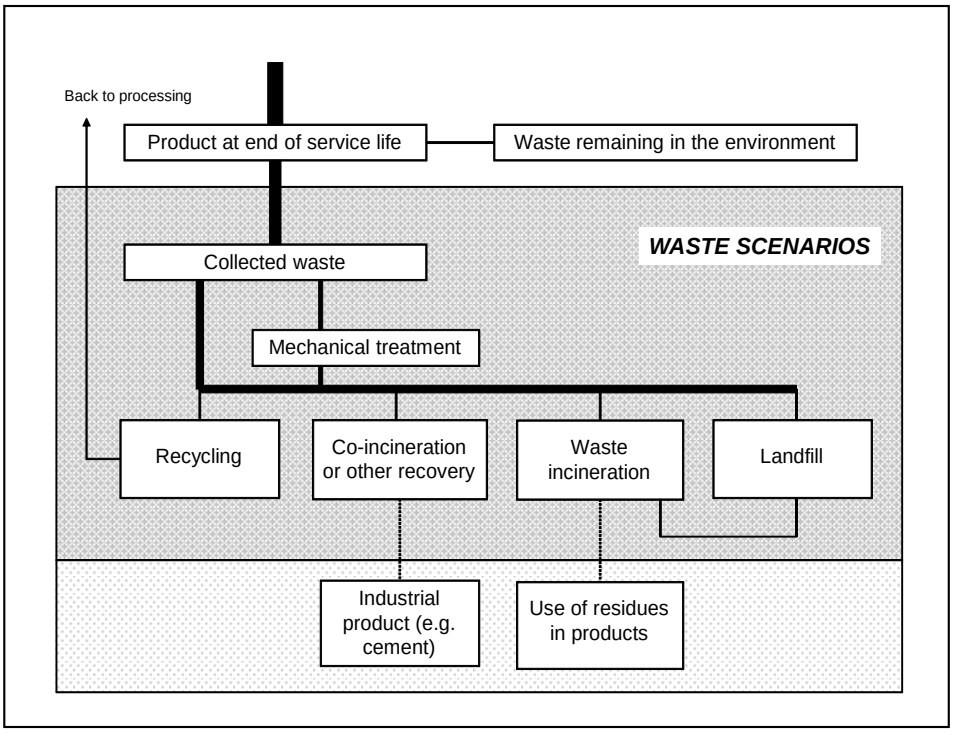

Figure 4: Schematic representation of the waste life stage of a substance

2.3.3.2 Types of emmissions, sources and emission pathways

Emission patterns vary widely from well-defined point sources (single or multiple) to diffuse releases from large numbers of small point sources (like households) or line sources (like a noise barrier). Releases may also be continuous or non-continues like peak or block emissions. The latter can be also intermittent (see also **section 2.3.3.4** of this guidance).

Continuous emissions are characterised by an almost constant emission rate flow over a prolonged period (e.g. the emission of a substance from a continuous preservation process such as in cooling towers).

Peak emissions are characterised by a relatively large amount discharged in a short time where the time intervals between peaks and the peak height can vary greatly (e.g. the discharge of spent disinfectants in a batch disinfection process e.g. in food production industry).

Block emissions are characterised by a flow rate which is reasonably constant over certain time periods with regular intervals (e.g. the emissions form harbours during the application and removal phase of antifouling to boat hulls at the beginning of the sailing season sailing). The quantities released from a certain process may vary from 100%, as is the case for example with household products like detergents or volatile solvents in paints, to below 1% for substances applied in closed systems.

Besides releases from point sources, diffuse emissions from treated articles during their service life may contribute to the total exposure for a substance. For substances used in

2. manufactured into a new type of product;
3. used as secondary fuel in heat production.

In the second and third option the substance may enter into processing and final products from which new types and amounts of releases could occur. In some cases, another substance or product may be recycled, and the substance assessed is present in this product. Releases in this situation may vary widely and information on them may not be readily available since the focus of attention is not on the substance assessed, but on the substance or product recovered. In addition to being incinerated or being disposed of in landfill, waste may be released, either intentionally or unintentionally, to the environment. Articles may intentionally be left in the environment after their service life.

long-life materials this may be a major source of emissions (e.g. cables buried in soil). Demolished building materials may be used as ballast at e.g. road constructions. Fragments of articles may also be lost during use (e.g. paint flakes, car undercoating).

Info-box 2: Emission pathways of biocides and receiving environmental compartments

The **STP** can be exposed to releases from indoor applications in industrial, public and private areas (e.g. indoor use of surface disinfectants) as well as by releases from outdoor applications (e.g. leaching from a noise barrier, treated with a wood preservative).

The substance may be released from the STP to the following consecutive environmental compartments:

Water → Sediment (sea/freshwater)
Air → Soil
Soil → Groundwater

Water (freshwater or seawater) can be either a direct recipient (e.g. from outdoor spray applications against insects or by leaching from e.g. antifouling agents applied on ships) or can be exposed indirectly via the effluent from an STP that contains residues.

The consecutive environmental compartment is freshwater- or seawater sediment.

Soil can receive direct emission of the active substance during application or service life of a biocidal product (e.g. emissions during outdoor in-situ applications or leaching from a house treated with wood preservatives) or indirect emissions from application of residue-containing sludge from an STP or manure from treated animal housings.

Emissions to soil result in the exposure of the following consecutive environmental compartments:

Groundwater

Surface water (not routinely assessed)

Air is exposed if a product contains volatile active substances or by direct emissions from aerosols or spray applications. Direct emission can also occur from evaporation and drift containing biocidal preservatives e.g. used in cooling systems (PT 11).

Emissions to air result in exposure of the following consecutive environmental compartments:

Soil (through deposition)

Water (through deposition, not routinely assessed) → Sediment

There are two main routes of exposure to **birds and mammals**; primary and secondary exposure. Primary exposure means that birds or mammals are either directly in contact with the substance (e.g. contact to rodenticides) or they are directly exposed via an environmental compartment to which the substance was released.

Secondary exposure entails the exposure to a substance through the natural food chain where the food of birds or mammals contains substances or their metabolites. In general, secondary exposure is assessed if 1) the substance has a high bioaccumulation potential and 2) the toxicity of the active substances to birds is high. For most organics, a cut off value of log K_{ow} of 3 is used to indicate the bioaccumulation potential. However, this cut off value of log K_{ow} is based on a QSAR and not all organic substances are suitable for this QSAR.

2.3.3.3 Emission estimation

Emission estimation applies either the tonnage of the substance or the average consumption/application rate as a starting point. In both cases emission factors (fractions released to the relevant environmental compartments) are used. Information on when to apply what type of calculation (i.e. tonnage or consumption based) and on emission factors is provided in the following chapters.

2.3.3.3.1 Consumption/application rate based approach

The consumption/application rate based approach is based on the quantity of a substance used in a single application or treatment. The application or dose rate of a substance is multiplied by the treatment area or volume or any other relevant unit or measure. Emission Scenario Documents (ESDs) provide default values per product-type[14] for the treatment areas and volumes or use rate such as e.g.:

- dimensions of external façade (range of scenarios) for the outdoor use of masonry/wood preservatives/paints;
- area treated (crack & crevice, barrier treatment, ant nest etc.) for indoor and outdoor use of insecticides;
- quantity used per person per day for the consumer use of disinfectants/personal care products.

The consumption/application rate based approach is particularly suited to situations where exposure is highly localised such as direct or indirect emission to soil. Further advantages of this approach are that it is standardised due to the ESDs, it is suited to point sources and it can be communicated in a transparent way.

The disadvantages are that emission estimations concern the local scale only although background contribution can be significant when a large number of uses is to be considered, they require a good understanding of the application, for some default values there is a lack of reliable data and there is no direct relation with the actual volume for the application. In addition the conduction of an aggregated exposure assessment is difficult.

Emission Scenario Documents:

For the emission estimation of most of the PTs respective ESDs and additional related documents are available which are provided on the ESD specific ECHA webpage: http://echa.europa.eu/guidance-documents/guidance-on-biocides-legislation/emission-scenario-documents).

Product-type specific amendments to the ESDs:

In the course of the ongoing review program for biocides, decisions were taken for several PTs which specify the emission estimation and should be taken into account when preparing an exposure assessment. These decisions are included in the Technical Agreements for Biocides (TAB) available on the ECHA website (http://echa.europa.eu/about-us/who-we-are/biocidal-products-committee/working-groups).

2.3.3.3.2 Tonnage based approach

The tonnage based approach takes into account the annual EU tonnage and it is primarily focused on emission to wastewater. In the emission estimation a fraction of the annual EU tonnage is defined which is used in a standard EU region (F_{region}) and a standard STP catchment ($F_{mainsource}$). The daily emission is then determined by taking account of number of emission days ($T_{emission}$).

The advantages of the tonnage based approach are that no use details are required, the tonnage will be known to the applicant, the emission is related to the used volume and it facilitates the conduction of an aggregated assessment.

[14] Product type as specified in Annex V of the Biocidal Product Regulation

The disadvantages are that tonnage data are confidential, the representation for a long term view is questionable (growth, share etc.), it is not suitable to cover direct emissions to soil and water and it bears a certain uncertainty with regard to the distribution of uses.

The tonnage based approach is described in several ESDs (e.g. ESD for PT 1 and PT 2). However it was developed for industrial chemicals and was originally described in the TGD of 2003. Since the text from the TGD (2003) is still relevant for this approach, the original text from the TGD is provided in the following (beside adapted Appendix/Annex numbers). The examples provided in the original text have been revised in order to be more specific for biocides.

Tonnage based approach (cited from TGD 2003):

Emissions of a substance are dependent on the use patterns.

Three categories are distinguished, i.e. main category, industry category and function or use category. An overview of these categories can be found in **Appendix 6** of this guidance. The main categories are intended to describe generally the exposure relevance of the use(s) of a substance. In the context of environmental risk assessment they are also used to characterise release scenarios for the estimation of emissions to the environment during specific stages of the life-cycle of the substance (production, formulation, and industrial/professional use and service life). They can therefore be allocated to release fractions, which are used as default values where specific information is missing. The following main categories are distinguished:

- use in closed systems: refers to the industrial/professional use stage when a substance is used for example as preservative in a closed cooling circuit,
- use resulting in inclusion into or onto a matrix: refers to the stage of formulation, e.g. when a substance is included in the emulsion layer of a photographic film. It also may refer to the stage of industrial/professional use, e.g. when a substance, applied e.g. as an in-can preservative in paint, ends up in the finished coating layer;
- non-dispersive use: relates to the number (and size) of the emission sources;
- wide dispersive use: relates also to the number (and size) of the emission sources.

The industry categories specify the branch of industry (including personal and domestic use, and use in the public domain) where considerable emissions occur by application of the substance as such, or by the application and use of preparations and products containing the substance. Some important emission sources have not been included specifically in this scheme and hence have to be allocated to category "Others" (no. 15/0), e.g. emissions of substances (in mixtures) other than fuels and fuel additives used in motor vehicles.

The use or function category specifies the specific function of the substance. There are 55 categories which have a varying level of detail. There is no general category as "Plastics additives" and many other specific categories lack as well; exceptions are categories like 47 "Softeners" (= plasticisers) and 49 "Stabilisers" (heat and UV-stabilisers).

The release of a substance at different stages of its life-cycle should be estimated by order of preference from:

- specific information for the given substance (e.g. from producers, product registers or open literature);
- specific information from the ESDs which are available for most of the 22 PTs;
- emission factors as included in the release tables of

Emissions may occur from a category other than the one to which a substance is allocated. A substance used in paint will normally be allocated to category 14 "Paints, lacquers and varnishes". Though the local emissions of solvents may be considerable at one point source (the paint factory) at the stage of formulation (paint production), most of the solvent will be emitted at paint application. The application could be classified in several industrial categories depending on the type of paint. In case of a do-it-yourself paint it would belong to category 5

"Personal/domestic", in case of motor car repair or professional house painting it would be category 15/0 "Others" (wide dispersive use, so diffuse releases) and in case of motor car production 16 "Engineering industry: civil and mechanical" (non-dispersive use, so few large point sources).

It is possible that confusion arises when the use of a substance, belonging to a certain specific process of an industrial category, occurs at another branch of industry. One example is the application of an additive for an epoxy resin applied in the electronic industry for the embedding of electronic components. Though the industrial/professional use takes place at category 4 "Electrical/electronic engineering industry" the industrial/professional use of epoxy resins belongs to category 11 "Polymers industry". The releases from the process will be found in the table for the latter category. Further information on main categories, industry categories and use categories is provided in **Appendix 6**, together with more examples.

For chemical industry, two separate industrial categories exist, one for basic chemicals and another for chemicals used in synthesis. Basic chemicals are considered to comprise commonly used chemicals such as solvents and pH-regulating agents such as acids and alkalis. Also the primary chemicals from the oil refining process are considered as basic chemicals. Substances used in synthesis fall in two classes, namely intermediates (substances produced from a starting material to be converted in a subsequent reaction into a next substance) and other substances. These other substances consist mainly of 'process regulators' (e.g. accelerators, inhibitors, indicators). For industrial category 5 (personal/domestic) the use and application of substances (as such or in formulations) is considered at the scale of households. The types of application are e.g. adhesives, cosmetics, detergents, and pharmaceuticals. Some applications have been covered in other industrial categories at the stage of private use. These applications comprise fuels and fuel additives (mineral oil and fuel industry), paint products (paints, lacquers and varnishes industry) and photochemicals (photographic industry). For industrial category 6 (public domain), use and application at public buildings, streets, parks, offices, etc. is considered.

The A-tables of **Appendix 6** provide the estimated total release fractions of the production volume (emission factors) to air, (waste) water and industrial soil during production, formulation, industrial/professional use, private use, and recovery, according to their industrial category. The production volume is defined as the total tonnage of a substance brought to the European market in one year, i.e. the total volume produced in the EU plus the total amount imported into the EU, and minus the total volume exported from the EU excluding the volume of the substance present in products imported/exported. The total volume released is averaged over the year and used for the PECregional calculation.

The B-tables of **Appendix 6** are used for the determination of the releases from point sources for the evaluation of PEClocal. They provide the fraction of the total volume released that can be assumed to be released through a single point source, and the number of days during which the substance is released, thus allowing the daily release rate at a main point source to be calculated.

Despite the need for applying expert judgement when determining the fraction of main source, the following general guidelines for the emission estimation should be applied:

- for production the input for the regional production volume is by default set at the EU production volume, which is also used as input for the **B-tables**. Based on the information available to the rapporteur on the number of production sites, size distribution and geographic distribution it can be decided to apply a 10% rule, where it is assumed that 10% of the amount that is produced and used in the EU is produced/used within a region and it is subsequently assumed that the size of the main local source can be obtained by multiplying this amount with the fraction of main source from the **B-tables**. Alternatively it can be decided to use another percentage or to use specific values as input for the regional model (e.g. the emissions from the largest source or the emissions from the largest emitter) where this reflects a more realistic worst case. Similarly this information can be used to set the fraction of main source for the local exposure calculation. It should be noted that

if site-specific data are available then it can be the case that the largest site is not the largest source of emissions;

- for formulation and processing (industrial use) a similar approach as for production is used: by default the EU volume is used as input for the region as well as for the **B-tables** unless it can be shown/is known that a large number of sites with a reasonable European distribution exists for the specific formulation/processing step of the substance involved. In that case again it can be decided to apply the 10% rule, to use another percentage or to use specific values. Whether or not the available information is sufficient for a specific substance will depend on the expert judgement by the rapporteur;
- for private use the 10% rule is applied by default both for the input of the regional volume and for the input volume for the B-table in agreement with the assumption of 10% of the use occurring in the region.

It must be realised that depending on the Industrial catergory/Use category (IC/UC) combination this approach may in some cases lead to unreasonable worst-case assumptions, especially for the estimation of the emissions during formulation/processing. Hence, a case-by-case assessment using expert judgement remains warranted. For new active substances the default should be overwritten anyway because it may be assumed that in most cases just one or at the most a few producers exist.

In general, the data supplied by industry will help to find the correct entry to the release tables of **Appendix 6**.

The production volume is expressed in tonnes/year in the data set and denoted by PRODVOL. TONNAGE is the volume of substance that is used for subsequent life-cycle stages. In the emission tables of **Appendix 6**, PRODVOL must be used for T when estimating releases at production whereas TONNAGE should be used as T for the subsequent life-cycle stages. If at the disposal stage the substance is recovered this amount should be added to the tonnage of the relevant life-cycle stages. Note that IMPORT and EXPORT refer to the EU, not Member States within the EU.

$$TONNAGE = PRODVOL + IMPORT - EXPORT \qquad \textbf{Equation 4}$$

Explanation of symbols

PRODVOL	production volume of substance	[tonnes·yr^{-1}]	data set
IMPORT	volume of substance imported	[tonnes·yr^{-1}]	data set
EXPORT	volume of substance exported	[tonnes·yr^{-1}]	data set
TONNAGE	tonnage of substance	[tonnes·yr^{-1}]	

The release (in tonnes.yr^{-1}) per stage of the life-cycle and to every environmental compartment is calculated with the equations given in **Appendix 6** and denoted by $RELEASE_{i,j}$ (where i is the stage in the life-cycle and j is the compartment):

i	**stage of the life-cycle**	***j***	**compartment**
1	Production (not relevant for biocides)	a	air
2	Formulation (only relevant for the formulation of the biocidal product into an end-product)	w	water
3	industrial/professional use	s	soil (regional only)
4	private use		
5	service life		
6	waste disposal (including waste treatment and recovery)		

The following table presents the variables used as input for the emission tables in **Appendix 6**, and the releases, which are the output from emission tables and the calculation routine of **Appendix 6**.

Input

MAINCAT	main category (for substances)	[-]	data set
INDCAT	industrial category	[-]	data set
USECAT	use category	[-]	data set
TONNAGE	tonnage of substance (production volume + import - export)	[tonnes·yr^{-1}]	**Equation 4**
PRODVOL	production volume of substance	[tonnes·yr^{-1}]	data set
S	water solubility	[mg·l^{-1}]	data set
VP	vapour pressure	[Pa]	data set
BP	boiling point (for some estimations)	[°C]	data set
Specific information on the use pattern of the substance			

Output

$RELEASE_{i,j}$	release to compartment *j* during life-cycle stage *i*	[-]
$Fmainsource_i$	fraction of release at the local main source at life-cycle stage *i*	[-]
$Temission_i$	total number of days for the emission at life-cycle stage *i*	[d]

For each stage other than production, the losses in the previous stage are taken into account (see calculation in **Appendix 6**). Releases during production are not taken into account in the other stages, as generally, these releases will not have been considered in the reported production volume. In certain cases this might lead to total releases exceeding 100%. It must be specified if releases during each stage are relevant or not. If the release during a certain life stage is not applicable, the release fraction will be set to zero.

Furthermore, few quantitative methods have been developed for estimation of the emissions during the service life of articles containing the substance (main category II) e.g. for emission of a flame retardant in plastics used for TV-sets, radios etc. However, though quantitative methodologies are at present scarce for these types of emissions, preliminary quantitative estimations may be performed on a case-by-case basis (see **section 2.3.3.5** of this guidance).

After accounting for losses during the six stages of the life-cycle, the part of the tonnage that remains is assumed to end up in waste streams completely. Quantitative methods for estimating emissions at the disposal stage are currently available for municipal waste incineration and municipal landfills. However, at present there is not sufficient information available, to set up an emission scenario which is representative at EU level. Nevertheless, preliminary quantitative estimations modelling a reasonable worst case for the regional scenario may be performed on a case-by-case basis. Quantitative methods for the various types of waste operations aiming at recovery are at the stage of development. Preliminary quantitative estimations may be performed on a case-by-case basis (see **sections 2.3.3.6** and **2.3.7.2** of this guidance).

For local emissions for every environmental compartment, the main point source and each stage of the life-cycle is considered. The emission rate is given averaged per day (24 hours). This implies that, even when an emission only takes place a few hours a day, the emission will be averaged over 24 hours. Emissions to air and water will be presented as release rates during an emission episode. Local emissions can be calculated for each stage of the life-cycle and each compartment:

$$Elocal_{i,j} = Fmainsource_i \cdot \frac{1000}{Temission_i} \cdot RELEASE_{i,j}$$ **Equation 5**

Explanation of symbols

$RELEASE_{i,j}$	release during life-cycle stage *i* to compartment *j*	[tonnes·yr^{-1}]
$F_{mainsource,\ i}$	fraction of release at the local main source at life-cycle stage *i*	[-]
$T_{emission,\ i}$	number of days per year for the emission in stage *i*	[d·yr^{-1}]
$Elocal_{i,j}$	local emission during episode to compartment *j* during stage *i*	[kg·d^{-1}]

For local release estimates, point sources (and therefore, presumably single stages of the life-cycle) need to be identified. It will normally be necessary to assess each stage of the life-cycle to determine whether adverse effects can occur since decisions need to be made to clarify or reduce any identified risk for all life-cycle stages. This is not required if it is obvious that a certain stage is negligible.

For the regional scale assessments, the release fractions for each stage of the life-cycle need to be summed for each compartment. The emissions are assumed to be a constant and continuous flux during the year. Regional emissions can be calculated as:

$$Eregional_j = \frac{1000}{365} \cdot \sum_{i=1}^{6} RELEASE_{i,j}$$ **Equation 6**

Explanation of symbols

$RELEASE_{i,j}$	release during life-cycle stage *i* to compartment *j*	[tonnes·yr^{-1}]
$Eregional_j$	total emission to compartment *j* (annual average)	[kg·d^{-1}]

When assessing the releases on local and regional scales, the following points must be noted:

- in particular High Production Volume Chemicals (HPVCs) often have more than one application, sometimes in different industrial categories. For these substances, the assessment proceeds by breaking down the production volume for every application according to data from industry. For the local situation, in principle, all stages of the life-cycle need to be considered for each application. Where more than one stage of the life-cycle occurs at one location, the PEClocal must be calculated by summing all the relevant emissions from that location. For releases to wastewater, only one point source for the local STP is considered. For the regional situation, the emissions to each compartment have to be summed for each stage of the life-cycle and each application. The regional environmental concentrations are used as background concentrations for the local situation;
- if substances are applied in products with an average life span of many years, after the initial arrival of the products onto the market the yearly emissions to the environment will increase. However, after a certain number of years with similar use of the products a steady-state situation will be reached. Examples are a plastic article or a paint coating where the substance assessed is applied as a plasticiser (see also **section 2.3.3.5** of this guidance).

Emission reduction techniques have not been taken into account in the tables of **Appendix 6** as the kind of techniques applied (with possibly large differences in efficiencies) as well as the degree of penetration may differ between Member States or industry sectors. Only when for a certain process a specific reduction measure is common practice this will be taken into account. In all other cases, reasonable worst-case applies."

2.3.3.4 Intermittent releases

Many substances are released to the environment from industrial sources as a result of batch, rather than continuous, processes. In extreme cases, substances may only be emitted a few times a year. Since the PECs associated with industrial releases can take into account both the amount released and the number of days of emission, the magnitude of the PECs in the risk assessment should not be affected. The local PEC is always calculated on the basis of a daily release rate, regardless of whether the discharge is intermittent or continuous. It represents the concentration expected at a certain distance from the source on a day when discharge occurs. The discharge is always assumed to be continuous over the 24-hour period. On the other hand, the regional PEC is calculated using the annual release rate. It represents the steady-state concentration to be expected, regardless of when the discharge occurred.

Intermittent release needs to be defined, although applicants and eCAs will have to justify the use of this scenario on a case-by-case basis. Intermittent release can be defined as "intermittent but only recurring infrequently i.e. less than once per month and for no more than 24 hours".

This would correspond to a typical batch process only required for a short period of the year (releases to the environment may be only of limited duration). Thus, for the aquatic compartment, transport processes may ensure that the exposure of aquatic organisms is of short duration. Calculation of the likely exposure period should take into account the potential of a substance to substantially partition to the sediment. Such partitioning, while reducing the calculated local PEC_{water} may also increase the exposure time by repartitioning to the water phase over an extended period. For intermittent releases to the aquatic compartment an intermittent PNEC is used in the risk characterisation (see **section 3.3.2** of this guidance) that has been derived using a method differing from the usual one.

Where the batch process occurs more frequently than above or is of a longer duration, protection against short-term effects cannot be guaranteed because fish, rooted plants and the majority of the macro-invertebrates are more likely to be exposed to the substance on the second and subsequent emissions. When intermittent release is identified for a substance, this is not necessarily applicable to all releases during the life-cycle.

2.3.3.5 Emissions during service-life of long-life articles

Long-life articles are here defined as articles having a service-life longer than one year. Substances in such articles may accumulate in society (landfills excluded). The emissions from long-life articles can be expected to be highest at steady state (i.e. when the flow of an article into society equals the outflow, see Consumption/application rate based approach). Estimating the emissions often requires knowledge of the substance use pattern in the preceding years.

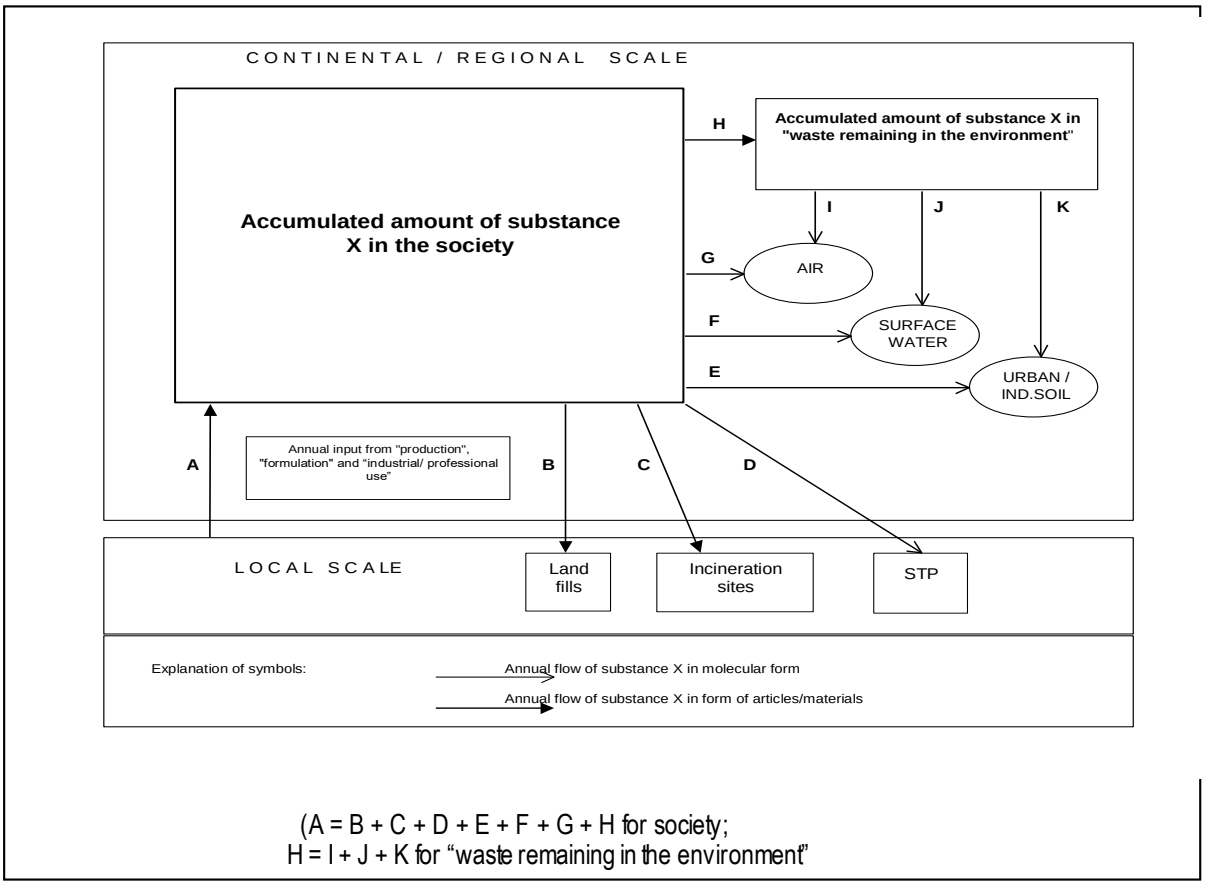

Figure 5: Emissions from long-life articles at Steady state

There are several mechanisms for diffuse emission such as evaporation, leaching, corrosion, abrasion and weathering effects. An additional release route that in some cases is of importance is when a substance diffuses from one material into another (e.g. from glue material into construction material). Substances that are slowly emitted from long-life materials are often characterised by inherent properties such as low water solubility and low vapour pressure (e.g. semi-volatile substances). Particulate emissions will have different fate and behaviour properties compared to molecular emissions e.g. lower bioavailability and longer persistence.

The emission from articles can be assumed to be proportional to the surface area. It is, however, not always possible to estimate this area. Weight based emission factors are then used.

For the emission of biocides from long-life materials, the emission can normally be expected to be highest in the beginning of the use period (due to diffusion mechanisms). It is necessary to be aware that the emission factors are normally an average for the whole service life.

The service life of an article can be defined as the average lifetime of the article. If a significant proportion of an article/material/substance is re-used or recycled leading to a second service life this should be considered in the exposure assessment. Depending on the re-use/recycle pattern this can be handled in different ways:

- if the recycling of an article leads to a second service life with the same or a similar use as the first service life this can be accounted for by adequately prolonging the first service life;
- if the recycling of an article leads to a second service life different from the first service life, emissions from both service lives are calculated separately;

- if the substance/material is recovered and used as raw material for production of new articles this amount should be added to the appropriate life-cycle stage (formulation, industrial/professional use), if not already accounted for.

The calculations of emissions from long-life articles can be performed as follows:

1) estimation of the service life of the article;

2) estimation of emission factors for the substance from the actual material (e.g. fraction/tonnes or mg.m^{-2} surface area). If emission data are missing:

   - compare with similar scenarios described in ESDs (e.g. ESD PT 8 and the City scenario (PT 10) for (in-can) preservation of paints (PT 6, 7) and polymers (PT 9), ESD PT 2 for in-can preservation of detergents (PT 6), or guidance note on leaching rate estimations of PT 07, 09 and 10)

   - search for data in the literature;

   - use a worst-case assumption or if necessary conduct/request an emission study;

3) calculation of the total releases of substance from articles at steady state.

   Assuming constant annual input of the substance and a constant emission factor the equation for the releases to a specific compartment and for the total of all compartments can be written as:

$$RELEASEtot\_steadystate_{i,j,k} = F_{i,j} \cdot Qtot\_accum\_steadystate_k \quad \textbf{Equation 7}$$

and:

$$RELEASEtot\_steadystate_{i,total,k} = F_{i,total} \cdot Qtot\_accum\_steadystate_k \quad \textbf{Equation 8}$$

where the amount accumulated in product *k* in the society at the end of service life (steady state) can be calculated as:

$$Qtot\_accum\_steadystate_k = Qtot_k \cdot \sum_{y=1}^{Tservice_k} (1 - F_{i,total})^{y-1} \quad \textbf{Equation 9}$$

In situations where the emission factor is low (< 1%.yr^{-1}) and the service life of the product is not very long, the emissions and accumulation at steady state (**Equations 7-9**) can be simplified as:

$$RELEASEtot\_steadystate_{i,j,k} = F_{i,j} \cdot Qtot_k \cdot Tservice_k \quad \textbf{Equation 10}$$

$$RELEASEtot\_steadystate_{i,total,k} = F_{i,total} \cdot Qtot_k \cdot Tservice_k \quad \textbf{Equation 11}$$

$$Qtot\_accum\_steadystate_k = Qtot_k \cdot Tservice_k \quad \textbf{Equation 12}$$

Explanation of symbols

$F_{i,,j}$	Fraction of tonnage released per year (emission factor) during life-cycle stage i (service life) to compartment j	[-]	data set[1)]
$F_{i,total}$	Fraction of tonnage released per year (emission factor) during life-cycle stage i (service life) to all relevant compartments	[-]	data set[2)]
RELEASEtot_steady state$_{i,j,k}$	Annual total release to compartment j at steady state for product k	[tonnes·yr^{-1}]	
RELEASEtot_steady state$_{i,total,k}$	Annual total releases to all relevant compartments at steady state for product k	[tonnes·yr^{-1}]	
$Qtot_k$	Annual input of the substance in product k	[tonnes·yr^{-1}]	data set
Qtot_accum_steady state$_k$	Total quantity of the substance accumulated in product k at steady state	[tonnes]	
$Tservice_k$	Service life of product k	[yr]	data set

1) Alternatively use **Equation 16**

2) Alternatively use **Equation 17**

The annual total amount that will end up as waste from product *k* at the end of service life at steady state (b+c+h in **Figure 5**) can be written as (assuming no degradation within the article):

Explanation of symbols

QWASTEtot_steady state$_k$	Total quantity of the substance in product k ending up as waste at steady state	[tonnes·yr^{-1}]	
$Qtot_k$	Annual input of the substance in product *k*	[tonnes·yr^{-1}]	data set
RELEASEtot_steady state$_{i,total,k}$	Annual total releases to all relevant compartments at steady state for product *k*	[tonnes·yr^{-1}]	**Equation 8**

Using a 10% default the annual regional release from article k to compartment j and for the total of all compartments can be calculated as:

$$RELEASEreg\_steadystate_{i,j,k} = RELEASEtot\_steadystate_{i,j,k} \cdot 0.1 \quad \textbf{Equation 13}$$

$$QWASTEtot\_steadystate_{k} = Qtot_{k} - RELEASEtot\_steadystate_{i,total,k} \quad \textbf{Equation 14}$$

$$RELEASEreg\_steadystate_{i,total,k} = RELEASEtot\_steadystate_{i,total,k} \cdot 0.1 \quad \textbf{Equation 15}$$

Explanation of symbols

RELEASEreg_steady state$_{i,j,k}$	Annual regional release to compartment *j* at steady state for product *k*	[tonnes·yr^{-1}]	
RELEASEreg_steady state$_{i,total,k}$	Annual regional release to all relevant compartments at steady state for product *k*	[tonnes·yr^{-1}]	
RELEASEtot_steady state$_{i,j,k}$	Annual total release to compartment *j* at steady state for product *k*	[tonnes·yr^{-1}]	**Equation 7**/ **Equation 10**
RELEASEtot_steady state$_{i,total,k}$	Annual total releases to all relevant compartments at steady state for product *k*	[tonnes·yr^{-1}]	**Equation 8**/ **Equation 11**

These regional diffuse releases are then added to the regional emissions calculated from non-diffuse emissions (Eregional$_j$; **Equation 6**).

If an emission factor is available as release per surface area, it can be converted to a product specific "fraction of tonnage released" ($F_{i,j}$ and $F_{i,total}$):

$$F_{i,j}\ (\text{product specific}) = \frac{\text{EMISSIONarea}_{i,j,k} * 1000}{\text{THICK}_k * \text{CONC}_k}$$ **Equation 16**

and:

$$F_{i,total}\ (\text{product specific}) = \frac{\text{EMISSIONarea}_{i,total,k} * 1000}{\text{THICK}_k * \text{CONC}_k}$$ **Equation 17**

Explanation of symbols

$F_{i,j}$	Fraction of tonnage released per year (emission factor) during life cycle stage *i* (service life) to comparment *j* from product *k*	[yr^{-1}]	
$F_{i,total}$	Fraction of tonnage released per year (emission factor) during life cycle stage *i* (service life) to all relevant compartments from product *k*	[yr^{--1}]	
$CONC_k$	Concentration of substance in product *k*	[kg·dm^{-3}]	data set
EMISSIONarea$_{i,j,k}$	Annual amount of substance emitted per area from product *k* to compartment *j*	[g·m^{-2}·yr^{-1}]	data set
EMISSIONarea$_{i,total,k}$	Annual total of amount substance emitted per area from product *k*	[g·m^{-2}·yr^{-1}]	data set
$THICK_k$	Thickness of the emitting material in product *k*	[mm]	data set

If the area based emissions can be expected to decrease with decreasing concentration in the product the equations 7-8 above are used. If the emission is expected to be independent of the remaining amount of the substance in the product the simplified **Equations 10-11** are used.

If the amount of a substance in use in the society has not reached steady state and the accumulation is still ongoing, the calculated PEC will represent a future situation. If this is the case this should be considered when comparing PEC with monitoring data.

Releases from articles will normally only contribute to the continental and regional releases. The emissions from indoor uses can be released to wastewater and therefore be regarded as a point source (stream "d" in **Figure 5**). Also outdoor uses may cause releases to STP if the storm water system is connected to the STP. This has to be considered case by case.

Quantitative methods for estimating emissions from waste remaining in the environment are currently not available. Therefore such releases have to be considered on a case-by-case basis. As for substances in long-life articles, substances in "waste remaining in the environment" will also accumulate. As a simplification the emissions at steady state can be assumed to be equal to the annually formed amount of "waste remaining in the environment" (see **Figure 5**). If the degradation rate of the substance in the waste material is known, this should be taken into consideration. When the emission of a substance from waste remaining in the environment is very slow it will take a long time to reach steady state. In that case the calculated emission may reflect a future situation.

As for emissions from articles, releases from waste remaining in the environment will also contribute mainly to the continental and regional releases.

2.3.3.6 Emmissions from waste disposal

If the major share of a substance placed on the market remains in products or articles at the end of their service life (releases during use and service life are comparatively small), the waste life-cycle stage of the substance may need particular attention. This refers e.g. to organic substances in landfills and metals in waste incineration processes. The underlying criterion for considering waste emissions in the risk assessment of substances is that the waste stage will contribute significantly to the overall human exposure or environmental concentration in comparison to the emissions from other parts of the life-cycle of the substance (e.g. use stages). If this is not the case, waste considerations could be excluded from the assessment process and general risk management measures based on EU waste legislation should be sufficient.

For certain types of substances, e.g. metals and persistent and toxic substances releases from waste may be slow compared to the release from the use phase but nevertheless the continued long-term release after use could be of concern. On a case-by-case basis, these aspects may be addressed in the risk assessment.

To guide the decision whether an estimation of the releases from the waste stage is pertinent, the following considerations may be used.

First, on the basis of the production volume and the use pattern a preliminary assessment on the volume that may end up in the waste streams should be performed. In doing so the toxicity and other adverse effects of the substance and of possible breakdown products should be taken into account to qualify the significance of the possible impact of such a volume entering the waste stream. Even a small volume of a highly toxic compound may be of concern.

Subsequently, information on anaerobic degradation in landfills or conditions simulating conditions in landfills may indicate that further assessment may not be needed. Water solubility, adsorption/desorption in soil (under landfill conditions) or if available from leaching experiments could also be included in the evaluation as an indicator for leaching potential. However, it is noted that even sorbed substances may leave the landfill via particle transport with leachates.

The substance may also leave the landfill with the produced landfill gas. The K_{ow} and Henry's law constant as well as the tropospheric persistency may be used to indicate whether the release through landfill gas may be of significance. A proposal for possible trigger values can be found in Danish EPA (2001).

For incineration, inorganic substances are the predominant substances of concern. The concern is especially associated with possible leaching of such substances from incineration products whether landfilled or used e.g. for road construction. Furthermore, substances that contain halogens need special attention due to the possible formation of hazardous

substances during incineration.

In order to evaluate whether emissions from incineration of a substance containing an inorganic substance of concern should be included in the risk assessment, the predicted occurrence of the substance in a waste stream should be compared with typical background-ranges. If a substance or a specific use of a substance may contribute unduly to the influent concentration further release calculation should be carried out.

2.3.3.7 Delayed releases from waste disposal and dilution in time

Releases from the waste life stage may occur several decades after processing of the substance under assessment. These delays are determined, inter alia, by:

- the service life span of the substance as such, or in a product or article;
- intermediate storage after service life before waste collection;
- exposure of residues from waste incineration to water. This source could be of particular relevance if the residues are re-introduced into the market as products (e.g. building material) exposed to water;
- intensity of gas production in landfills;
- exposure of landfilled waste to water and deterioration of the landfill bottom liner.

The releases from landfills and residues from waste incineration residues usually take place over a long time period. Hence the daily or annual release may result in a very small PEC. If available, monitoring data may be a valuable source of information (see **section 2.2.2** of this guidance). The need for a long-term release assessment should be decided on a case-by-case basis, in particular for metals or organic substances that are persistent and toxic.

2.3.3.8 Exposure from treated articles

Articles treated with or incorporating biocidal products can lead to consumer and environmental exposure if chemical constituents of the active substances are released in any way. Exposure from treated articles during service life may be the most significant exposure to the active substance. Specifically, articles consisting of different types of polymers can be used in a large range of consumer applications, which makes the exposure situation very complex. Such applications also can belong to a wide range of product types (PTs). The diversity of applications has consequences for the exposure of the environment. Uses with similar exposure patterns (e.g. down the drain, direct exposure to soil, etc.) should be summed up in an aggregated exposure assessment (see **section 4.7** of this guidance).

When treated articles are imported into the EU, the only possible way to carry out a risk assessment is by active substance evaluation. The risk assessment of the intended uses in treated articles is therefore to be included in the Competent Authority Report (CAR).

Definitions

The ***use*** of the biocidal product can include the application of the biocidal product itself (professional or amateur use), the formulation of a treated article (e.g. conversion and compounding of plastic materials; spraying, dipping, thermal impregnation, etc. for wood) as well as the use of the treated article itself (e.g. painting a façade with an outdoor paint containing an algicide or fungicide).

Service life: Use of a treated article in service, e.g. treated wood on a children's playground, a painted façade; shower curtains, fillers, treated kitchen tops, treated apparel, etc. in use (see also **section 2.1**).

Environment

Due to the diversity of uses in treated articles, the exposure has to be related to both the PTs and the specific use of the treated article. Both of these are needed to describe the

exposure pattern. For use in treated articles, besides the properties of the active substance, more aspects have to be taken into account:

- physical condition of the treated article (solid, liquid). This can change during different use phases (e.g. for paints and coatings);
- material the treated article consists of and the structure of the material (wood, plastic, hard or porous surface);
- duration of the service life of the treated article and possible accumulation in the technosphere (see also **section 2.3.3.5**);
- use pattern of the treated article (open space, outside under roof, in-house, in contact with water/soil; regular washing, occasional wiping, etc.).

It is important to consider which of these parameters have effects on the exposure situation. As it is impossible to take into account every single use in detail, it is necessary to summarize similar uses to exposure categories (e.g. regularly washed textiles, treated wood exposed to rain and in contact with soil). It can also be meaningful to estimate which uses probably will have a big impact on the emission situation for a certain compartment (e.g. regularly washed treated textiles) and which uses probably have a small impact (e.g. articles used in-house and wiped occasionally). If the variety of possible uses cannot be handled otherwise, focus should be laid on the uses with a big impact.

For more information on the estimation of exposure from articles please consult REACH *Guidance on information requirements and chemical safety assessment,* Chapter R.15: Consumer exposure estimation and Chapter R.16: Environmental exposure estimation) available at http://echa.europa.eu/guidance-documents/guidance-on-information-requirements-and-chemical-safety-assessment.

Please refer also to the OECD Guideline on how to write emission scenarios for the life-cycle step service life (document No 19 at http://www.oecd.org/chemicalsafety/risk-assessment/emissionscenariodocuments.htm)

To estimate the exposure from treated articles, it might be the easiest way forward to apply the tonnage approach. As a default, the whole tonnage of the active substance, possibly from different suppliers, is used for the emission calculations. The different shares of the tonnage then have to be allocated to the different use patterns or exposure categories. The notifier of the active substance has to help with these allocations. In case the tonnage approach is not used, typical concentrations of the active substance have to be considered for each use and a quantitative estimation of the amount of treated material/articles with a certain use-pattern (e.g. antimicrobial/anti-fungal treated floors in public buildings) has to be made. Possibly, different concentrations of the active substance for different use patterns or different parts of the EU/EEA have to be taken into account (e.g. for treated wood). To consider the different fields of use, use patterns, concentrations of the active substance in a material and different leaching rates from different materials are a precondition for a realistic estimation of environmental exposure of the active substance. Information on the estimated life time of the treated article and possible re-applications, if relevant, are necessary.

Leaching

In higher-tier estimations, leaching rates out of the treated article can be applied to refine the exposure estimations. The assessment can be based on model calculations with well supported default values and/or measured laboratory leaching values, or based on the results of a field or semi-field exposure study. It is important to consider different types of materials/uses which may show different leaching patterns. The duration of the field- or semi-field study should reflect the exposure situation and enable an extrapolation to the service life of the treated article. For polymers, it has to be taken into account that leaching rates can vary quite significantly depending on the type of polymer (e.g. polyethylene leaches less than polyamide, etc.), the type of application (incorporation or coating) and of the use (a regularly washed textiles leaches much more than a kitchen worktop). For wood preservatives, guidance on extrapolation of leaching rates for life time calculations can be

found in 'ESD for PT 8: Revised Emission Scenario Document for Wood Preservatives' (OECD series No 2, 2013) available at http://echa.europa.eu/guidance-documents/guidance-on-biocides-legislation/emission-scenario-documents.

No reliable method exists to predict the leaching rate based on physico-chemical properties of the active substance and therefore leaching studies are normally required. In general a tiered approach should be followed:

- Tier 1: worst-case assumption where 50% of the active substance is assumed to leach after an initial time period of 30 days and 100% of the active substance is assumed to leach after a given longer time period. The longer time period (equal to the life time) can vary and depends on the PT and use of the treated article. Default values for the life time of a number of consumer articles are given in the PT specific ESDs or additional PT related documents (see **section 2.3.3.3.1**).
- Tier 2: validated laboratory leaching test. The uncertainty of using a laboratory test to predict environmental concentrations should be addressed by using an assessment factor.
- Tier 3: semi-field tests or monitoring studies.

For some PTs like e.g. PT 2, 4, 7, 9, and 10, the biocidal product is often added as a master batch to a polymer. The polymer may subsequently be applied to a surface and/or incorporated into a matrix from which leaching of the active substance(s) will take place. As these surfaces/matrices may have many different characteristics, it is important to take into account data for the leaching behaviour for different types of surfaces/matrices which is likely to cover the worst-case leaching behaviour.

The emissions during service life are considered to be diffuse emissions that usually cause exposure on a regional scale. In some cases, however, local exposure scenarios should also be considered. Examples of local scenarios are e.g. wood preservatives or other substances leaching from construction materials, as described in the ESDs for PT 8, 10 and in the 'Guidance note on leaching rate estimations for substances used in biocidal products in PT 07, 09 and 10 of 2010 (endorsed at the 36th CA meeting). The document is available on ECHA website at http://echa.europa.eu/guidance-documents/guidance-on-biocides-legislation/biocidal-products-directive under "Additional guidance on specific issues". Laboratory and semi field leaching test methods for PT 7, 9 and 10 are further provided in the TAB (chapter 2.4.1).

Emissions of the diffuse/wide dispersive type have to be summed up in an aggregated exposure scenario. Possible environmental emissions from articles treated with the same active substance should be summed up. Exposure categories, i.e. uses with the same emission pattern, can be helpful to simplify the aggregated exposure assessment.

Exposure from the waste stage of the treated articles should also be taken into account, if relevant. For this, please consult *Guidance on information requirements and chemical safety assessment. Chapter R.15: Consumer exposure estimation* and *Chapter R.16: Environmental exposure estimation*) available at (http://echa.europa.eu/guidance-documents/guidance-on-information-requirements-and-chemical-safety-assessment).

Further guidance and documents related to emission estimation from treated articles:

- 'Report of the leaching workshop assessing leaching from treated wood to the environment' available at http://echa.europa.eu/guidance-documents/guidance-on-biocides-legislation/emission-scenario-documents under 'Product Type 8. Wood preservatives';
- OECD 313:2007: Estimation of Emissions from Preservative-Treated Wood to the Environment: Laboratory Method for Wooden Commodities That Are Not Covered And Are In Contact with Fresh Water or Seawater;
- CEN/TS 15119-2:2012 Durability of Wood and Wood-Based Products, Determination of Emissions from Preservative Treated Wood to the Environment -

Part 2: Wooden Commodities Exposed in Use Class 4 or 5 (In Contact with the Ground, Fresh Water or Sea Water) - Laboratory Method. CEN/TC 38: 2012. CEN-CENELEC Management Centre, Brussels; 2007;

- OECD Test Guideline 107: Preservative - Treated wood to the environment: For wood held in storage after treatment and for wooden commodities that are not covered and are not in contact with ground (OECD, 2009) available at http://echa.europa.eu/guidance-documents/guidance-on-biocides-legislation/emission-scenario-documents under 'Product Type 8. Wood preservatives';
- OECD Series on Emission Scenario Documents, Number 3: Emission Scenario Document on plastic additives. (2004, revised in 2009) available at http://www.oecd.org/chemicalsafety/risk-assessment/emissionscenariodocuments.htm;
- OECD Series on Emission Scenario Documents, Number 19: Complementing Guideline for Writing ESDs: The Life-Cycle Step "service-life" (2008) available at http://www.oecd.org/chemicalsafety/risk-assessment/emissionscenariodocuments.htm;
- CEN/TR 16663 : 2014 Determination of emissions from preservative treated wood in the environment - wooden commodities exposed in Use Class 3 (Not covered, not in contact with ground) – Semi-field method;
- BAM Guidance on a laboratory leaching test method for materials that are treated with biocides for PT 7, 9, 10 (2015), available in TAB v1.2, entry ENV 26;
- BAM Guidance on a semi-field test method for materials that are treated with biocides for PT 7, 9, 10 (2015), available in TAB v1.2, entry ENV 26.

2.3.4 Characterisation of the environmental compartments

In this section, the following parameters are derived:

- definition of the standard environmental characteristics (**Table 3**);
- bulk densities for soil, sediment, and suspended matter.

For the derivation of PECs a standardised generic environment needs to be defined since the general aim is to obtain conclusions regarding risks of the substance at EU level. The characteristics of the real environment will, obviously, vary in time and space. In **Table 3**, average or typical default values are given for the parameters characterising the environmental compartments. The standard assessment needs to be performed with the defaults, as given in **Table 3**. When more specific information is available on the location of the emission sources, this information can be applied in refinement of the PEC by deviating from the parameters of **Table 3**.

Several other generic environmental characteristics, mainly relevant for the derivation of regional PEC (e.g. the sizes of the environmental compartments, mass transfer coefficients) are given in **section 2.3.7.7** (**Tables 11-13**) of this guidance.

Table 3: Definition of the standard environmental characteristics

Parameter	Symbol	Unit	Value
General			
Density of the solid phase	RHO_{solid}	$[kg_{solid} \cdot m_{solid}^{-3}]$	2,500
Density of the water phase	RHO_{water}	$[kg_{water} \cdot m_{water}^{-3}]$	1000
Density of air	RHO_{air}	$[kg_{air} \cdot m_{air}^{-3}]$	1.3
Temperature (12°C)	TEMP	[K]	285
Surface water			
Concentration of suspended matter (dry weight)	$SUSP_{water}$	$[mg_{solid} \cdot l_{water}^{-1}]$	15
Suspended matter			
Bulk density of (wet) suspended matter	RHO_{susp}	$[kg \cdot m^{-3}]$	1,150
Volume fraction solids in susp. matter	$F_{solid, susp}$	$[m_{solid}^3 \cdot m_{susp}^{-3}]$	0.1
Volume fraction water in susp. matter	$F_{water, susp}$	$[m_{water}^3 \cdot m_{susp}^{-3}]$	0.9
Weight fraction organic carbon in susp. solids	$F_{oc, susp}$	$[kg_{oc} \cdot kg_{solid}^{-1}]$	0.1
Sediment			
Bulk density of (wet) sediment	RHO_{sed}	$[kg \cdot m^{-3}]$	1,300
Volume fraction solids in sediment	$F_{solid, sed}$	$[m_{solid}^3 \cdot m_{sed}^{-3}]$	0.2
Volume fraction water in sediment	$F_{water, sed}$	$[m_{water}^3 \cdot m_{sed}^{-3}]$	0.8
Weight fraction organic carbon sediment solids	$F_{oc, sed}$	$[kg_{oc} \cdot kg_{solid}^{-1}]$	0.05
Soil			
Bulk density of (wet) soil	RHO_{soil}	$[kg \cdot m^{-3}]$	1,700
Volume fraction solids in soil	$F_{solid, soil}$	$[m_{solid}^3 \cdot m_{soil}^{-3}]$	0.6
Volume fraction water in soil	$F_{water, soil}$	$[m_{water}^3 \cdot m_{soil}^{-3}]$	0.2
Volume fraction air in soil	$F_{air, soil}$	$[m_{air}^3 \cdot m_{soil}^{-3}]$	0.2
Weight fraction organic carbon in soil solids	$F_{oc, soil}$	$[kg_{oc} \cdot kg_{solid}^{-1}]$	0.02
Weight fraction organic matter in soil solids	$F_{om, soil}$	$[kg_{om} \cdot kg_{solid}^{-1}]$	0.034

Transfer from wet weight to dry weight

The densities of soil and suspended matter provided in the Table 3 are expressed in wet weight, they can be recalculated into dry weight as follows:

The conversion factors for soil and sediment are derived from the compartment definition in phases. The conversion to dry weight can also be used for entering toxicity data.

$$CONV_{soil} = \frac{RHO_{soil}}{Fsolid_{soil} \cdot RHOsolid}$$ **Equation 18**

$$CONV_{susp} = \frac{RHO_{susp}}{Fsolid_{susp} \cdot RHOsolid}$$ **Equation 19**

Input

RHO_{soil}	wet bulk density of soil	[$kg_{wwt}.m^{-3}$]	O[c]
$Fsolid_{soil}$	volume fraction of solids in soil	[$m^3.m^{-3}$]	D
RHO_{susp}	wet bulk density of suspended matter	[$kg_{wwt}.m^{-3}$]	O[c]
$Fsolid_{susp}$	volume fraction of solids in suspended matter	[$m^3.m^{-3}$]	D
RHOsolid	density of solid phase	[$kg.m^{-3}$]	D

Output

$CONV_{soil}$	conversion factor for soil concentrations: wwt to dwt	[$kg_{wwt}.kg_{dwt}^{-1}$] O[c]
$CONV_{susp}$	conversion factor for suspended matter conc.: wwt to dwt	[$kg_{wwt}.kg_{dwt}^{-1}$] O[c]

Each of the compartments soil, sediment, and suspended matter is described as consisting of three phases: air (only relevant in soil), solids, and water. The bulk density of each compartment is thus defined by the fraction and bulk density of each phase. Both the fractions solids and water, and the total bulk density are used in subsequent calculations. This implies that the bulk density of a compartment cannot be changed independently of the fractions of the separate phases and vice versa.

The bulk densities of the compartments soil, sediment, and suspended matter are defined by the fractions of the separate phases:

$$RHO_{comp} = Fsolid_{comp} \bullet RHOsolid + Fwater_{comp} \bullet RHOwater + Fair_{comp} \bullet RHOair$$
$$with\ comp \in \{soil, sed, susp\}$$

Equation 20

Application of the formulas above for the values mentioned leads to the following bulk densities of each standard environmental compartment, provided in Table 3 above.

When deriving the bulk density of different environmental compartments care should be taken to ensure that the expression of exposure and effect concentrations is consistent for both (for example always comparing PEC values in dry weight with PNEC values in dry weight or use the corresponding wet weight values for both).

2.3.5 Partition coefficients

In this section, the following processes are described:

- fraction of substance in air associated with aerosol;
- partitioning between air and water;
- partitioning between solids and water in soil, sediment and suspended matter.

Transport and transformation ("fate") describe the distribution of a substance in the environment, or in organisms, and its changes with time (in concentration, chemical form, etc.). Since measured data on fate processes for different compartments are usually not available, they must be extrapolated from the primary data listed in **section 2.3.2** of this guidance. This section describes the derivation of the partitioning processes between air-aerosol, air-water, and solids-water in the various compartments.

It should be noted that for ionising substances, partitioning behaviour between air-water and solids-water is dependent on the pH of the environment. **Section 4.5.3** of this guidance gives more specific guidance for the assessment of these compounds.

Fate estimates based on "partitioning" are limited to distribution of a substance in molecular form. For substances that also will be distributed in the environment as particles (caused by

abrasion/weathering of anthropogenic materials) extrapolation based on partitioning may not be relevant. In such a case the partitioning method may underestimate exposure of soil and sediment environments and overestimate the exposure of water. If the particle size is small also air distribution may occur, at least in the local perspective. There are no estimation methods available for particle distribution so this has to be dealt with on a case-by-case basis.

2.3.5.1 Adsorption to aerosol particles

The fraction of the substance associated with aerosol particles can be estimated on the basis of the substance's vapour pressure, according to Junge (1977). In this equation, the sub-cooled liquid vapour pressure should be used.

$$Fass_{aer} = \frac{CONjunge \bullet SURF_{aer}}{VP + CONjunge \bullet SURF_{aer}}$$ **Equation 21**

Explanation of symbols

CONjunge	constant of Junge equation	[Pa·m]	*
$SURF_{aer}$	surface area of aerosol particles	[$m^2 \cdot m^{-3}$]	*
VP	vapour pressure	[Pa]	data set
$F_{ass, aer}$	fraction of the substance associated with aerosol particles	[-]	

* as a default the product of CONjunge and $SURF_{aer}$ is set to 10^{-4} Pa (Van de Meent, 1993; Heijna-Merkus and Hof, 1993).

Alternatively the octanol-air partition coefficient could be used as described by Finizio et al. (1997).

For solids, a correction of the vapour pressure is required to derive the sub-cooled liquid vapour pressure (Mackay, 1991; van Noort, 2004):

$$VPL = \frac{VP}{e^{6.79 \cdot (1 - \frac{T_{melt}}{T})}}$$ **Equation 22**

Explanation of symbols

T	environmental temperature	[K]	285
T_{melt}	melting point of substance	[K]	data set
VPL	sub-cooled liquid vapour pressure	[Pa]	
VP	vapour pressure	[Pa]	data set

2.3.5.2 Volatilisation

The transfer of a substance from the aqueous phase to the gas phase (e.g. stripping in the aeration tank of a STP, volatilisation from surface water) is estimated by means of its Henry's law constant. If the value is not available in the input data set, the required Henry's Law constant and the Kair-water (also known as the "dimensionless" Henry's law constant) can be estimated from the ratio of the vapour pressure to the water solubility, both

expressed at T_{env}, which is the temperature of the environmental compartment of interest. For water miscible compounds direct measurement of the Henry's law constant is recommended (see also REACH *Guidance on information requirements and chemical safety assessment Chapter R.7a: Endpoint specific guidance, Appendix R.7.1-1* = Henry's law constant and evaporation rate). If an experimentally determined Henry's law constant is available, it can be corrected for temperature using **Equation 23**[15].

$$H(T_{env}) = \frac{VP(\mathrm{T_{env}}) \cdot M}{S(\mathrm{T_{env}})}$$ **Equation 23**

$$K_{air\text{-}water} = \frac{H(T_{env})}{R \cdot T_{env}}$$ **Equation 24**

$$H(T_{env}) = \mathrm{H}(T_{test}) \cdot e^{\left(\frac{H_{0vapor} - H_{0solut}}{R} \cdot \left(\frac{1}{T_{test}} - \frac{1}{T_{env}}\right)\right)}$$ **Equation 25**

Explanation of symbols

$VP(T_{env})$	vapour pressure at the environmental temperature	[Pa]	**Equation 2**
M	molecular weight	[g · mol^{-1}]	data set
$S(T_{env})$	solubility at the environmental temperature	[mg · l^{-1}]	data set
R	gas constant	[Pa · m^3 · mol^{-1} · k^{-1}]	8.314
T_{env}	environmental temperature (scale-dependent)	[K]	285
T_{test}	temperature of the measured experimental Henry's law constant	[K]	data set
$H(T_{env})$	Henry's law constant at the environmental temperature	[Pa · m^3 · mol^{-1}]	
$H(T_{test})$	Henry's law constant at the test temperature	[Pa · m^3 · mol^{-1}]	data set
$K_{air\text{-}water}$	air-water partition coefficient	[-]	
H_{0vapor}	enthalpy of vapourisation	[J · mol^{-1}]	5·10^4
H_{0solut}	enthalpy of solution	[J · mol^{-1}]	1·10^4

If no reliable data for vapour pressure and/or solubility can be obtained with the present OECD guidelines, QSARs are available, but are not addressed in this guidance. For further information please refer to *Guidance on information requirements and chemical safety assessment Chapter R.6: QSARs and grouping of chemicals* (http://echa.europa.eu/guidance-documents/guidance-on-information-requirements-and-chemical-safety-assessment).

2.3.5.3 Adsorption/desorption

In addition to volatilisation, adsorption to solid surfaces is the main partitioning process that drives distribution in soil, surface waters, and sediments. The adsorption of a substance to

[15] It is noted that temperature correction in EUSES is implemented in a slightly different way (parameters first converted to 25°C and then to the temperature of environmental compartment of interest), but for the local compartment, results are identical to the routine given here.

soil, sediment, suspended matter and sludge can be obtained or estimated from:

- K_{oc} measured in a screening test on adsorption/desorption (EC method C.18/OECD Test Guideline 106)
- K_{oc} estimated by the HPLC method (EC method C.19/OECD Test Guideline 121);
- column leaching study (OECD 312);
- lysimeter studies/Field leaching studies (OECD Test Guideline 22);
- adsorption control within an inherent biodegradability test;
- if no K_{oc} is available, it may be estimated from K_{ow} "(for metabolites or substances for which a K_{oc} is technically impossible to derive)).

It should be noted that for surfactants the octanol/water partition coefficient (K_{ow}) is experimentally difficult to determine and this parameter may not be sufficiently descriptive of surface activity or adsorption/desorption (surfactant behaviour).

If no measured data are available for a specific adsorbing material, it is assumed that all adsorption can be related to the organic matter of the medium, via standardisation to K_{oc} (this is only valid for non-ionic substances) based on the organic carbon content of different media (e.g. soil, sediment, suspended matter, sewage sludge). For organic, non-ionic substances, K_{oc} can be estimated from K_{ow} as outlined in *Guidance on information requirements and chemical safety assessment Chapter R.6: QSARs and grouping of chemicals* available at http://echa.europa.eu/guidance-documents/guidance-on-information-requirements-and-chemical-safety-assessment. The equation for "non-hydrophobic" substances is preferred as default. For specific groups of substances, other QSARs are given in *Chapter R.6.* For ionic substances, a measured adsorption coefficient is needed, or it may be possible to first investigate how significant the value might be by using a high value of K_{oc} in the assessment. Cationic substances are generally known to adsorb strongly.

For water soluble, highly adsorptive substances the use of K_{ow} as input into SimpleTreat may lead to an overestimation of the aquatic exposure concentration. SimpleTreat will predict a low elimination on the basis of the log K_{ow} (and small Henry's law constant), while adsorption onto sludge may be a significant elimination mechanism for these substances. For those substances either a K_{oc} experimentally determined *in activated sludge with measured organic carbon content* or the approach described in the following should be used.

In the absence of better adsorption/desorption data, the Zahn-Wellens elimination level can be used as an estimate of the extent of adsorption to sludge. The 3h value is recommended. For slowly adsorbing substances, consideration should be given to the hydraulic retention time in the aeration tank of the STP (default is 6.8 h in SimpleTreat 3.1). Values beyond 24 h would not normally be used. Where data are not available for adsorption up to 24 h, data from time scales beyond this can only be used if adsorption is the only removal mechanism, with an upper limit of 7 d.

The solid-water partition coefficient (K_p) in each compartment (soil, sediment, suspended matter) can be calculated from the K_{oc} value, and the fraction of organic carbon in the compartment. Initially, the fraction of organic carbon in the standard environment should be used, as given in **Table 3.**

$$Kp_{comp} = Foc_{comp} \bullet Koc \qquad with\ comp \in \{soil, sed, susp\}$$ **Equation 26**

Explanation of symbols

K_{oc}	partition coefficient organic carbon-water	[l·kg^{-1}]	data set
$F_{oc, comp}$	weight fraction of organic carbon in compartment *comp*	[kg·kg^{-1}]	**Table 3**

$K_{p,\ susp}$	partition coefficient solid-water in suspended matter	[l·kg^{-1}]
$K_{p,\ sed}$	partition coefficient solid-water in sediment	[l·kg^{-1}]
$K_{p,\ soil}$	partition coefficient solid-water in soil	[l·kg^{-1}]

In all cases, i.e. less or more than three measurements of K_{oc} for parent and major metabolites are available for neutral, organic, non-ionised substances from a range of contrasting test systems, within a specific compartment (e.g. different soils or sediments respectively), it is recommended to use the **geometric mean** value in calculations. This is recommended to account for the variability in Koc values and is based on the assumption that the underlying populations typically follow a log-normal distribution. Note that such an approach would not be appropriate when the partition coefficient was dependent on system properties other than organic carbon content (e.g. when pH dependent partitioning is observed). In those cases the guidance provided in **section 2.3.2** should be considered. K_p is expressed as the concentration of the substance sorbed to solids (in $mg_{chem}·kg_{solid}^{-1}$) divided by the concentration dissolved in (pore)water ($mg_{chem}·l_{water}^{-1}$). The dimensionless form of K_p, or the total compartment-water partition coefficient in $(mg·m_{comp}^{-3})/(mg·m_{water}^{-3})$, can be derived from the definition of the compartment in multiple phases (i.e. solid, water and air fractions in soil; solid and water fractions in suspended matter and sediment):

$$K_{comp\text{-}water} = \frac{Ctotal_{comp}}{Cporew_{comp}}$$

$$K_{comp\text{-}water} = Fair_{comp} \cdot K_{air\text{-}water} + Fwater_{comp} + Fsolid_{comp} \cdot \frac{Kp_{comp}}{1000} \cdot RHOsolid \qquad \textbf{Equation 27}$$

$$with\ comp \in \{soil\ , susp\ , sed\}$$

Explanation of symbols

$F_{water,\ comp}$	fraction water in compartment *comp*	[$m_{water}^3 \cdot m^{-3}$]	**Table 3**
$F_{solid,\ comp}$	fraction solids in compartment *comp*	[$m^3 \cdot m^{-3}$]	**Table 3**
$F_{air,\ comp}$	fraction air in compartment comp (only relevant for soil)	[$m_{air}^3 \cdot m^{-3}$]	**Table 3**
RHO_{solid}	density of the solid phase	[$kg_{dwt} \cdot m^{-3}$]	**Table 3**
$K_{p,comp}$	solids-water part. coeff. in compartment *comp*	[$l \cdot kg^{-1}$]	**Equation 26**
$K_{air\text{-}water}$	air-water partition coefficient	[-]	**Equation 24**
$K_{soil\text{-}water}$	soil-water partition coefficient	[$m^3 \cdot m^{-3}$]	
$K_{susp\text{-}water}$	suspended matter-water partition coefficient	[$m^3 \cdot m^{-3}$]	
$K_{sed\text{-}water}$	sediment-water partition coefficient	[$m^3 \cdot m^{-3}$]	

2.3.6 Abiotic and biotic degradation rates

In this section, the following processes are described:

- hydrolysis in surface water;
- photolysis in surface water and in the atmosphere;

- biodegradation in the sewage treatment plant;
- biodegradation in the environmental compartments (surface water, soil, sediment).

Transport and transformation ("fate") describe the distribution of a substance in the environment, or in organisms, and its changes with time (in concentration, chemical form, etc.), thus including both biotic and abiotic transformation processes. In general, the assessment of degradation processes should be based on data, which reflect the environmental conditions as realistically as possible. Data from studies where degradation rates are measured under conditions that simulate the conditions in various environmental compartments are preferred. The applicability of such data should, however, be judged in the light of any other degradation data including results from screening tests. Most emphasis is put on the simulation test results but in the absence of simulation test data, degradation rates and half-lives have to be estimated from screening test data. The rates of degradation of a substance in the environment are determined by a combination of substance-specific properties and environmental conditions.

For substances where a range of degradation data is available, the use of average input parameters (artithmetic mean, median or geometric mean) is recommended.

Please refer also to FOCUS (2006) Guidance Document on Estimating Persistence and Degradation Kinetics from Environmental Fate Studies on Pesticides in EU Registration (Sanco/10058/2005) and FOCUS (2011), Generic guidance for Estimating Persistence and Degradation Kinetics from Environmental Fate Studies on Pesticides in EU Registration.

In this section, methods for derivation of degradation rate constants are described for abiotic degradation (hydrolysis and photolysis) and biotic degradation (in soil, sediment, water, and sewage treatment). For hydrolysis and photolysis, only primary degradation is measured.

In general, risk assessment focuses on the parent compound. If relevant metabolites or transformation products are formed, the risk assessment should include these. It is possible that the rate of reaction is such that only the resulting products need to be considered, or in intermediate cases both the substance and the degradation products will require consideration. It is important to have information about which chemical species were responsible for any effects that were observed in the aquatic toxicity studies.

Where substances degrade by complex interaction mechanisms, for example abiotic degradation followed by biodegradation, and where there are no internationally recognised protocols for simulation tests, the use of relevant field data could be considered provided that the kinetics of full mineralisation or formation of possible metabolites have been determined.

2.3.6.1 Hydrolysis

Values for the half-life (DT_{50}) of a hydrolysable substance can be converted to degradation rate constants, which may be used in the models for calculating the PEC, if not already covered by results on biodegradation. The results of a ready biodegradability study will show whether or not the hydrolysis products are themselves biodegradable. Similarly, for substances where DT_{50} is less than 12 hours, environmental effects are likely to be attributed to the hydrolysis products rather than to the parent substance itself. These effects should also be assessed. QSAR methods are available for certain groups of substances, e.g. the EPIWIN program (US EPA, 2002) and other methods described in *Guidance on information requirements and chemical safety assessment Chapter R.6: QSARs and grouping of chemicals*.

For many substances, the rate of hydrolysis will be heavily dependent on the specific environmental pH and temperature and in the case of soil, also moisture content. For risk assessment purposes for fresh water, sediment and soil, a pH of 7 and a temperature of 12 °C (285 K) will normally be established which conform to the standard environmental parameters of **Table 3**. However, for some substances, it may be necessary to assume a different pH and temperature to fully reflect the potential of the substance to cause adverse

effects. This may be of particular importance where the hydrolysis profile shows significantly different rates of hydrolysis over the range pH 4 - 9 and the relevant toxicity is known to be specifically caused by either the stable parent substance or a hydrolysis product.

Rates of hydrolysis always increase with increasing temperature. When hydrolysis half-lives have been determined in standard tests, they should be recalculated to reflect an average EU outdoor temperature by the equation:

$$DT50(X\,°C) = DT50(t) \cdot e^{(0.08 \cdot (T-X))}$$ **Equation 28**

where X = 12 °C for fresh water and 9 °C for seawater. Note that this equation for the correction of DT_{50} values for temperature also applies to other degradation data.

When it is documented for a specific substance that the typical pH of the environmental compartment to be assessed also affects the hydrolysis rate in addition to temperature, the most relevant hydrolysis rate should be taken or extrapolated from the results of the standard test in different pH values. Thereafter the temperature correction is to be applied, where relevant.

When the use of an alternative pH will affect the environmental distribution and toxicity by changing the nature of the soluble species, for example with ionisable substances, care should be taken to ensure that this is fully taken into account when making a final PEC/PNEC comparison.

The half-life for hydrolysis (if known) can be converted to a pseudo first-order rate constant:

$$khydr_{water} = \frac{\ln 2}{DT50\,hydr_{water}}$$ **Equation 29**

Explanation of symbols

$DT50hydr_{water}$	half-lifetime for hydrolysis in surface water	[d]	data set
$khydr_{water}$	first order rate constant for hydrolysis in surface water	[d^{-1}]	

2.3.6.2 Photolysis in water

In the vast majority of surface water bodies dissolved organic matter is responsible for intensive light attenuation. Thus photolysis processes are normally restricted to the upper zones of water bodies. Indirect processes like photo-sensitisation or reaction with oxygen transients ($^1O_2$, OH-radicals, ROO-radicals) may significantly contribute to the overall breakdown rate. Photochemical degradation processes in water may only become an important fate process for substances, which are persistent to other degradation processes (e.g. biodegradation and hydrolysis). The experimental determination of the quantum yield (OECD, 1992c) and the UV-absorption spectrum of the substance are prerequisites for estimating the rate of photodegradation in surface water. Due to high seasonal variation in light flux, photochemical degradation should only be based on average EU conditions. Methods to derive average degradation rates which can be used in the model calculation of regional PEC are described in Zepp and Cline (1977) and Frank and Klöppfer (1989).

The following aspects have to be considered when estimating the photochemical transformation in natural water bodies:

- the intensity of the incident light depends on seasonal and geographic conditions and varies within wide ranges. For long-term considerations average values can be used

while for short-term exposure an unfavourable solar irradiance (winter season) should be chosen;

- in most natural water bodies, the rate of photoreaction is affected by dissolved and suspended matter. Since the concentration of the substance under consideration is normally low compared to the concentration of e.g. dissolved humic acids, the natural constituents absorb by far the larger portion of the sunlight penetrating the water bodies.

Using the standard parameters of the regional model (i.e. a water depth of 3 m and a concentration of suspended matter of 15 mg/l), the reduction in light intensity is higher than 98% through the water column. Indirect (sensitised) photochemical reactions should only be included in the overall breakdown rate of water bodies if there is clear evidence that this pathway is not of minor importance compared to other processes and its effectiveness can be quantified. For facilitating the complex calculation of phototransformation processes in natural waters computer programmes have been developed (e.g. ABIWAS by Frank and Klöppfer, 1989; GC-SOLAR by Zepp and Cline, 1977).

In practice it will not be possible to easily demonstrate that photodegradation in water is significant in the environment. A value for the half-life for photolysis in water (if known) can be converted to a pseudo first-order rate constant:

$$kphoto_{water} = \frac{\ln 2}{DT50\ photo_{water}}$$ **Equation 30**

Explanation of symbols

$DT_{50}photo_{water}$	half-lifetime for photolysis in surface water	[d]	data set
$kphoto_{water}$	first order rate constant for photolysis in surface water	[d^{-1}]	

2.3.6.3 Photochemical reactions in the atmosphere

Although for some substances direct photolysis may be an important breakdown process, the most effective elimination process in the troposphere for most substances results from reactions with photochemically generated species like OH radicals, ozone and nitrate radicals. The specific first order degradation rate constant of a substance with OH-radicals (k_{OH} in $cm^3 \cdot molecule^{-1} \cdot s^{-1}$) can either be determined experimentally (OECD, 1992c) or estimated by (Q)SAR-methods like AOPWIN (US EPA, 2012). By relating kOH to the average OH-radical concentration in the atmosphere, the pseudo-first order rate constant in air is determined:

$$kdeg_{air} = k_{OH} \cdot OHCONC_{air} \cdot 24 \cdot 3600$$ **Equation 31**

Explanation of symbols

k_{OH}	specific degradation rate constant with OH-radicals	[$cm^3 \cdot molec^{-1} \cdot s^{-1}$]	data set
$OHCONC_{air}$	concentration of OH-radicals in atmosphere	[$molec \cdot cm^{-3}$]	$5 \cdot 10^5$ *
$kdeg_{air}$	pseudo first order rate constant for degradation in air (24-hour day)	[d^{-1}]	

* The global annual average OH-radical concentration can be assumed to be 5.10^5 molecules.cm^{-3} (BUA, 1992).

Degradation in the atmosphere is an important process and it is essential to consider whether it can affect the outcome. Photodegradation data in the atmosphere must be evaluated with some care. Highly persistent substances may be reported as rapidly degraded in air under environmental conditions where the chemical could be in large

amounts in the gas phase. In the real environment, most of the substance may be associated to particles or aerosol and the real atmospheric half-life could be orders of magnitude higher.

2.3.6.4 Biodegradation in a sewage treatment plant

The assessment of biodegradability and/or removal in sewage treatment plants should preferably be based on results from tests simulating the conditions in treatment plants (e.g. OECD Test guideline 303 A). For further guidance on use of STP simulation test results, see **section 2.3.6.7** of this guidance.

The ready biodegradability tests that are used at the moment are aimed at measuring the ultimate biodegradability of a substance. They do not give a quantitative estimate of the removal percentage in a wastewater treatment plant. Therefore, in order to make use of the biodegradation test results that are available and requested in the present chemical legislation, it is necessary to assign rate constants to the results of the standard tests for use in STP-models. These constants are based on a relatively limited number of empirical data. However, since direct measurements of degradation rates at environmentally relevant concentrations are often not available, a pragmatic solution to this problem has been found. For the purpose of modelling a sewage treatment plant (STP), the rate constants of **Table 4** below were derived from the biodegradation screening tests. All constants in **Table 4** have the following prerequisites:

- they are only used for the water-dissolved fraction of the substance. Partitioning between water and sludge phases should be calculated prior to the application of the rate constant;
- sufficiently valid data from internationally standardised tests are preferred;

Data from non-standardised tests and/or tests not performed according to the principles of GLP may be used if expert judgement has confirmed them to be equivalent to results from the standardised degradation tests on which the calculation models, e.g. SimpleTreat, are based. The same applies to STP-measured data, i.e., in-situ influent/effluent measurements.

If measured degradation rates for the STP are available from a simulation test, they should be corrected to the environmental temperature of the standard STP (288.15 K), using SimpleTreat.

A water-sediment simulation study can be considered as an alternative to a STP simulation test. The resulting DT_{50} value (biodegradation in water phase, not dissipation) from this test can be used as a worst-case value for degradation in the STP.
The opposite is not acceptable, i.e. using the DT_{50} value from a STP simulation test as a substitute for degradation in a water-sediment system.

Table 4: Elimination in sewage treatment plants: Extrapolation from test results to rate constants in STP model (SimpleTreat) [a)]

Test result	Rate constant k.(h-1)
Readily biodegradable [b)]	1
Readily, but failing 10-d window [b)]	0.3
Inherently biodegradable, fulfilling specific criteria [c)]	0.1
Inherently biodegradable, not fulfilling specific criteria [c)]	0
Not biodegradable	0

Notes on Table 4:

a) For use in STP models, these rate constants do not need to be corrected for different environmental temperatures as they are generic values.

b) Ready biodegradability testing (28 d) e.g. according to OECD test guidelines 301 A-F.

Ready biodegradability tests are screening tests for identifying substances that, based on general experience, are assumed to undergo rapid and ultimate biodegradation in the aerobic environment. However, a negative result does not necessarily mean that the substance will not be biodegraded in, e.g., a sewage treatment plant.

The degree of ultimate degradation may be followed by determination of the loss of dissolved organic carbon (DOC), the evolution of carbon dioxide or the amount of oxygen consumed. It is generally accepted that a substance is considered to be readily biodegradable if the substance fulfils the pass criteria of a test for ready biodegradability (cf. the Annex V methods or the OECD guidelines) which may include the concept of the 10 days time window as a simple kinetic criterion. All percentage biodegradation results refer to true biodegradation i.e. mineralisation excluding abiotic elimination processes (e.g. volatilisation, adsorption). This means that corresponding data in adequate control vessels must be generated during biodegradation testing. The test may be continued beyond 28 days if biodegradation has started but does not reach the required pass criteria for final mineralisation: in this case however, the substance would not be regarded as being readily biodegradable. If the substance reaches the biodegradation pass levels within 28 days but not within the 10-day time window, a biodegradation rate constant of 0.3 h^{-1} is assumed. In case that only old ready biodegradation test results (i.e. tests executed prior to the introduction of the 10 days time window criterion and documenting only on the pass level) are available a rate constant of 0.3 h^{-1} should be applied in case the pass level is reached. Based on weight of evidence (e.g. several old test results) a rate constant of 1 h^{-1} may be justified by expert judgement.

If the substance is found to be not readily biodegradable, it is necessary to check whether it was inhibitory to microbial activity at the concentration used in the biodegradability test. If the substance is inhibitory, it may be re-tested at low, non-inhibitory concentrations in a test simulating the conditions in a sewage treatment plant. If appropriate, re-testing in another more suitable ready biodegradability test may be considered. Re-testing in a modified ready biodegradability test at a much lower concentration (i.e. more than 10 times lower than prescribed) cannot generally be recommended because suitable simulation test methods are available.

c) Inherent biodegradability testing (28d) e.g. according to OECD test guidelines 302 B-C.

Inherent biodegradability tests are designed to assess whether the substance has any potential for biodegradation. A negative result will normally mean that non-biodegradability (persistence) should be assumed. A positive result, on the other hand, indicates that the substance will not persist indefinitely in the environment. In those cases where a more accurate prediction of degradation kinetics in treatment plants is required, sewage treatment plant simulation tests should be conducted (OECD test guideline 303 A).

In tests for inherent biodegradability, the test conditions are designed to be more favourable to the microorganisms in that the ratio of substance to cells is lower than in the ready tests and there is no requirement for the (bio)degradation to follow a time pattern as in the ready tests. Also, pre-exposure of the inoculum resulting in pre-adaptation of the microorganisms may be allowed. The time permitted for the study is limited to 28 days, but it may be continued for much longer; 6 months has been suggested as the maximum duration for the test. The results obtained in a test of more than 28 days are not comparable with those obtained in less than this period.

Usually, more than 70% (bio)degradation within 28 days indicates that the substance is inherently biodegradable. However, extrapolation of the results of the inherent tests should be done with great caution because of the strongly favourable conditions for biodegradation that are present in these tests. Therefore, a substance that passes an inherent test should in principle be given a rate constant of zero.

However, if it can be shown that:

- The elimination in the test can really be ascribed to biodegradation, and;
- No recalcitrant metabolites are formed, and;
- The adaptation time in the test is limited;

then a rate constant of 0.1 h^{-1} in the STP-model can be used. These qualitative criteria are transformed into the following more specific criteria that the different inherent biodegradation tests must fulfil:

Zahn-Wellens test: Pass level must be reached within 7 days, log-phase should be no longer than 3 days, and percentage removal in the test before biodegradation occurs should be below 15%.

MITI-II test: Pass level must be reached within 14 days, log-phase should be no longer than 3 days.

No specific criteria have been developed for positive results in a SCAS test (OECD test guideline 302 A). A rate constant of 0 h^{-1} will be assigned to a substance, irrespective whether it passes this test or not.

2.3.6.5 Biodegradation in surface water, sediment and soil

The rate of biodegradation in surface water, soil and sediment is related to the structure and concentration of substances, microbial numbers, organic carbon content, and temperature. These properties vary spatially and an accurate estimate of the rate of biodegradation is very difficult even if laboratory or field data are available. Fate and exposure models normally assume the following simplifications:

- the kinetics of biodegradation are pseudo-first order;
- only the dissolved portion of the substance is available for biodegradation.

In some circumstance specific information on biodegradability in water, sediment or soil may not be available. However any deviations from the core and PT-specific information requirements (see *Guidance on the Biocidal Product Regulation: Volume IV Environment, Part A Information Requirements* available at http://echa.europa.eu/web/guest/guidance-documents/guidance-on-biocides-legislation) should be clearly justified. In these cases it may be justifiable that rate constants for these compartments have to be estimated from the results of standardised tests.

In deeper sediment layers anaerobic conditions normally prevail. A prediction of anaerobic biodegradation from aerobic biodegradability is not possible.

The assessment of biodegradation in surface waters, sediments and soil should, whenever possible, be based on results from tests simulating the conditions in the relevant environmental compartments.

Temperature influences the activity of microorganisms and thus the biodegradation rate in the environment. When biodegradation rates or half-lives have been determined in simulation tests, it should be considered to recalculate the degradation rates obtained to reflect an average EU outdoor temperature by **Equation 28**. When it is documented for a specific substance that a difference between the temperature employed in the test and the average outdoor temperature has no influence on the degradation half-life, no correction is needed.

Surface water

Use of simulation test results:
Preference of simulation tests (e.g. OECD Test guideline 309 or 308) also applies to estimation of degradation half-life in surface waters. An assessment of the applicability of such test results should always be conducted taking into account the prescribed standard conditions for surface waters applied in the risk assessment scenarios relative to the conditions employed in simulation tests.

Use of screening test results:
When results from biodegradation tests simulating the conditions in surface waters are not available, the use of results from various screening tests may be considered. **Table 5** gives a proposal for first order rate constants for surface water to be used in local and especially regional models, based on the results of screening tests for biodegradability. The proposal is based on general experience in relation to available data on biodegradation half-lives in surface waters of readily and not readily biodegradable substances.

The assigned degradation half-lives of an inherently biodegradable substance of 150 days in

surface water (**Table 5**) and 300 – 30,000 days in soil and sediment (**Table 6**) will not affect the local concentration but only the predicted regional concentration, provided that the residence time of the substance is much larger than the assigned half-life (i.e. only for substances present in soil compartment and sediment).

It is noted that the conditions in laboratory screening tests are very different from the conditions in various environmental compartments. The concentration of the test substance is several orders of magnitude greater in these screening tests than the concentrations of xenobiotic substances generally occurring in the environment and thus the kinetic regimes are significantly different. The temperature is also higher in screening tests than those generally occurring in the environment. Furthermore the microbial biomass is normally lower under environmental conditions than those occurring in these screening tests, especially in the tests for inherent biodegradability. These factors are taken into account in the proposed degradation rates and half-lives in **Tables 5** and **6**.

Table 5: First order rate constants and half-lives for biodegradation in surface water based on results of screening tests on biodegradability [a)]

Test result	Rate constant k (d-1)	Half-life (d)
Readily biodegradable	$4.7 \cdot 10^{-2}$	15
Readily, but failing 10-d window [b)]	$1.4 \cdot 10^{-2}$	50
Inherently biodegradable [c)]	$4.7 \cdot 10^{-3}$	150
Not biodegradable	0	∞

Notes on Table 5:

a) For use in exposure models these half-lives do not need to be corrected for different environmental temperatures.

b) The 10-day time window concept does not apply to the MITI test. The value obtained in a 14-d window is regarded as acceptable in the Closed Bottle method, if the number of bottles that would have been required to evaluate the 10-d window would cause the test to become too unwieldy.

c) Only those inherently degradable substances that fulfil the criteria described in note b) to Table 6 above. The half-life of 150 days reflects a present "best expert judgement".

The general experience is that a substance passing a test for ready biodegradability may under most environmental conditions be rapidly degraded and the estimated half-lives for such substances (cf. **Table 5**) should therefore be regarded as being in accordance with "the realistic worst-case concept". An OECD guidance document for classification of chemicals hazardous for the aquatic environment (OECD, 2001c) contains a chapter on interpretation of degradation data. Even though this guidance relates to hazard classification and not risk assessment, many of the considerations and interpretation principles may also apply in a risk assessment context. One difference is of course that in the risk assessment context not only a categorisation of the substance (i.e. a classification) is attempted, but instead an approximate half-life is estimated. Another difference is that for risk assessment, the availability of high quality test data is required in virtually all cases and further testing may therefore be required in the case of low quality data.

In distribution models, calculations are performed for compartments each consisting of homogeneous sub-compartments, i.e. surface water containing dissolved organic carbon and suspended matter, sediment containing porewater as well as a solid phase and soil containing air, porewater as well as a solid phase. Since it is assumed that no degradation takes place in the sorbed phase, the rate constant for the surface water, bulk sediment or soil in principle depends on the suspended matter/water, sediment/water or soil/water partition coefficient of the substance. With increasing hydrophobicity (sorption) of the

substance, the freely dissolved fraction present in the water phase available for degradation decreases, and therefore the overall rate constant should also decrease. However, for surface waters the influence of sorption is already comprised in the degradation rates when they are determined for bulk water in simulation tests employing the same conditions as in the aquatic environment. Neither is it needed to consider the influence of sorption processes when rate constants are established from screening test results due to the well-established practice to conclude on biodegradability in the environment from such data.

If no aquatic simulation or screening test data are available, a degradation rate for surface water may be established from a result of a simulation test for soil biodegradation. A substance may be considered readily biodegradable (but failing 10-d window) if it is ultimately degraded within 28 days in soil with a half-life <16 days (corresponding to >70% mineralization), no pre-exposure has taken place and a realistic concentration has been employed (cf. OECD, 2000b). In this case the respective default rate constant according to **Table 5** may be used. However, this has to be considered on a case-by-case basis.

Soil and sediment:

Use of simulation test results:

Also for assessment of biodegradation in soil or sediment, data from relevant simulation tests (e.g. OECD Test guideline 307 and 308) are preferred. Of course these tests do not directly simulate the conditions in non-disturbed soil or sediment. The measured half-life in water/sediment tests may be dependent on the relative volume of water and sediment employed in the test. However if up to three DT_{50}-values from different water-sediment or soil systems are available, the worst case value will be used whereas when more than three DT_{50}-values for the respective compartment are available then the geometric mean will be used.

When such simulation test data are available, the applicability of the results from the tests should be evaluated on a case-by-case basis employing expert judgement when used in a risk assessment. For field degradation/dissipation studies, where the compound might be lost not only because of actual degradation but also because of photolysis, volatilization, leaching or surface runoff, the significance of loss due to transport should be estimated based on known compound properties (e.g. Henry's law constant, solubility or the K_{ow}). If considerable losses to other compartments cannot be excluded, preference should be given to degradation data obtained under controlled laboratory conditions for the evaluation of the substance´s persistence. Another possible approach for soil is that in case of a biphasic decline only the slow phase of this decline should be taken into account for estimating the half-life since this reflects the degradation in the soil matrix rather than loss-processes at the soil surface. Information on how to address long term matrix $degT_{50}$ from field studies is further provided in the EFSA Journal 2014;12(5):3662 [67 pp.] (http://www.efsa.europa.eu/en/efsajournal/pub/3662).

Use of screening test results:

When no data from tests simulating the conditions in soil or sediment are available, the use of screening test data may be considered. The guidance for use of such data is based on the general recognition that for substances with low K_p values at present not enough empirical data is available to assume some sort of dependence of the soil biodegradation half-life on the solids/water partition coefficient. Nevertheless, for substances with high K_p values there is evidence that some sort of K_p dependence exists. Therefore, degradation half-life classes for (bulk) soil, partly based on K_p, are presented in **Table 6**. If a half-life from a surface-water simulation test is available it may, in a similar manner, form the basis for the establishment of a half-life in soil. The half-lifes indicated in the table are considered conservative.

Table 6: Half-lives (days) for (bulk) soil based on results from standardised biodegradation test results

Kp, soil * [l.kg-1]	Readily biodegradable	Readily biodegradable, failing 10-d window	Inherently biodegradable
≤ 100	30	90	300
>100, ≤ 1000	300	900	3,000
>1000, ≤ 10,000	3,000	9,000	30,000
etc.	etc.	etc.	etc.
* Measured Kp, soil values are preferred, but if not available and assuming an EU standard soil these values correspond to log Kow values of 4.4 (Kp, soil = 100), 5.7 (Kp, soil = 1000), and 6.9 (Kp, soil = 10,000) using the QSAR equations for Kp, soil as a function of Kow			

The following equation can be used to convert DT_{50} to a rate constant for biodegradation in soil:

$$kbio_{soil} = \frac{\ln 2}{DT50\,bio_{soil}}$$ **Equation 32**

Explanation of symbols

$DT_{50}bio_{soil}$	half-life for biodegradation in bulk soil	[d]	**Table 6**
$kbio_{soil}$	first order rate constant for degr. in bulk soil	[d^{-1}]	

The extrapolation of results from biodegradation tests to rate constants for sediment is problematic given the fact that sediment in general consists of a relatively thin oxic top layer and anoxic deeper layers. For the degradation in the anoxic layers a rate constant of zero (infinite half-life) can be assumed unless specific information on degradation under anaerobic conditions is available. For the oxic zone, similar rate constants as the ones for soil can be assumed. For the present regional model, a 3 cm thick sediment compartment is assumed with aerobic conditions in the top 3 mm. The sediment compartment is assumed to be well mixed with respect to the substance concentration. This implies that the total half-life for the sediment compartment will be a factor of ten higher than the half-life in soil. The degradation half-life for sediment is given by:

$$kbio_{sed} = \frac{\ln 2}{DT50\,bio_{soil}} \cdot Faer_{sed}$$ **Equation 33**

Explanation of symbols

$DT_{50,\,bio,\,soil}$	half-life for biodegradation in bulk soil	[d]	**Table 6**
$F_{aer,\,sed}$	fraction of the sediment compartment that is aerobic	[$m^3 \cdot m^{-3}$]	0.10
$k_{bio,\,sed}$	first order rate constant for degr. in bulk sediment	[d^{-1}]	

The remarks in the section on soil biodegradation regarding use of half-lives derived in surface water simulation tests may also apply for sediments.

2.3.6.6 Overall rate constant for degradation in surface water

In surface water, the substance may be transformed through photolysis, hydrolysis, and biodegradation. For calculation of the regional PEC, the rate constants for these processes can be summed into one, overall degradation rate constant. It should be noted that different types of degradation (primary and ultimate) are added. This is done for modelling purposes only. It should be noted that measurements on one degradation process might in fact already include the effects of other processes. For example, hydrolysis can occur under the conditions of a biodegradation test or a test of photodegradation, and so may already be comprised by the measured rate from these tests. In order to add the rates of different processes, it should be determined that the processes occur in parallel and that their effects are not already included in the rates for other processes. If exclusion of hydrolysis from the other degradation rates cannot be confirmed its rate constant should be set to zero. The equation below relates to primary degradation. If the primary degradation is not the rate-limiting step in the total degradation sequence and degradation products accumulate, then also the degradation product(s) formed in the particular process (e.g. hydrolysis) should be assessed. If this cannot be done or is not practical, the rate constant for the process should be set to zero.

$$kdeg_{water} = khydr_{water} + kphoto_{water} + kbio_{water}$$ **Equation 34**

Explanation of symbols

$khydr_{water}$	first order rate constant for hydrolysis in surface water	[d^{-1}]	**Equation 29**
$kphoto_{water}$	first order rate constant for photolysis in surface water	[d^{-1}]	**Equation 30**
$kbio_{water}$	first order rate constant for biodegradation in surface water	[d^{-1}]	**Table 5**
$kdeg_{water}$	total first order rate constant for degradation in surface water	[d^{-1}]	

2.3.6.7 Wastewater treatment

In this section, the following parameters are derived:

- emission from a sewage treatment plant to air;
- concentration in sewage sludge;
- concentration in effluent of a sewage treatment plant;
- PEC for microorganisms in a sewage treatment plant.

Elimination refers to the reduction in the concentration of substances in gaseous or aqueous discharges prior to their release to the environment. Elimination from the water phase may occur by physical as well as chemical or biochemical processes. In a sewage treatment plant (STP), one of the main physical processes is settling of suspended matter which will also remove adsorbed material. Physical processes do not degrade a substance but transfer it from one phase to another e.g. from liquid to solid. In the case of volatile substances, the aeration process will enhance their removal from the water phase by "stripping" them from the solid/liquid phases to the atmosphere. Substances may be removed from exhaust gaseous streams by scrubbing e.g. by adsorption on a suitable material or by passing through a trapping solution.

Wastewater treatment

One of the critical questions to answer in determining the PEC for the aquatic environment is whether or not the substance will pass through a wastewater treatment plant and if yes, through which kind of treatment plant before being discharged into the environment. The situation in the Member States concerning percentage connection to sewage works is quite

diverse (see **Appendix 4**). The percentage connection rate across the Community is subject to improvement due to the implementation of Council Directive 91/271/EEC of 21 May 1991 concerning the Urban Waste Water Treatment Directive (UWWTD, 91/271/EEC). This directive requires Member States (via transposition into national legislation) to ensure that wastewater from all agglomerations of > 2,000 population equivalents is collected and treated minimally by secondary treatment. A figure of 90% connection to wastewater treatment is proposed for the regional standard environment (see **Appendix 4**). Article 6 of the UWWTD allows Member States to declare non sensitive areas for which discharged wastewater from agglomerations between 10,000 and 150,000 population equivalents, which are located at the sea and from agglomerations between 2,000 and 10,000 population equivalents located at estuaries does not have to be treated biologically but only mechanically (primary treatment).

The situation with respect to wastewater treatment at industrial installations is less clear. It may be assumed that many of the larger industrial installations are either connected to a municipal wastewater treatment plant or have treatment facilities on site. In many cases, these treatment plants are not biological treatment plants but often physico-chemical treatment plants in which organic matter is flocculated by auxiliary agents e.g. by iron salts followed by a sedimentation process resulting in a reduction of organic matter measured as COD of about 25-50%.

In the present document, the above-described situation is taken into account as follows:

- on a local scale, it is assumed that wastewater will pass through a STP before being discharged into the environment. Nevertheless, for the largest PEClocal in surface water, it is necessary to determine an aquatic PEClocal assuming that no sewage treatment will take place. This value should be determined in addition to the normal PEC that assumes sewage treatment to flag for possible local problems (this PEC/PNEC ratio will not normally be used in risk characterisation). The alternative/additional PEC can be used to explore the possibility of environmental impact in regions or industrial sectors where percentage connection to sewage works is currently low, so as to give indications to local authorities for needs of possible local risk reductions. The PEC without considering a STP-treatment will not be used in the exposure assessment, unless the substance considered has a specific use category where direct discharge to water is widely practised;
- for a standard regional scale environment (definition see **section 2.3.7.1** of this guidance) it is assumed that 90% of the wastewater is treated in a biological STP and the remaining 10% released directly into surface waters (although mechanical treatment has some effect on eliminating organic matter, this is neglected because on the other hand stormwater overflows usually result in direct discharges to surface water even in the case of biological treatment. It is assumed that these two adverse effects compensate each other more or less with regard to the pollution of the environment).

The degree of removal in a wastewater treatment plant is determined by the physico-chemical and biological properties of the substance (biodegradation, adsorption onto sludge, sedimentation of insoluble material, volatilisation) and the operating conditions of the plant. As the type and amount of data available on degree of removal may vary, the following order of preference should be considered:

Measured data in full scale STP

The percentage removal should preferably be based upon measured influent and effluent concentrations. As with measured data from the environment, the measured data from STPs should be assessed with respect to their adequacy and representativeness.

Consideration must be given to the fact that the effectiveness of elimination in treatment plants is quite variable and depends on operational conditions, such as retention time in the aeration tank, aeration intensity, influent concentration, age and adaptation of sludge, extent of utilisation, rainwater retention capacity, etc. The data may be used provided that certain minimum criteria have been met, e.g. the measurements have been carried out over

a longer period of time. Furthermore, consideration should be given to the fact that removal may be due to stripping or adsorption (not degradation). In case no mass balance study has been performed, the percentage of transport to air or sludge should be estimated by using EUSES or Simple Treat.

Data from dedicated STPs should be used with caution. For example, when measured data are available for highly adapted STPs on sites producing high volume site-limited intermediates, these data should only be used for the assessment of this specific use category of the substance.

Simulation test data

Simulation testing is the examination of the potential of a substance to biodegrade in a laboratory system designated to represent either the activated sludge-based aerobic treatment stage of a sewage treatment plant or other environmental situations, for example a river (see *Guidance on the Biocidal Product Regulation: Volume IV Environment, Part A Information Requirements* available at http://echa.europa.eu/web/guest/guidance-documents/guidance-on-biocides-legislation).

There is insufficient information available on the applicability of elimination data from the laboratory test to the processes of a real sewage treatment plant. The results can be extrapolated to degradation in the real environment only if the concentrations that were used in the test are in the same order of magnitude as the concentrations that are to be expected in the real environment. If this is not the case, extrapolation can seriously overestimate the degradation rates especially when the extrapolation goes from high to low concentrations. If concentrations are in the same order of magnitude then the results of these tests can be used quantitatively to estimate the degree of removal of substances in a mechanical-biological STP.

If a complete mass balance is determined, the fraction removed by adsorption and stripping should be used for the calculation of sludge and air concentrations. In case no mass balance study has been performed, the percentage of transport to air or sludge should be estimated using EUSES or Simple Treat.

Info-box 3: EUSES

EUSES is a decision-support tool which enables the user to calculate the risk for the environment. The TGD (2003) as well as finalised emission scenario documents for biocides are included in EUSES 2.1.2. EUSES software and a manual can be downloaded free of charge from https://ec.europa.eu/jrc/en/scientific-tool/european-union-system-evaluation-substances and can be run on a normal PC. EUSES can be used for the environmental exposure estimation with the release estimation from **section 2.3.3.3** of this guidance. Beside the release estimation, only a few data on substance properties are needed to calculate PECs. If the use of default exposure estimates does not lead to a conclusion on the safe use, a refined assessment is possible, for example by including more specific information on releases and improved data on substance properties.

Output: The output of EUSES consists of the predicted environmental concentrations (PECs) for environmental risk assessment. EUSES can prepare an electronic report of all the input and output data in a Word or Excel format.

Modelling STP

If there are no measured data available, the degree of removal can be estimated by means of a sewage treatment plant model using log K_{ow} (K_{oc} or more specific partition coefficients can also be used; see **section 2.3.5** of this guidance), Henry's law constant and the results of biodegradation tests as input parameters. However, it should be remembered that the distribution behaviour of transformation products is not considered by this approach. It is proposed to use in the screening phase of exposure assessment a revised version of the sewage treatment plant model SimpleTreat (Struijs et al., 1991). This model is a multi-compartment box model, calculating steady-state concentrations in a sewage treatment

plant, consisting of a primary settler, an aeration tank and a liquid-solid separator. With SimpleTreat, the sewage treatment plant is modelled for an average size treatment plant based on aerobic degradation by active sludge, and consisting of 9 compartments (see **Figure 6**). Depending on the test results for ready and/or inherent biodegradability of a substance, specific first order biodegradation rate constants are assigned to the compound. An improved process formulation for volatilisation from the aeration tank, which is also applicable to semi-volatile substances (Mikkelsen, 1995), has been incorporated in the revised version.

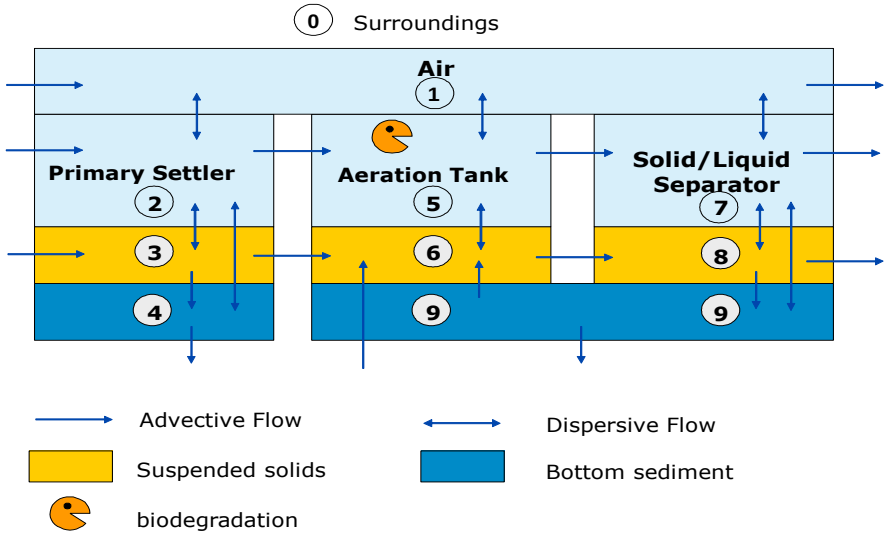

Figure 6: Schematic design of the sewage treatment plant model Simple Treat

For the purpose of modelling an STP, the rate constants presented in **Table 5** have been derived from the biodegradation screening tests.

Typical characteristics of the standard sewage treatment plant are given in **Table 7** on the next page. The amount of surplus sludge per person equivalent and the concentration of suspended matter in influent are taken from SimpleTreat (run at low loading rate).

At a higher tier in the risk assessment process more specific information on the biodegradation behaviour of a substance may be available. In order to take this information into account a modified version of the SimpleTreat model may be used. In this version the following scenarios are optional:

- temperature dependence of the biodegradation process;
- degradation kinetics according to the Monod equation;
- degradation of the substance in the adsorbed phase;
- variation in the sludge retention time;
- not considering a primary settler.

Table 7: Standard characteristics of a municipal sewage treatment plant

Parameter	Symbol	Unit	Value
Capacity of the local STP	$CAPACITY_{stp}$	[eq]	10,000
Amount of wastewater per inhabitant*	WASTEWinhab	$[l \cdot d^{-1} \cdot eq^{-1}]$	200
Surplus sludge per inhabitant	SURPLUSsludge	$[kg \cdot d^{-1} \cdot eq^{-1}]$	0.019
Concentration susp. matter in influent	$SUSPCONC_{inf}$	$[kg \cdot m^{-3}]$	0.45

* including rainwater

Calculation of the STP influent concentration

For local scale assessments, it is assumed that one point source is releasing its wastewater to one STP. The concentration in the influent of the STP, i.e. the untreated wastewater, can be calculated from the local emission to wastewater and the influent flow to the STP. The influent flow equals the effluent discharge.

$$Clocal_{inf} = \frac{Elocal_{water} \cdot 10^6}{EFFLUENT_{stp}}$$ **Equation 35**

Explanation of symbols

$Elocal_{water}$	local emission rate to (waste) water during episode	$[kg \cdot d^{-1}]$	**Equation 5**
$EFFLUENT_{stp}$	effluent discharge rate of STP	$[l \cdot d^{-1}]$	**Equation 35**
$Clocal_{inf}$	concentration in untreated wastewater	$[mg \cdot l^{-1}]$	

Calculation of the STP-effluent concentration

The concentration of the effluent of the STP is given by the fraction directed to effluent and the concentration in untreated wastewater as follows:

$$Clocal_{eff} = Clocal_{inf} \cdot Fstp_{water}$$ **Equation 36**

Explanation of symbols

$Clocal_{inf}$	concentration in untreated wastewater	$[mg \cdot l^{-1}]$	**Equation 35**
$Fstp_{water}$	fraction of emission directed to water by STP	[-]	Estimation by EUSES/Simple Treat
$Clocal_{eff}$	concentration of substance in the STP effluent	$[mg \cdot l^{-1}]$	

If no specific data are known, $EFFLUENT_{stp}$ should be based on an averaged wastewater flow of 200 l per capita per day for a population of 10,000 inhabitants (see **Table 7**):

$$EFFLUENT_{stp} = CAPACITY_{stp} \cdot WASTEWinhab$$ **Equation 37**

Explanation of symbols

$CAPACITY_{stp}$	capacity of the STP	[eq]	10000 (see **Table 7**)
WASTEWinhab	sewage flow per inhabitant	$[l \cdot d^{-1} \cdot eq^{-1}]$	200 (see **Table 7**)
$EFFLUENT_{stp}$	effluent discharge rate of STP	$[l \cdot d^{-1}]$	2×10^6

For calculating the PEC in surface water without sewage treatment, the fraction of the emission to wastewater, directed to effluent ($F_{stp, water}$) should be set to 1. The fractions to air and sludge ($F_{stp, air}$ and $F_{stp, sludge\ resp.}$) should be set to zero.

Info-box 4: Recommended method to calculate the concentration in the STP effluent

The EUSES/Simple Treat method should be used for calculating the fate and behaviour of a substance in the STP instead of the formerly used tables in Appendix II of TGD (2003).

Calculation of the emission to air from the STP

The indirect emission from the STP to air is given by the fraction of the emission to wastewater, which is directed to air:

$$Estp_{air} = Fstp_{air} \cdot Elocal_{water}$$ **Equation 38**

Explanation of symbols

$F_{stp, air}$	fraction of the emission to air from STP	[-]	Estimation by EUSES/Simple treat
$Elocal_{water}$	local emission rate to (waste) water during emission episode	$[kg \cdot d^{-1}]$	**Equation 5** or the outcome of biocide ESDs with emission to STP
$Estp_{air}$	local emission to air from STP during emission episode	$[kg \cdot d^{-1}]$	

Calculation of the STP sludge concentration

The concentration in dry sewage sludge is calculated from the emission rate to water, the fraction of the emission sorbed to sludge and the rate of sewage sludge production:

$$C_{sludge} = \frac{Fstp_{sludge} \cdot Elocal_{water} \cdot 10^6}{SLUDGERATE}$$ **Equation 39**

Explanation of symbols

$Elocal_{water}$	local emission rate to water during episode	$[kg \cdot d^{-1}]$	**Equation 5**
$Fstp_{sludge}$	fraction of emission directed to sludge by STP	[-]	Estimation by EUSES/Simple treat
SLUDGERATE	rate of sewage sludge production	$[kg \cdot d^{-1}]$	**Equation 38**
C_{sludge}	concentration in dry sewage sludge	$[mg \cdot kg^{-1}]$	

The rate of sewage sludge production can be estimated from the outflows of primary and secondary sludge as follows:

$$SLUDGERATE = \frac{2}{3} \cdot SUSPCONC_{inf} \cdot EFFLUENT_{stp} + SURPLUSsludge \cdot CAPACITY_{stp}$$ **Equation 40**

Explanation of symbols

$SUSPCONC_{inf}$	concentration of suspended matter in STP influent	[kg · m^{-3}]	**Table 7**
$EFFLUENT_{stp}$	effluent discharge rate of STP	[m^3 · d^{-1}]	**Equation 37**
SURPLUSsludge	surplus sludge per inhabitant equivalent	[kg · d^{-1} · eq^{-1}]	**Table 7**
$CAPACITY_{stp}$	capacity of the STP	[eq]	**Table 7**
SLUDGERATE	rate of sewage sludge production	[kg·d^{-1}]	

Anaerobic degradation may lead to a reduction of the substance concentration in sewage sludge during digestion. This is not yet taken into account.

Calculation of the STP concentration for evaluation of inhibition to microorganisms

As explained above in the section on STP modeling, the removal of a chemical in the STP is computed from a simple mass balance. For the aeration tank this implies that the inflow of sewage (raw or settled, depending on the equipment with a primary sedimentation tank) is balanced by the following removal processes: degradation, volatilization and outflow of activated sludge into the secondary settler. Activated sludge flowing out of the aeration tank contains the chemical at a concentration similar to the aeration tank, which is the consequence of complete mixing. It consists of two phases: water, which is virtually equal to effluent flowing out of the solids-liquid separator (this is called the effluent of the STP), and suspended particles, which largely settle to be recycled into the aeration tank. Assuming steady state and complete mixing in all tanks (also the aeration tank), the effluent concentration approximates the really dissolved concentration in activated sludge. It is assumed that only the dissolved concentration is bioavailable, i.e. the actual concentration to which the microorganisms in activated sludge are exposed. For the risk characterisation of a substance upon microorganisms in the STP, it can therefore be assumed that homogeneous mixing in the aeration tank occurs which implies that the dissolved concentration of a substance is equal to the effluent concentration:

$$PEC_{stp} = Clocal_{eff}$$ **Equation 41**

Explanation of symbols

$Clocal_{eff}$	total concentration of substance in STP effluent	[mg · l^{-1}]	**Equation 36**
PEC_{stp}	PEC for microorganisms in the STP	[mg · l^{-1}]	

In the case of intermittent release the situation is much more complex. During an interval shorter than several sludge retention times (SRT), presumably a small portion of the competent microorganisms will remain in the system. If the interval between two releases is shorter than one month (three times an average SRT), adaptation of the activated sludge is maintained resulting in rapid biodegradation when a next discharge enters the STP. In line with **section 2.3.3.4** of this guidance such a situation is not considered as an intermittent release and the PEC_{stp} can still be considered equal to $Clocal_{eff}$. After longer intervals the specific bacteria that are capable to biodegrade the compound, may be completely lost.

If the activated sludge is de-adaptated, the concentration in the aeration tank may increase during the discharge period. In that case the concentration in influent of the STP is more representative for the PEC for microorganisms:

$$PEC_{stp} = Clocal_{inf}$$ **Equation 42**

Explanation of symbols

$Clocal_{inf}$	total concentration of substance in STP influent	$[mg \cdot l^{-1}]$	**Equation 35**
PEC_{stp}	PEC for microorganisms in the STP	$[mg \cdot l^{-1}]$	

However, it needs to be noted that when the discharge period is shorter than the hydraulic retention time of the aeration tank (7-8 h), the maximum concentration in the effluent will be lower than the initial concentration at the discharge, due to peak dispersion, dilution and sorption in the sewer system, the primary settler and the activated sludge process. It is estimated that this maximum concentration will be at least a factor of three lower than the initial concentration. Whether or not this correction factor must be applied needs to be decided on a case-by-case basis. For such short emission periods care must be taken that the emission rates are in fact calculated over the actual emission period (as $kg \cdot h^{-1}$) and not averaged out over one day.

The choice of using the effluent concentration is also reflected in the choice of the assessment factors used for deriving a PNEC for the STP microorganisms. In modern sewage treatment plants with a denitrification stage, an additional tank is normally placed at the inlet of the biological stage. As the main biological degradation processes are taking place in the second stage, the microbial population in the denitrification tank is clearly exposed to higher concentrations of the substance as compared to the effluent concentration. As the technical standard of the STPs improves, this will have to be addressed in this assessment scheme in the near future.

2.3.7 Calculation of PEC

2.3.7.1 Introduction

In the following sections, guidance is given for the calculation of the local PEC for all relevant environmental compartments. In **section 2.3.7.7** of this guidance, the calculation of regional steady-state concentrations (PECregional) in relevant compartment is presented.

Other pathways than those described in this guidance, like deposition from air to surface waters, could be of relevance. No guidance for those pathways is currently available. Guidance on exposure assessment of the marine environment is presented in **section 2.6** of this guidance.

The following **Figure 7** shows the relationship between the local emission routes and the subsequent distribution processes in case of release via an STP. For each compartment, specific fate and distribution models are applied.

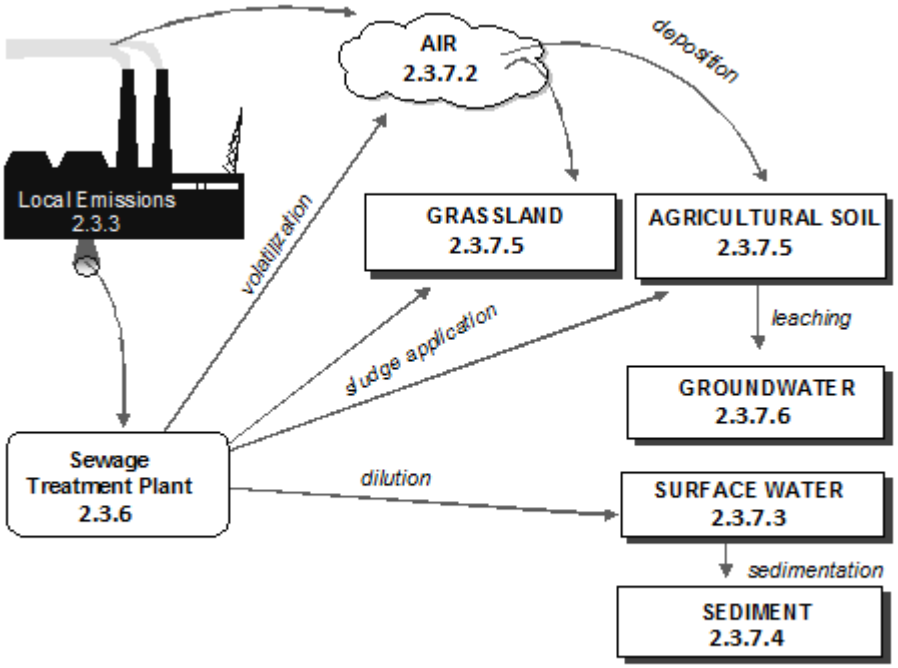

Figure 7: Local relevant emission and distribution routes

Calcuclation on the next pages presents an overview of the PEC values that need to be estimated.

Table 8: Overview of different exposure scenarios and the respective PECs

Target	Medium of exposure	Exposure scenario			
		Regional	section	Local	section
Aquatic compartment	surface water	steady-state concentration in surface water	2.3.7.7	concentration during emission period taking into account dilution, sorption, and, if relevant, sedimentation, volatilisation and degradation	**2.3.7.3**
	sediment	steady-state concentration in sediment		equilibrium concentration in freshly deposited sediment based on the properties of suspended matter, related to the local surface water concentration	**2.3.7.4**

Terrestrial compartment	(agricultural) soil	steady-state concentration in agricultural soil		Initial concentration in non-agricultural soil / concentration in agricultural soil, fertilised with manure or STP sludge over 10 years and receiving input through continuous aerial deposition, are either initial or averaged over 30 days	**2.3.7.5**
	groundwater	steady-state concentration in groundwater under agricultural soil		concentration in groundwater under agricultural soil.	**2.3.7.6**
Air compartment	air	steady-state concentration in air		concentration in air, at 100 m from point source or STP	**2.3.7.2**
Microorganisms	STP aeration tank	-	-	concentration during emission period	**0**

2.3.7.2 Calculation of the local PEC for the atmosphere

In this section, the following parameters are derived:

- local concentration in air during emission episode;
- annual average local concentration in air;
- total deposition flux (annual average).

The air compartment receives its input from direct emission to air, and volatilisation from the sewage treatment plant. The most important fate processes in air, are schematically drawn in **Figure 8**.

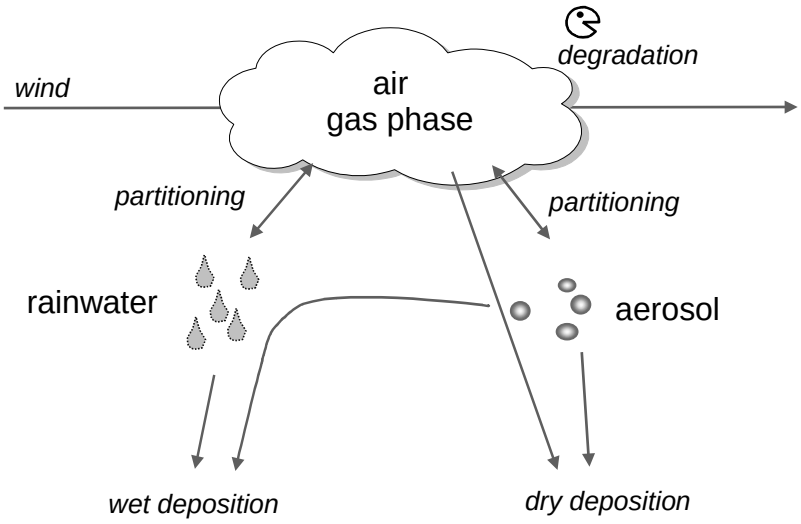

Figure 8: Fate processes in the air compartment

PEClocal for air cannot be compared with the PNEC for air because the latter is usually not available. The PEClocal for air is used as input for the calcu-lation of the intake of substances through inhalation in the indirect exposure of humans. Deposition fluxes are used as input for the calculation of PEClocal in soil. Therefore, both deposition flux and concentration are calculated as annual average values.

Many air models are available that are highly flexible and can be adjusted to take specific information on scale, emission sources, weather conditions etc. into account. For active substances or substances of concern, this type of information is normally not available. Hence a standardised exposure assessment is carried out making a number of explicit assumptions and using a number of fixed default parameters.

The gaussian plume model OPS, as described by Van Jaarsveld (1990) is proposed using the standard parameters as described by Toet and de Leeuw (1992). These authors used the OPS model and carried out a number of default calculations in order to describe a relationship between the basic characteristics of substances (vapour pressure and Henry's law constant) and the concentration in air and deposition flux to soil near to a point source.

The following assumptions/model settings are made:

- realistic average atmospheric conditions are used, obtained from a 10-year data set of weather conditions for The Netherlands;
- transport of vaporised and aerosol-bound substances is calculated separately. The partitioning between gas and aerosol is determined by means of the equation of Junge (see **Equation 21**);
- the atmospheric reaction rate is estimated by using AOPWIN (US EPA, 2012). Please refer also to **section 2.3.6.3** of this guidance when calculating the atmospheric reaction rate.
- losses due to deposition are neglected for estimation of the concentration and deposition fluxes at this short distance from the source;
- assumed source characteristics are:

- source height: 10 meters, representing the height of buildings in which production, processing or use take place;
- heat content of emitted gases: 0; this assumes there is no extra plume rise caused by excess heat of vapours compared to the outdoor temperature;
- source area: 0 meter; representing an ideal point source which is obviously not always correct but which is an acceptable choice;

- calculated concentrations are long-term averages.

The concentration in air at a distance of 100 meters from the point source is estimated. This distance is chosen to represent the average distance between the emission source and the border of the industrial site. The deposition flux of gaseous and aerosol-bound substances is estimated analogous to the estimation of atmospheric concentrations by means of an estimation scheme and with help of the OPS model. The deposition flux to soil is averaged over a circular area around the source, with a radius of 1000 m to represent the local agricultural area. Deposition velocities are used for three different categories:

- dry deposition of gas/vapour: estimated at 0.01 cm/s;
- wet deposition of gas/vapour: determined with the OPS model;
- dry and wet deposition of aerosol particles; determined within the OPS model using an average particle size distribution.

Based on the assumptions and model settings as listed above, calculations with the original OPS-model were performed for both gaseous and aerosol substances (Toet and de Leeuw, 1992). These calculations were only carried out for a source strength of 1 g/s, as it was proven that concentrations and deposition fluxes are proportional to the source strength. From these calculations it was concluded that local atmospheric concentrations are largely independent of the physical-chemical properties of the compounds. Hence, once the emission from a point source is known, the concentration at 100 meter from the source can be estimated from a simple linear relationship.

In the calculation of PEClocal for air both, emission from a point source as well as the emission from a STP is taken into account. The concentration on the regional scale (PECregional) is used as background concentration if the exposure assessment is performed using the tonnage based approach and therefore, summed to the local concentration.

The STP is assumed as a point source and the concentration of the chemical is calculated at a 100 m distance from it. The maximum from the two concentrations (direct and via STP) is used as the PEClocal:

$$Clocal_{air} = \max\left(Elocal_{air} , Estp_{air} \right) \cdot Cstd_{air}$$ **Equation 43**

$$Clocal_{air,ann} = Clocal_{air} \cdot \frac{Temission}{365}$$ **Equation 44**

Explanation of symbols

$Elocal_{air}$	local direct emission rate to air during episode	[kg · d^{-1}]	**Equation 5**
$Estp_{air}$	local indirect emission to air from STP during episode	[kg · d^{-1}]	**Equation 38**
$Cstd_{air}$	concentration in air at source strength of 1 kg·d^{-1}	[mg · m^{-3}]	$2.78.10^{-4}$

$T_{emission}$	number of days per year that the emission takes place	[d · year^{-1}]	**Appendix 6**
$Clocal_{air}$	local concentration in air during emission episode	[mg · m^{-3}]	
$Clocal_{air,ann}$	annual average concentration in air, 100 m from point source	[mg · m^{-3}]	

$$PEClocal_{air,ann} = Clocal_{air,ann} + PECregional_{air}$$ **Equation 45**

Explanation of symbols

$Clocal_{air,ann}$	annual average local concentration in air	[mg · m^{-3}]	**Equation 44**
$PECregional_{air}$	regional concentration in air	[mg · m^{-3}]	**2.3.7.7**
$PEClocal_{air,ann}$	annual average predicted environmental conc. in air	[mg · m^{-3}]	

The calculation of deposition flux is slightly more complex because of the dependence of the deposition flux on the fraction of the substance that is associated with the aerosols. In calculating the deposition flux, the emissions from the two sources (direct and STP) are summed:

$$DEPtotal = \left(Elocal_{air} + Estp_{air} \right) \cdot \left(Fass_{aer} \cdot DEPstd_{aer} + (1 - Fass_{aer}) \cdot DEPstd_{gas} \right)$$ **Equation 46**

$$DEPtotal_{ann} = DEPtotal \cdot \frac{Temission}{365}$$ **Equation 47**

Explanation of symbols

$Elocal_{air}$	local direct emission rate to air during emission episode	[kg · d^{-1}]	**Equation 5**
$Estp_{air}$	local indirect emission to air from STP during episode	[kg · d^{-1}]	**Equation 38**
$F_{ass, aer}$	fraction of the substance bound to aerosol	[-]	**Equation 21**
$DEP_{std, aer}$	standard deposition flux of aerosol-bound compounds at a source strength of 1 kg·d^{-1}	[mg · m^{-2} · d^{-1}]	1·10^{-2}
$DEP_{std, gas}$	deposition flux of gaseous compounds as a function of Henry's law constant, at a source strength of 1 kg·d^{-1}	[mg · m^{-2} · d^{-1}]	
	^{10}logH ≤ -2:		5·10^{-4}
	-2 < ^{10}logk_H ≤ 2:		4·10^{-4}
	^{10}logH > 2:		3·10^{-4}
$T_{emission}$	number of days per year that the emission takes place	[d · yr^{-1}]	**Appendix 6**
DEP_{total}	total deposition flux during emission episode	[mg · m^{-2} · d^{-1}]	
$DEP_{total, ann}$	annual average total deposition flux	[mg·m^{-2} · d^{-1}]	

2.3.7.3 Calculation of PEClocal for the aquatic compartment

2.3.7.3.1 Indirect release

The effluent of the sewage treatment plant is diluted into the surface water.

Figure 9 on the next page shows the most important fate processes of the aquatic compartment.

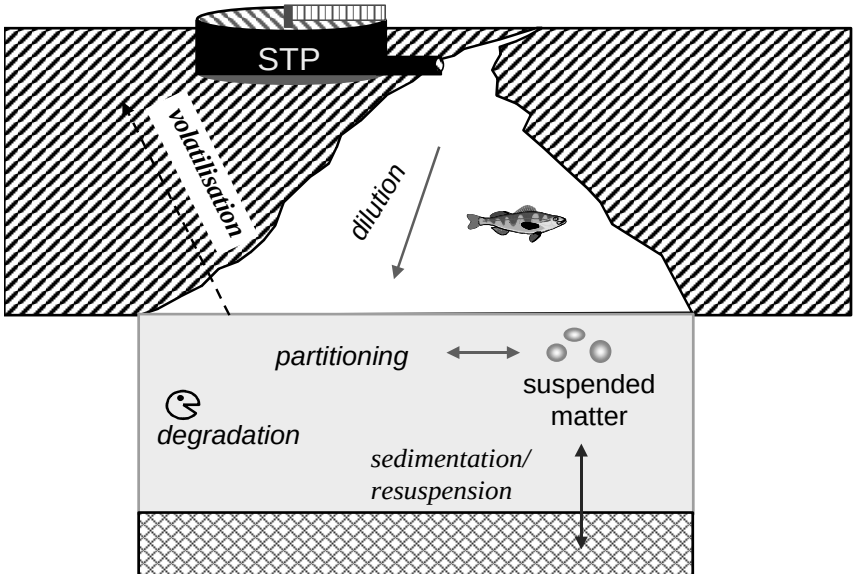

Figure 9: Fate processes in surface water

For the calculations, the following assumptions are made:

- complete mixing of the effluent in surface water is assumed as a representative exposure situation for the aquatic eco-system;
- for the first approach in the local assessments, volatilisation, degradation, and sedimentation are ignored because of the short distance between the point of effluent discharge and the exposure location.

The calculation of the PEClocal for the aquatic compartment involves several sequential steps (see also **Figure 9**). It includes the calculation of the discharge concentration of a STP to a water body, dilution effects and removal from the aqueous medium by adsorption to suspended matter.

Dilution in the receiving surface water and adsorption to suspended matter

The distance from the point of discharge where complete mixing may be assumed will vary between different locations. A fixed dilution factor may be applied. Dilution factors are dependent on flow rates and the industry-specific discharge flow. Due to the different seasonal, climatic and geographical conditions in the Member States, those dilution factors may vary over wide ranges. They have been reported in a range from 1 (e.g. dry riverbeds in summer) up to 100,000 (de Greef and de Nijs, 1990). The dilution factor depends on the dimensions of the STP and the receiving surface water and on the flow rate of effluent discharge of the STP in relation to the flow rate of the receiving surface water. The dilution factor is generally linked to the release scenario of the use category. For example, for consumer products an average dilution factor for sewage from municipal treatment plants of 10 is recommended. This is also regarded as a default dilution value for other types of substances if no specific data are available.

When a substance is released to surface water predominately as particles (e.g. as

precipitates or incorporated in small material pieces, like e.g. preservatives in polymerised materials or antifouling active substances in paint fragments lost during maintenance activities – see **section 2.3.3.5** of this guidance) this may lead to overestimation of $PEC_{surface\ water}$ and underestimation of $PEC_{sediment}$. If this is expected to occur it should be considered in the further evaluation (e.g. when comparing PEC with monitoring data and in the risk characterisation).

In certain circumstances, it may be possible to identify specific emission points which would allow the use of more precise information regarding the available distribution and fate processes. Such site-specific assessments should only be used when it is known that all the emissions emanating from the particular point in the life-cycle e.g. manufacture, arise from a limited number of specific and identifiable sites. In these circumstances each specific point of release will need to be assessed individually. If it is not possible to make this judgement, then the default assumptions should be applied. In site-specific assessments, due account can be taken of the true dilution available to the given emission as well as the impact of degradation, volatilisation, etc. in the derivation of the PEC. Normally, only dilution and adsorption to suspended sediment need to be considered but site-specific conditions may indicate that local distribution models can be used.

It must be noted that with the assumption of complete mixing of the effluent in the surface water no account is taken of the fact that in reality in the mixing zone higher concentrations will occur. For situations with relatively low dilution factors this mixing-zone effect can be accepted. For situations with very high dilution factors, however, the mixing zones may be very long and the overall area that is impacted by the effluent before it is completely mixed can be very substantial. Therefore, in case of site-specific assessments the dilution factor that is applied for calculation of the local concentration in surface water should not be greater than 1000.

If no measured data are available on the partition coefficient between suspended matter and water, $K_{p,\ susp}$, it can be estimated directly from the K_p or calculated from the K_{oc} of the substance, determined for other sorbents like soil or sediments (**section 2.3.5** of this guidance) by taking into account different organic carbon contents of the media.

For some substances it may be possible that PECs are calculated in water which exceed the water solubility of the substance. These results need to be interpreted carefully on a case-by-case basis. The concentration in surface water will not be corrected, but the result needs to be flagged. The PEC has to be interpreted based on the effects found in the aquatic toxicity tests.

In a situation where a substance is released through several point sources into the same river, the resulting cumulative concentration may in a first approach be estimated by assuming it to be released from one point source. If this PEC leads to "concern" then refined approaches may be used, such as river flow models, e.g. OECD (1992a) which addresses the specific emission pattern as well as river parameters. The local concentration in surface water is calculated as follows:

$$Clocal_{water} = \frac{Clocal_{eff}}{(1 + Kp_{susp} \cdot SUSP_{water} \cdot 10^{-6}) \cdot DILUTION}$$

Equation 48

Explanation of symbols

$C_{local,\ eff}$	concentration of the substance in the STP effluent	[mg · l^{-1}]	
$K_{p,susp}$	solids-water partition coefficient of suspended matter	[l · kg^{-1}]	**Equation 26**
$SUSP_{water}$	concentration of suspended matter in the river	[mg · l^{-1}]	15
DILUTION	dilution factor	[-]	10
$C_{local,\ water}$	local concentration in surface water during emission episode	[mg · l^{-1}]	

When considering dilution factors, account should be taken of the fluctuating flow-rates of typical receiving waters. The low-flow rate (or 10th percentile) should always be used. Where only average flows are available, the flow for dilution purposes should be estimated as one third of this average. When a site-specific assessment is appropriate, the actual dilution factor after complete mixing can be calculated from the flow rate of the river and the effluent discharge rate (this approach should only be used for rivers, not for estuaries or lakes):

$$DILUTION = \frac{EFFLUENT_{stp} + FLOW}{EFFLUENT_{stp}}$$ **Equation 49**

Explanation of symbols

$EFFLUENT_{stp}$	effluent discharge rate of stp	$[l \cdot d^{-1}]$	**Equation 37**
FLOW	flow rate of the river	$[l \cdot d^{-1}]$	data set
DILUTION	dilution factor at the point of complete mixing	[-]	(max. = 1000)

For indirect human exposure and secondary poisoning, an annual average concentration in surface water is calculated:

$$Clocal_{water,ann} = Clocal_{water} \cdot \frac{Temission}{365}$$ **Equation 50**

Explanation of symbols

$C_{local,\ water}$	local concentration in surface water during emission episode	$[mg \cdot l^{-1}]$	**Equation 48**
$T_{emission}$	number of days per year that the emission takes place	$[d \cdot yr^{-1}]$	**Appendix 6**
$C_{local,\ water,ann}$	annual average local concentration in surface water	$[mg \cdot l^{-1}]$	

The concentration at the regional scale ($PECregional_{,\ water}$) is used as background concentration for the local scale if the exposure assessment is performed using the tonnage based approach. Therefore, these concentrations are summed:

$$PEClocal_{water} = Clocal_{water} + PECregional_{water}$$ **Equation 51**

$$PEClocal_{water,ann} = Clocal_{water,ann} + PECregional_{water}$$ **Equation 52**

Explanation of symbols

$Clocal_{water}$	local concentration in surface water during episode	$[mg \cdot l^{-1}]$	**Equation 48**
$Clocal_{water,ann}$	annual average concentration in surface water	$[mg \cdot l^{-1}]$	**Equation 50**
$PECregional_{water}$	regional concentration in surface water	$[mg \cdot l^{-1}]$	**2.3.7.7**
$PEClocal_{water}$	predicted environmental concentration during episode	$[mg \cdot l^{-1}]$	
$PEClocal_{water,ann}$	annual average predicted environmental concentration	$[mg \cdot l^{-1}]$	

2.3.7.3.2 Direct release

In the following product-types, passing an STP is not an option but direct emission to surface water (fresh water or seawater) occurs:

PT 2: Swimming pools

PT 4: Seawater desalination

PT 6: Preservatives for product during storage

PT 7: Film preservatives

PT 8: Wood preservatives (use classes 3: bridge over pond, 4b: jetty in a lake/sheet piling in a waterway and 5: harbour wharf)

PT 9: Specifically fiber, rubber and polymerised materials preservatives

PT 11: Preservatives for liquid cooling and processing systems (e.g. "once through" cooling systems)

PT 12: Paper and wood pulp/Oil extraction

PT 17 Piscicides

PT 18: Control of mosquito larvae

PT 19: Repellents and attractants

PT 21: Antifouling products

For these cases specific guidance on how to perform the exposure assessment for surface water is provided in the respective ESD (see http://echa.europa.eu/guidance-documents/guidance-on-biocides-legislation/emission-scenario-documents). Please note that PT 6, PT 7, PT 9 and PT 10 are covered with regard to exposure assessment of surface water by the ESD for PT 8.

2.3.7.4 Calculation of PEClocal for sediment

In this section, the following parameter is derived:

- local concentration in sediment during the emission episode.

PEClocal for sediment can be compared to the PNEC for sediment dwelling organisms. The concentration in freshly deposited sediment is taken as the PEC for sediment; therefore, the properties of suspended matter are used. The concentration in bulk sediment can be derived from the corresponding water body concentration, assuming a thermodynamic partitioning equilibrium (see also Di Toro et al., 1991):

$$PEClocal_{sed} = \frac{K_{susp\text{-}water}}{RHO_{susp}} \cdot PEClocal_{water} \cdot 1000 \qquad \textbf{Equation 53}$$

Explanation of symbols

$PEClocal_{water}$	concentration in surface water during emission episode	$[mg \cdot l^{-1}]$	**Equation 52**
$K_{susp\text{-}water}$	suspended matter-water partition coefficient	$[m^3 \cdot m^{-3}]$	**Equation 27**
RHO_{susp}	bulk density of suspended matter	$[kg \cdot m^{-3}]$	**Equation 20**
$PEClocal_{sed}$	predicted environmental concentration in sediment	$[mg \cdot kg^{-1}]$	

Highly adsorptive substances may not be considered adequately with the approach described above, as they are often not in equilibrium distribution between water and

suspended matter because of their cohesion to the suspended matter; however they may be desorbed after ingestion by benthic or soil organisms. However as a first step the adsorption to suspended matter should be considered when calculating the PEC value for sediment based on the $PEClocal_{water}$ also for strong adsorbing substances and metals.

In the case when release to the surface water predominately occurs as particles (see **section 2.3.7.3** of this guidance) this calculation may underestimate the sediment concentration. If this is expected to occur it should be considered in the further evaluation (e.g. when comparing PEC with monitoring data and in the risk characterisation).

2.3.7.5 Calculation of PEClocal for the soil compartment

The concentration in soil ($PEClocal_{soil}$) is calculated either following **indirect release**, when another environmental compartment is exposed before, as

- concentration in soil, fertilised with sludge from an STP or liquid manure from stable applications and
- concentration in soil receiving continuous aerial deposition from a nearby point source (e.g. application sites like cooling towers and STP aeration tank),

or following **direct release** (e.g. leaching from a painted house wall, some outdoor insect treatments), when soil is the first receiving environmental compartment.

The processes by which the substance is removed from the soil compartment also need to be considered (degradation, volatilisation and leaching). **Figure 10** below shows the most important fate processes in the soil compartment.

For sewage sludge application, two different soil types are distinguished: agricultural land and grassland. They differ in the amount of sludge applied and the mixing depth.

The concentration in groundwater is calculated below this agricultural area.

The PEC in agricultural soil is used for the risk characterisation of terrestrial ecosystems (**section 4** of this guidance) and as a starting point for the calculation of indirect human exposure via crops and cattle products (see *Guidance on the Biocidal Products Regulation Volume III Human health - Part B Risk Assessment*, http://echa.europa.eu/web/guest/guidance-documents/guidance-on-biocides-legislation).

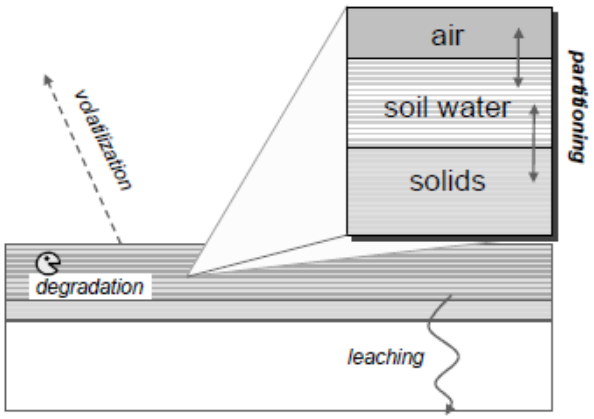

Figure 10: Fate processes in the soil compartment

2.3.7.5.1 Indirect release

In this section, the following endpoints and underlaying parameters are derived:

- local concentration in agricultural soil (averaged over a certain time period);
- local concentration in grassland (averaged over a certain time period);
- percentage of steady-state situation (to indicate persistency).

Guidance for calculating PEClocal in soil is given for the following exposure routes:

- application of sewage sludge in agriculture;
- dry and wet deposition from the atmosphere.

For **sludge application** to agricultural soil, an application rate of 5,000 kg/ha dry weight per year is assumed. For grassland a rate of 1000 kg/ha/yr should be used. Sludge application is treated as a single event once a year. Furthermore, it is impossible to indicate when the emission episode takes place within a year. In the beginning of the growing season any impact on exposure levels will be large. After the growing season, the impact may well be insignificant. Therefore, averaging represents an appropriate scenario choice.

Atmospheric deposition is assumed to be a continuous flux throughout the year. It should be noted that the deposition flux is averaged over a year. This is obviously not fully realistic, since the deposition flux is linked to the emission episode. Averaging is done to facilitate calculation of a steady-state level. The contribution to the overall impact from wet and dry deposition is based on the emission calculation of a point source (**section 2.3.7.2** of this Guidance) and is related to a surrounding area within 1000 m from that source. The deposition is averaged over the whole area. For the exposure assessment of soil, a simplified model is used. The top layer of the soil compartment is described as one compartment, with an average influx through aerial deposition and sludge application, and a removal from the box by degradation, volatilisation, leaching, and other processes if relevant. The concentration in this soil box can now be described with a simple differential equation.

Derivation of the removal rate constants:

The total rate constant for removal is made up of several parts:

- biodegradation rate constant (please refer to **section 2.3.6.5** of this guidance);
- volatilisation of substance from soil;
- leaching to deeper soil layers.

The rate constant for diffusive transfer from soil to air is estimated as the reciprocal of the sum of mass transfer resistances at the air and soil sides of the soil/air interface. Given a substance-independent air-side partial mass transfer coefficient, $kasl_{air}$, and the soil-referenced overall mass transfer coefficient, $kasl_{soil}$, the rate constant for volatilisation, $k_{volat\ i}$, becomes:

$$\frac{1}{k_{volati}} = \left(\frac{1}{kasl_{air} \cdot K_{air\text{-}water} / K_{soil-water}} + \frac{1}{kasl_{soil}} \right) \cdot DEPTH_i \qquad \textbf{Equation 54}$$

Explanation of symbols

$kasl_{air}$	partial mass transfer coefficient (PMTC) at the air-side of the air-soil interface	[m · s^{-1}]	1.05·10^{-3}
$kasl_{soil}$	partial mass transfer coeff. at soil-side of the air-soil interface	[m · d^{-1}]	**Equation 72**
$K_{air\text{-}water}$	air-water partition coefficient	[m^3 · m^{-3}]	**Equation 24**
$K_{soil\text{-}water}$	soil-water partition coefficient	[m^3 · m^{-3}]	**Equation 27**
$DEPTH_i$	mixing depth of soil type *i*	[m]	**Table 10**
$k_{volat\ i}$	rate constant for volatilisation from soil *i*	[d^{-1}]	

A pseudo first-order rate constant for leaching can be calculated from the amount of rain flushing the liquid-phase of the soil compartment:

$$k_{leach} = \frac{Finf_{soil} \cdot RAINrate}{K_{soil\text{-}water} \cdot DEPTH_{soil}}$$ **Equation 55**

Explanation of symbols

$F_{inf, soil}$	fraction of rain water that infiltrates into soil	[-]	0.25
RAINrate	rate of wet precipitation (700 mm/year)	[m · d^{-1}]	1.92·10^{-3}
$K_{soil\text{-}water}$	soil-water partition coefficient	[m^3 · m^{-3}]	**Equation 27**
$DEPTH_{soil}$	mixing depth of soil	[m]	**Table 10**
k_{leach}	pseudo first-order rate constant for leaching from soil layer	[d^{-1}]	

Other removal processes may be important in some cases (e.g. uptake by plants). If rate constants are known for these processes, they may be added to the total removal. The overall removal rate constant is given by:

$$k = k_{volat} + k_{leach} + kbio_{soil}$$ **Equation 56**

Explanation of symbols

k_{volat}	pseudo-first order rate constant for volatilisation from soil	[d^{-1}]	**Equation 52**
k_{leach}	pseudo-first order rate constant for leaching from top soil	[d^{-1}]	**Equation 53**
$kbio_{soil}$	pseudo-first order rate constant for biodegradation in soil	[d^{-1}]	**Table 6**
k	first order rate constant for removal from top soil	[d^{-1}]	

General description of modelling degradation in soil

Initial concentration:

The initial concentration, $C_{soil}(0)$, is governed by the input of the substance through sludge application.

$$\frac{dC_{soil}}{dt} = - k \cdot C_{soil} + D_{air}$$ **Equation 57**

Explanation of symbols

D_{air}	aerial deposition flux per kg of soil	[mg · kg^{-1} · d^{-1}]	**Equation 56**
t	time	[d]	
k	first order rate constant for removal from top soil	[d^{-1}]	**Equation 54**
C_{soil}	concentration in soil	[mg · kg^{-1}]	

In the formula above, the aerial deposition flux is used in mg substance per kg of soil per day. D_{air} can be derived by converting the total deposition flux ($DEPtotal_{ann}$) as follows:

$$D_{air} = \frac{DEPtotal_{ann}}{DEPTH_{soil} \cdot RHO_{soil}}$$ **Equation 58**

Explanation of symbols

$DEPtotal_{ann}$	annual average total deposition flux	[mg · m^{-2} · d^{-1}]	**Equation 47**
$DEPTH_{soil}$	mixing depth of soil	[m]	**Table 10**
RHO_{soil}	bulk density of soil	[kg · m^{-3}]	**Equation 20**
D_{air}	aerial deposition flux per kg of soil	[mg · kg^{-1} · d^{-1}]	

The differential **Equation 55** has an analytical solution, given by:

$$C_{soil}(t) = \frac{D_{air}}{k} - \left[\frac{D_{air}}{k} - C_{soil}(0) \right] \cdot e^{-k\,t}$$ **Equation 59**

Explanation of symbols

C_{soil} (0)	initial concentration in soil after sludge application	[mg · kg^{-1}]	**Equation 59**
C_{soil} (t)	concentration in soil at a specific moment in time after sludge application	[mg · kg^{-1}]	

With this equation, the concentration can be calculated at each moment in time, when the initial concentration in that year is known.

Derivation of the initial concentration after 10 years of sludge application:

The previous section showed general equations describing how degradation in soil is modelled. In this section, specific equations are provided how both degradation and deposition are taken into account in the modelling. Parameter names for the concentration in soil resulting from spreading of sludge and deposition via air are therefore different from the ones used in the previous section. The parameters contain an index to indicate the year of sludge application and a value between brackets to indicate the point in time for which the concentration is valid. E.g. Cdepsoil10 (0) is the initial (0) concentration in soil resulting from deposition (dep) after 10 years (index '10').

As a realistic worst-case assumption for exposure, it is assumed that sludge application takes place for 10 consecutive years. To be able to calculate the concentration in this year averaged over the time period T (**Equation 64**), an initial concentration in this year needs to be derived. For this purpose, the contributions of deposition and sludge applications are considered separately.

The concentration due to 10 years of continuous deposition only, is given by applying **Equation 58** with an initial concentration of zero and 10 years of input:

$$Cdep_{soil10}(0) = \frac{D_{air}}{k} - \frac{D_{air}}{k} \cdot e^{-365 \cdot 10 \cdot k}$$ **Equation 60**

For sludge application, the situation is more complicated as this is not a continuous process. The concentration just after the first year of sludge application is given by:

$$Csludge_{soil\,1}(0) = \frac{C_{sludge} \cdot APPL_{sludge}}{DEPTH_{soil} \cdot RHO_{soil}}$$ **Equation 61**

Explanation of symbols

C_{sludge}	concentration in dry sewage sludge	[mg · kg^{-1}]	Equation 39
$APPL_{sludge}$	dry sludge application rate	[kg · m^{-2} · yr^{-1}]	**Table 10**
$DEPTH_{soil}$	mixing depth of soil	[m]	**Table 10**
RHO_{soil}	bulk density of soil	[kg · m^{-3}]	Equation 20
$Csludge_{soil\ 1}$ (0)	concentration in soil due to sludge in first year at t=0	[mg · kg^{-1}]	

The fraction of the substance that remains in the top soil layer at the end of a year is given by:

$$Facc = e^{-365\,k}$$ **Equation 62**

Explanation of symbols

k	first order rate constant for removal from top soil	[d^{-1}]	**Equation 56**
F_{acc}	fraction accumulation in one year	[-]	

At the end of each year, a fraction F_{acc} of the initial concentration remains in the top-soil layer. The initial concentration after 10 applications of sludge is given by:

$$Csludge_{soil\ 10}\ (0) = Csludge_{soil\ 1}\ (0) \cdot \left[1 + \sum_{n=1}^{9} Facc^{n} \right]$$ **Equation 63**

The sum of both the concentration due to deposition and sludge is the initial concentration in year 10:

$$C_{soil\ 10}\ (0) = Cdep_{soil\ 10}\ (0) + Csludge_{soil\ 10}\ (0)$$ **Equation 64**

This initial concentration can be used in Equation 62 to calculate the average concentration in soil over a certain time period.

Average concentration:

Accumulation of a substance may occur when sludge or manure is applied over consecutive years. The scenario is further worked out for sludge. As a realistic worst-case exposure scenario, it is assumed that sludge is applied for 10 consecutive years. The local emission scenario to soil via the STP also includes indirect emission via air. This is accounted for in the calculation of the PEC_{soil} on a local scale (application of STP sludge onto land) and is addressed in **section 2.3.7.5**. For spreading of manure, indirect exposure of soil via air is

not taken into account. To indicate for potential persistency of the substance, the percentage of the steady-state situation is calculated.

As shown in Figure 11, the concentration in soil is not constant in time.

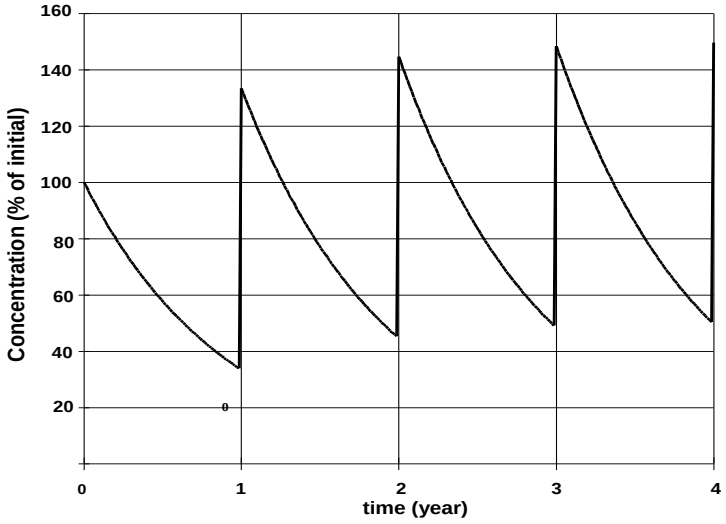

Figure 11: Cumulation in soil due to several years of sludge application

The exposure pattern for sludge is characterised by repeated applications with a one-year time interval. The concentration will be high just after sludge application (in the beginning of the growth season), and lower at the end of the year due to removal processes. When performing risk assessment for the terrestrial compartment, care should be taken that the PEC and PNEC soil are based on comparable exposure patterns. The results of currently available standardised terrestrial ecotoxicity tests are generally expressed on the basis of initial, nominal concentrations in test with single applications. Consequently, a $PNEC_{soil}$ based on those tests is most accurately described in terms of initial concentrations too. In that case the $PNEC_{soil}$ should be compared with the initial PEC_{soil}, which is the PEC_{soil} directly after the last sludge application. The $PNEC_{soil}$ may also be derived by equilibrium partitioning from a $PNEC_{aquatic}$ for chronic exposure. If this $PNEC_{aquatic}$ is based on study results that are expressed as time averaged concentrations, the $PNEC_{soil}$ is representative for time averaged exposure concentrations too. In that case, it is reasonable to average the PEC_{soil} over a certain time period, and a period of 30 days after the last application of sludge is used. In order to assess the risks of secondary poisoning in the terrestrial compartment (using porewater concentration, see **section 3.8.3.7**) and indirect human exposure, it is more appropriate to use an extended averaging period of 180 days. The approach for sludge is also applicable to the indirect emissions of biocides to soil via manure, e.g. biocides for veterinary hygiene (PT3) and biocides for the control of arthropods in stables (PT18).

Other biocide use types result in a variety of exposure patterns that are not reflected by the profile for sludge and manure described in Figure 11. Indirect exposure of soil occurs in PT11 (cooling fluids) via deposition, but results in a different exposure pattern than emissions via STP or manure. Direct emission to soil occurs during the application phase or service life of biocides in several product types, such as preservatives applied in paints and coatings (PT07), wood (PT08), polymerised materials (PT09) and masonry (PT10). For wood preservatives in PT08, losses during the application phase give a single emission, followed by a continuous emission due to leaching in service life. Repeated applications of insecticides (e.g. terraces in PT18) may lead to multiple emissions within a relatively short period of time. The combination of the emission profile and the behaviour of the substance in soil determine the pattern of PEC_{soil} over time.

For compounds that are nondegradable or very slowly degrading (see **section 3.10** of this

guidance), involatile and/or less mobile, and which are continuously emitted (e.g. via leaching from preserved materials or drift from cooling towers), the exposure pattern results in soil concentrations that increase with time. In this case, the highest PEC should be taken for risk assessment, i.e. the plateau concentration in case of repeated pulses or continuous exposure. As indicated above, existing soil ecotoxicity tests are developed for single applications. Especially for compounds that degrade during the test, the exposure profile in the ecotoxicity tests may differ from the exposure pattern in the receiving soil compartment. A case-by-case decision on the selection of initial or time averaged PEC and $PNEC_{soil}$ should be taken to ensure that the risk assessment is protective. For this, information about the likely exposure in the toxicity test system is needed, and plotting the development of the PEC_{soil} over time and the concentration pattern in the critical ecotoxicity test may be useful for decision making.

The procedure for deriving an averaged PEC_{soil} is illustrated in **Figure 12**, where the average concentration is given by the area of the shaded surface, divided by the number of days.

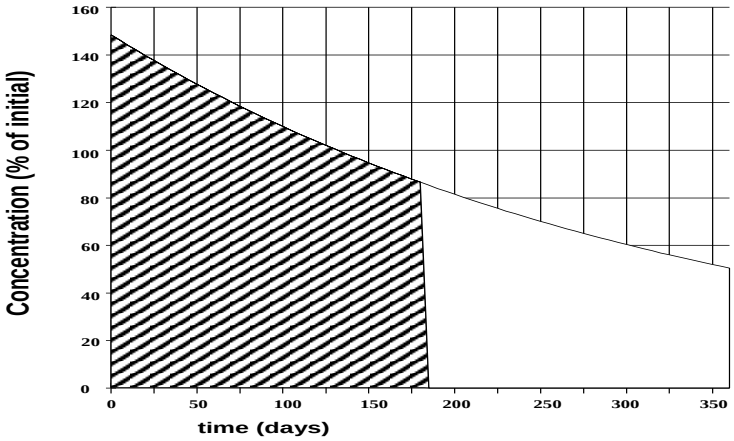

Figure 12: The concentration in soil after 10 years. The shaded area is the integrated concentration over a period of 180 days.

The local concentration in soil is defined as the average concentration over a certain time period T. The average concentration over T days is given by:

$$Clocal_{soil} = \frac{1}{T} \cdot \int_0^T C_{soil}(t)\,dt$$ **Equation 65**

Solving this equation for the range 0 to T gives the final equation for the average concentration in this period:

$$Clocal_{soil} = \frac{D_{air}}{k} + \frac{1}{kT}\left[C_{soil10}(0) - \frac{D_{air}}{k} \right] \cdot \left[1 - e^{-kT}\right]$$ **Equation 66**

Explanation of symbols

D_{air}	aerial deposition flux per kg of soil	[mg · kg^{-1} · d^{-1}]	**Equation 58**
T	averaging time	[d]	**Table 9**
k	first order rate constant for removal from top soil	[d^{-1}]	**Equation 56**
$C_{soil\ 10}$ (0)	initial concentration in soil (after sludge application) in year 10	[mg · kg^{-1}]	**Equation 64**
$C_{local,\ soil}$	average concentration in soil over T days	[mg · kg^{-1}]	

Indicating persistency of the substance in soil

Ten consecutive years of accumulation may not be sufficient for some substances to reach a steady-state situation. These substances may accumulate for hundreds of years. To indicate potential problems of persistency in soil, the fraction of the steady-state concentration can be derived:

$$Fst\text{-}st = \frac{C_{soil\ 10}\ (0)}{C_{soil\ \infty}\ (0)}$$ **Equation 67**

Explanation of symbols

$C_{soil\ 10}$ (0)	initial concentration after 10 years	[mg · kg^{-1}]	**Equation 62**
$C_{soil\ \infty}$ (0)	initial concentration in steady-state situation	[mg · kg^{-1}]	**Equation 66**
$F_{st\text{-}st}$	fraction of steady-state in soil achieved	[-]	

The initial concentration in the steady-state year is given by:

$$C_{soil\ \infty}\ (0) = \frac{D_{air}}{k} + Csludge_{soil\ 1}\ (0) \cdot \frac{1}{1 - Facc}$$ **Equation 68**

Explanation of symbols

D_{air}	aerial deposition flux per kg of soil	[mg · kg^{-1} · d^{-1}]	**Equation 58**
k	first order rate constant for removal from top soil	[d^{-1}]	**Equation 56**
F_{acc}	fraction accumulation in one year	[-]	**Equation 62**
$C_{sludge,\ soil\ 1}$ (0)	concentration in soil due to sludge in first year at t=0	[mg · kg^{-1}]	**Equation 61**
$C_{soil\infty}$(0)	initial concentration in steady-state situation	[mg · kg^{-1}]	

Calculation of PEClocal$_{soil}$

For soil, three different PECs are calculated, for different endpoints:

Table 9: Characteristics of soil and soil-use for the three different endpoints

	Depth of soil compartment [m]	**Averaging time** [days]	**Rate of sludge application** [kg$_{dwt}$.m^{-2}.year^{-1}]	**Endpoint**
PEClocal$_{soil}$	0.20	None (initial PEC) /30 (time averaged)	0.5	terrestrial ecosystem
PEClocal$_{agr.\ soil}$	0.20	180	0.5	crops for human consumption, porewater
PEClocal, grassland	0.10	180	0.1	grass for cattle, porewater

The "depth of soil" represents the depth range for the top soil layer which is of interest. The depth of 20 cm is taken because this range usually has a high root density of crops, and represents the ploughing depth. For grassland, the depth is less since grasslands are not ploughed.

The averaging period of 180 days for crops is chosen as a representative growing period for crops. For grassland this period represents a reasonable assumption for the period that cattle are grazing on the field. The average period of 180 days for agricultural soil and grassland is also the relevant period for the derivation of porewater concentrations (see **Equation 71**). For the ecosystem a period of 30 days is taken as a relevant time period with respect to chronic exposure of soil organisms or the initial PEC is used (see the discussion on average concentration on page 89).

The concentration at the regional scale is used as background concentration for the local scale if the exposure assessment is performed using the tonnage based approach. For this purpose, the concentration in unpolluted soil needs to be applied ("natural soil", only input through deposition). Otherwise, sludge application is taken into account twice.

$$PEClocal_{soil} = Clocal_{soil} + PECregional_{natural\ soil} \qquad \textbf{Equation 69}$$

Explanation of symbols

$Clocal_{soil}$	local concentration in soil	[mg·kg^{-1}]	**Equation 67**
$PECregional_{natural\ soil}$	regional concentration in natural soil	[mg·kg^{-1}]	**2.3.7.7**
$PEClocal_{soil}$	predicted environmental conc. in soil	[mg·kg^{-1}]	

The equation for deriving the concentration in the pore water is:

$$PEClocal_{soil,porew} = \frac{PEClocal_{soil} \cdot RHO_{soil}}{K_{soil\text{-}water} \cdot 1000} \qquad \textbf{Equation 70}$$

Explanation of symbols

$PEClocal_{soil}$	predicted environmental conc. in soil[16]	[mg·kg^{-1}]	**Equation 67**
$K_{soil\text{-}water}$	soil-water partition coefficient	[m^3·m^{-3}]	**Equation 27**
RHO_{soil}	bulk density of wet soil	[kg·m^{-3}]	**Equation 20**
$PEClocal_{soil,porew}$	predicted environmental conc. in porewater	[mg·l^{-1}]	

2.3.7.5.2 Direct release

In the following product-types, substances can potentially be directly released to soil without passing an STP or any other environmental compartment before:

PT 6: Preservatives for product during storage

PT 7: Film preservatives

PT 8: Wood preservatives (use classes 3, 4b and 5)

PT 9: Fibre, leather, rubber and polymerised materials preservatives

PT 10: Construction material preservatives

PT14: Rodenticides

PT18: Insecticides, acaricides and products to control other arthropods

[16] The worst case agricultural PEC value for arable land should be used.

For these cases specific guidance on how to perform the exposure assessment for soil is provided in the respective ESD (see http://echa.europa.eu/guidance-documents/guidance-on-biocides-legislation/emission-scenario-documents). Please note that PT 6, PT 7, PT 9 and PT 10 are coverd with regard to exposure assessment of soil by the ESD for PT 8.

The same considerations concerning the comparision of initial and time averaged PEC and PNEC values provided for indirect release also applies to direct release (see **section 2.3.7.5.1**).

2.3.7.5.3 Mixing depth depending on release- and soil type

Depending on how the release to soil occurs (direct/indirect) and on the type of soil (agricultural land/grassland/soil in general) different mixing depth are considered in the exposure assessment.

An overview of default values for mixing depth/depth of soil compartment as given the ESDs and partly revised in the TAB is provided in Table 10 on the next page.

Table 10: Default values for mixing depth/depth of soil compartment as given the ESDs[17]

PT/scenario	Target soil	DEPTHs (m)	Source
PT 3 Veterinary hygiene			
- disinfection of animal housings (manure) - non-medicinal - teat dips (manure) - footwear (manure) - animal's feet	arable land grassland	0.20 0.05	ESD for PT 3: Emission scenarios for veterinary hygiene biocidal products (JRC Scientific and Technical Reports, 2011)
PT6			
In can preservatives used in paints (house scenario)		0.5	See decision for PT 10 (TAB v1.3, section 2.4.11)
PT7			
Film preservatives (house scenario)		0.5	See decision for PT 10 (TAB v1.3, section 2.4.11)
PT8			
Storage place In situ treatment Treated wood in service		0.5 0.5 0.5	ESD for PT 8: Revised Emission Scenario Document for Wood Preservatives (OECD series No. 2, 2013)
PT 9 Fibre, leather, rubber and polymerised materials preservatives			
Roof membranes	-	0.2	Use-based approaches for the estimation of environmental exposure due to roof membranes (UBA, 2014)
PT 10 Construction material preservatives			

[17] ESDs contain binding values. TAB should be consulted where ESD values may have been overwritten.

PT/scenario	Target soil	DEPTHs (m)	Source
House scenario, countryside	-	0.5	TAB v1.3, section 2.4.11)
PT 14 Rodenticides			
- a sewer system, - in and around buildings, - open areas, waste dumps.	-	0.1	ESD for PT 14: Emission scenarios for biocides used as rodenticides (EUBEES, 2003)
PT 15 Avicides			
		0.1	ESD for PT 15: Emission scenarios for biocides used as avicides (EUBEES, 2003)
PT 18 Insecticides, acaricides and products to control other arthropods			
Restricted areas	-	0.5	Emission Scenario Document for Insecticides, Acaricides and products to control other arthropods for household and professional uses / TAB
Manure/sewage sludge application	arable land	0.20	Emission Scenario Document for Insecticides for Stables and Manure Storage Systems
Manure/sewage sludge application	grassland	0.05	
	- surface application (broad cast)	0.05	
PT 19 Repellents and attractants			
Insect repellents applied on animal skin - application	-	0.5	ESD for PT 19: Emission scenarios for repellents and attractants (ECHA, 2015)
Insect repellents applied on animal skin - Rolling of horses	-	0.1	
Insect repellents applied on animal skin - hosing of horses	-	0.5	
Application of repellents in the environment of humans and animals- Application on unpaved ground	-	0.5	
Insect repellents used for factory-treated textiles Emissions during the service life of tents	-	0.1	
PT 21 Antifouling products			
New building pleasurecraft in an average OECD boatyard for both realistic worst case and typical case scenario	-	0.5	Emission scenarios for antifouling products in OECD countries (European Commission, DG Environment, 2004

PT/scenario	Target soil	DEPTHs (m)	Source
Professional application of paint during M&R of pleasure craft in an average OECD boat yard/marina for both realistic worst case and typical case scenario	-	0.5	Referring to the OECD ESD for PT 8.
Non-professional application of paint during M&R of pleasure craft in an average OECD marina for both realistic worst case and typical case scenario	-	0.5	
Professional removal of the paint layer during M&R of pleasure craft in an average OECD boatyard for both realistic worst and typical case	-	0.5	
Nonprofessional removal of the paint layer in an average OECD boatyard/marina (see M&R) for both realistic worst and typical case	-	0.5	
PT 22 Embalming and taxidermist fluids			
Embalming – releases in cemetries	-	0.5	ESD for PT 22: Emission scenarios for biocides used in taxidermy and embalming processes (EUBEES, 2001)

2.3.7.6 Calculation of concentration in groundwater

In this section, the following parameter is derived:

- local concentration in groundwater.

The concentration in groundwater is calculated for indirect exposure of humans through drinking water. As an indication for potential groundwater levels, the concentration in porewater of agricultural soil is taken.

$$PEClocal_{grw} = PEClocal_{agr.soil,porew}$$ **Equation 71**

Explanation of symbols

$PEClocal_{, agr.soil,porew}$	predicted environmental conc. in porewater	$[mg \cdot l^{-1}]$	**Equation 68**
$PEClocal_{, grw}$	predicted environmental conc. in groundwater	$[mg \cdot l^{-1}]$	

If no data on degradation in soil are available for exposure modelling in groundwater, the result is a worst-case $PEC_{porewater}$ estimate as the substance is assumed to accumulate over a 10 year period. In case data on degradation in soil are used, $PEClocal_{agr. soil, porew}$ is a realistic worst-case estimate since biodegradation, leaching and volatilisation are taken into account over a 10 year period and over a limited soil depth ($DEPTH_i$ depending on the ESD, see **Table 10**). If the risk assessment for the groundwater compartment indicates a inacceptable risk based on this first tier $PEC_{porewater}$ and data on degradation in soil had been

taken into account, refinement of $PEClocal_{gw}$, using available groundwater simulation models developed for assessment of pesticide mobility, is the next step to be taken. See also **Info-box 5**.

As refinement option, the $PEClocal_{,gw}$ can be estimated by using available groundwater simulation models developed for assessment of the pesticide mobility in soil reflecting, more realistic groundwater conditions, or by using measured data (lysimeter studies or monitoring data).

Info-box 5: Cut off criteria for groundwater assessment of biocides

The following basic cut-off criteria are applicable to avoid the need for a full formal refinement of FOCUS groundwater assessment:

- For active substance only assessments (i.e. where no major metabolites are formed) the standard cut-off criteria (DT50 <21 d at 20°C and Koc >500 L/kg) could be used for biocide application rates up to 100 kg a.s./ha per year.
- For assessments including metabolites, the standard cut-off criteria could be used if a) both parent and metabolites meet the standard cut-off criteria and b) the biocide application rates are less than 10 kg a.s./ha per year
- Where a parent assessment is triggered based on the cut-off criteria (i.e. because it has a DT50 > 21 d at 20°C or Koc <500L/kg), metabolites should always be included irrespective of their properties.

The following tiered approach to biocide groundwater assessments is proposed:
Tier 1: Estimation of PECgw as soil pore water concentration
Tier 2: Consideration of parent and all major metabolites against the cut-off criteria listed above
Tier 3: Refinement of Tier 1 estimates using FOCUS PEARL (or PELMO) and relevant Product Type specific guidance.

Groundwater criteria evaluation summary

The BPR implies that for biocides the trigger value for pesticides in groundwater is applied (BPR Annex VI, point 68). The concentration in groundwater should therefore be <0.1 µg/L for active substance, relevant metabolites or breakdown/reaction products and substances of concern. The total concentration should be <0.5 µg/L. In addition, the trigger value applies for each separate biocide. A decision tree is given in **Figure 13**.

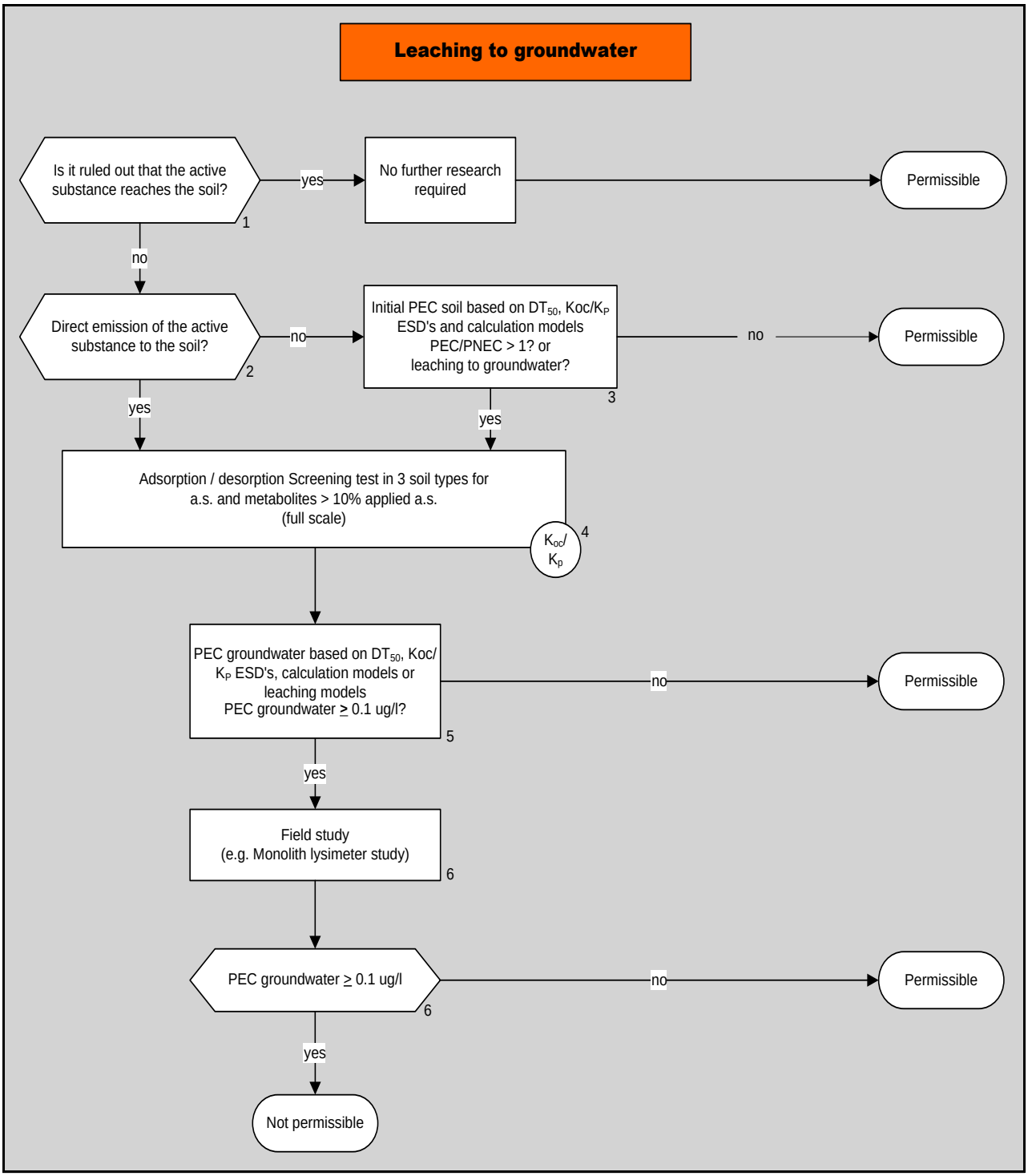

Figure 13: Decision tree for the groundwater assessment

2.3.7.7 Calculation of PECregional

In this section, the following parameters are derived:

- regional exposure concentrations in all environmental compartments

  Regional computations are done by means of multimedia fate models based on the fugacity concept. Recently, models have been described by Mackay et al. (1992), Van de Meent (1993) and Brandes et al. (1996) (SimpleBox). These models are box

models, consisting of a number of compartments (see **Figure 7**) which are considered homogeneous and well mixed. A substance released into the model scenario is distributed between the compartments according to the properties of both the substance and the model environment.

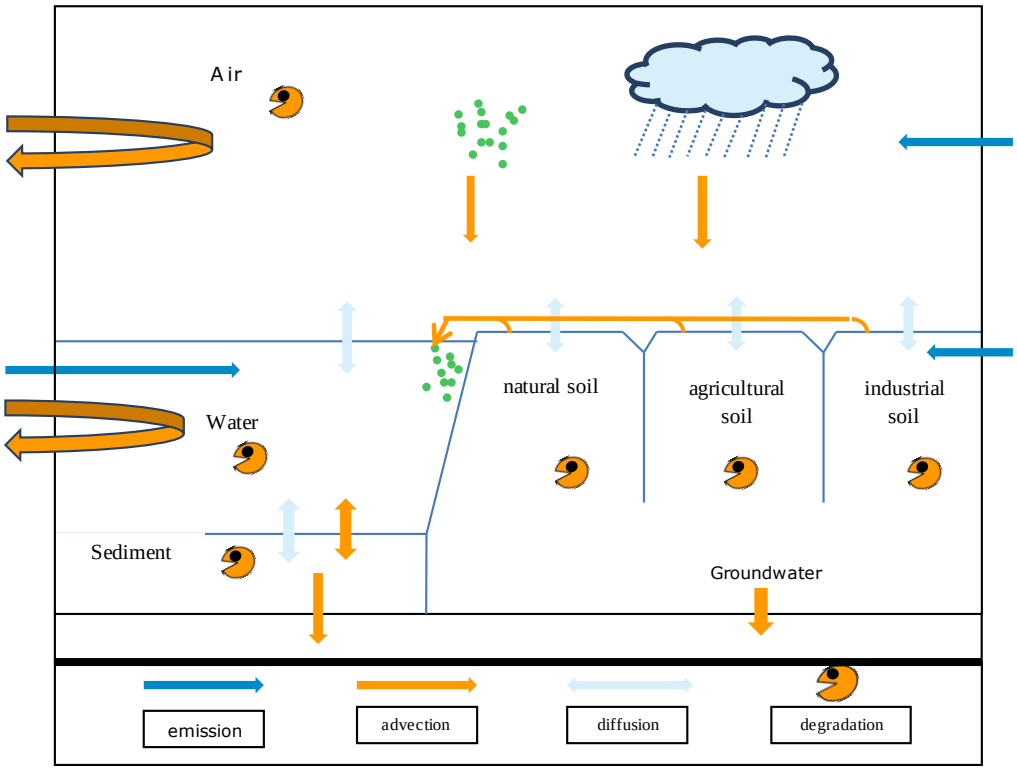

Figure 14: The relevant emission and distribution routes

Several types of fate processes are distinguished in the regional assessment, as drawn in **Figure 14**:

- emission, direct and indirect (via STP) to the compartments air, water, industrial soil, and agricultural soil;
- degradation, biotic and abiotic degradation processes in all compartments;
- diffusive transport, as e.g. gas absorption and volatilisation. Diffusive mass transfer between two compartments goes both ways, the net flow may be either way, depending on the concentration in both compartments;
- advective transport, as e.g. deposition, run-off, erosion. In the case of advective transport, a substance is carried from one compartment into another by a carrier that physically flows from one compartment into the other. Therefore, advective transport is strictly one-way.

Substance input to the model is regarded as continuous and equivalent to continuous diffuse emission. The results from the model are steady-state concentrations, which can be regarded as estimates of long-term average exposure levels. The fact that a steady state between the compartments is calculated does not imply that the compartment to which the emission takes place is of no importance.

In a Mackay-type level III model, the distribution and absolute concentrations may highly depend upon the compartment of entry.

Advective import and export (defined as inflow from outside the model or outflow from the model environment) can be very important for the outcome of both regional and local model calculations. Therefore, the concentration of a substance at the "border" of the region must be taken into account. This is defined as the background concentration of a substance. The background concentration in a local model can be obtained from the outcome of the regional model. For substances with many relatively small point sources, this background concentration may represent a significant addition to the concentration from a local source. The background concentration in the regional model has to be calculated using a similar box model of a larger scale, e.g. with the size of the European continent. In this continental model, however, it is assumed that no inflow of air and water across the boundaries occurs. Furthermore it is assumed that all substance releases enter into this continental environment. The resulting steady-state concentrations are then used as transboundary or background concentrations in the regional model. The continental and regional computations should thus be done in sequence. **Figure 1** visualises the relationship between the concentrations calculated for the different model scales. For both the regional and continental scale, the total emission amounts (through diffuse and point sources, summed over all stages of the life-cycle) are used.

For the PECregional calculation, in contrast to PEClocal, an average percentage connection rate to STPs should be included in the calculation. This leads to a more realistic estimation of the likely background concentration on a regional scale. For the purposes of the generic regional model, a STP connection rate of 90% (the EU average according to **Appendix 4**) will be assumed.

The results from the regional model should be interpreted with caution. The environmental concentrations are averages for the entire regional compartments (which were assumed well mixed). Locally, concentrations may be much higher than these average values. Furthermore, there is a considerable degree of uncertainty due to the uncertainty in the determination of input parameters (e.g. degradation rates, partitioning coefficients).

Model parameters for PECregional

When calculating the PECregional it is important which modelling parameters are chosen and what fraction of the total emissions is used as emission for the region. There are two different possibilities:

- calculation of a PECregional on the basis of a standardised regional environment with agreed model parameters;
- calculation of a PECregional on the basis of country specific model parameters.

A standardised regional environment should be used for the first approach in the calculation of PECregional. When more specific information is available on the location of production /emission sites, this information can be applied to refine the regional assessment. The second approach may sometimes result in a better estimation of the concentrations for a specific country. However, depending on the information on production site location, it will lead to a number of different PEC values which makes a risk characterisation at EU level more complicated.

Calculations are performed for a densely populated area of 200·200 km with 20 million inhabitants. Unless specific information on use or emission per capita is available, it is assumed that 10% of the european production and use takes place within this area, i.e. 10% of the estimated emission is used as input for the region. The model parameters proposed for this standard region are given in **Table 11**. It should be noted that it is extremely difficult to select typical or representative values for a standard European region. Therefore, the rationale behind the values of **Table 11** is limited. Nevertheless, these values present a starting point for the regional scale assessments. Characterisation of the environmental compartments for the regional model should be done according to the values in **Table 3**.

Table 11: Proposed model parameters for regional model

Parameter	Value in regional model
area of the regional system	4.104 km^2
area fraction of water	0.03
area fraction of natural soil	0.60
area fraction of agricultural soil	0.27
area fraction of industrial/urban soil	0.10
mixing depth of natural soil	0.05 m
mixing depth of agricultural soil	0.2 m
mixing depth of industrial/urban soil	0.05 m
atmospheric mixing height	1000 m
depth of water	3 m
depth of sediment	0.03 m
fraction of the sediment compartment that is aerobic	0.10
average annual precipitation	700 mm· yr^{-1}
wind speed	3m · s^{-1}
residence time of air	0.7 d
residence time of water	40 d
fraction of rain water infiltrating soil	0.25
fraction of rain water running off soil	0.25
EU average connection percentage to STP	80%

The area fractions for water and for natural, agricultural and industrial/urban soils, are average values obtained from ECETOC (1994b), supplemented with data received from Sweden and Finland. Data for Norway and Austria are obtained from the FAO statistical databases available at http://www.fao.org/statistics/en/. The residence time for air (defined as the time between air entering and leaving the region) of 0.7 days is derived from the wind speed of 3 m/s and the area of the region. The residence time of water of 40 days is selected as a reasonable average for the european situation.

The amount of wastewater discharged, is the product of the amount of wastewater discharged per person equivalent and the number of inhabitants of the system. Using a flow per capita of 200 l · d^{-1} (equivalent to the value used in the SimpleTreat model, see **Table 7**) and a population of 20 million, this results in an additional water flow through the model environment of 4.0 · 10^6 m^3 · d^{-1}. The inflow caused by inflowing riverwater, is 6.5 · 10^7 m^3 · d^{-1}.

In addition to the environmental characteristics of the region, selected intermedia mass transfer coefficients are required in the multimedia fugacity model to ensure comparability of the outcome with other models. These transfer coefficients are summarised in **Table 12**.

Table 12: Intermedia mass transfer coefficients

Parameter	Value
air-water interface: air side partial mass transfer coefficient (k aw_{air})	**Equation 82**
air-water interface: water side partial mass transfer coefficient (k aw_{water})	**Equation 81**
Aerosol deposition rate	0.001 m · s^{-1}
air-soil interface: air side partial mass transfer coefficient (k asl_{air})	1.05 · 10^{-3} m · s^{-1}
air-soil interface: soil side partial mass transfer coefficient (k asl_{soil})	**Equation 70**
sediment-water interface: water side partial mass transfer coefficient (ksw_{water})	2.78 · 10^{-6} m · s^{-1}
sediment-water interface: pore water side partial mass transfer coefficient (k $sw_{pore\ water}$)	2.78 · 10^{-8} m · s^{-1}
net sedimentation rate	3 mm · yr^{-1}

Mass transfer at air-soil and air-water interface on the regional and continental scales.

Soil–air interface

A substance-dependent soil-side partial mass transfer coefficient (PMTC) at the soil-air interface $kasl_{soil}$ ($m.d^{-1}$) is deduced from the exponential concentration profile in an undisturbed soil:

$$kasl_{soil} = \left(Veff_{soil} + \frac{Deff_{soil}}{d_p} \right)$$ **Equation 72**

In undisturbed soil, processes of downward advection (pore water + small particles), *diff*usion (air, water, solids), and degradation take place simultaneously. These processes are included in Simplebox 3.0 (Den Hollander et al., 2004). The result is an exponential decrease of the concentration with depth, characterised by a substance-dependent penetration depth (d_p) (Hollander, 2004 and 2006).

$$d_p = \frac{Veff_{soil} + \sqrt{Veff_{soil}^{\ 2} + Deff_{soil} \cdot 4 \cdot k\deg_{soil}}}{2 \cdot k\deg_{soil}}$$ **Equation 73**

In which:

$$Veff_{soil} = FRw.soil \frac{RAINRATE \cdot F\inf_{soil}}{Fwater_{soil}} + FRs.soil. \frac{SOLIDadv.soil}{Fsolid_{soil}}$$ **Equation 74**

$$Deff_{soil} = FRa.soil \frac{DIFFgas \cdot Fair_{soil}^{\ 1.5}}{Fair_{soil}} + FRw.soil. \frac{DIFFwater \cdot Fwater_{soil}^{\ 1.5}}{Fwater_{soil}} + FRs.soil \cdot \frac{SOLIDdiff.soil}{Fsolid_{soil}}$$ **Equation 75**

$$FRw.soil = \frac{Fwater_{soil}}{Fair_{soil} \cdot K_{air-water} + Fwater_{soil} + Fsolid_{soil} \cdot Kp_{soil} \cdot RHO_{solid}/1000}$$ **Equation 76**

$$FRs.soil = \frac{Fsolid_{soil}}{Fair_{soil} \cdot K_{air-water}/(\ Kp_{soil} \cdot RHO_{solid}/1000\ ) + Fwater_{soil}/(\ Kp_{soil} \cdot RHO_{solid}/1000\ ) + Fsolid_{soil}}$$ **Equation 77**

$$FRa.soil = 1 - FRw.soil - FRs.soil$$ **Equation 78**

$$DIFFgas = 2.57 \cdot 10^{-5} \sqrt{\frac{18}{M \cdot 1000}}$$ **Equation 79**

$$DIFFwater = 2.0 \cdot 10^{-9} \sqrt{\frac{32}{M \cdot 1000}}$$ **Equation 80**

Explanation of symbols

M	molecular weight of the substance	[$kg_c \cdot mol^{-1}$]	
kdegsoil	rate constant for degradation in bulk soil	[d^{-1}]	
RAINRATE	average daily rate of wet precipitation	[$m \cdot d^{-1}$]	1.92·10-3
Finfsoil	fraction of precipitation that penetrates into the soil	[-]	0.25
dp	substance-dependent penetration depth	[m]	**Equation 73**
Veffsoil	effective advection (with penetrating porewater)	[m]	**Equation 74**
Deffsoil	effective diffusion coefficient	[$m^2 \cdot d^{-1}$]	**Equation 75**
FRa.soil	mass fraction of the substance in the air phase of soil	[-]	**Equation 78**
FRw.soil	mass fraction of the substance in the water phase of soil	[-]	**Equation 76**
FRs.soil	mass fraction of the substance in the solid phase of soil	[-]	**Equation 75**
Fairsoil	volume fraction of air in the soil compartment	[$m_{air}^3 \cdot m_{soil}^{-3}$]	**Table 3**
Fwaters	volume fraction of water in the	[$m_{water}^3 \cdot m_{soil}^{-3}$]	**Table 3**

oil	soil compartment		
$Fsolid_{soil}$	volume fraction of solids in the soil compartment	$[m_{solid}^3 \cdot m_{soil}^{-3}]$	**Table 3**
$K_{air-water}$	air-water partition coefficient	$[m^3 \cdot m^{-3}]$	**Equation 24**
Kpsoil	partition coefficient solid-water in soil	$l \cdot kg^{-1}$	**Equation 26**
RHOsolid	Density of solid phase	$kg_{dwt} \cdot m^{-3}$	**Table 3**
DIFFgas	molecular diffusivity of the substance in the gas phase	$[m^2 \cdot s^{-1}]$	**Equation 77**
DIFFwater	molecular diffusivity of the substance in the water phase	$[m^2 \cdot s^{-1}]$	**Equation 78**
SOLIDadv.soil	rate of advective downward transport of soil particles	$[m \cdot s^{-1}]$	$6.34 \cdot 10^{-12}$
SOLIDdiff.soil	solid phase diffusion coefficient in the soil compartment	$[m^2 \cdot s^{-1}]$	$6.37 \cdot 10^{-12}$
kaslsoil	partial mass-transfer coefficient at soil side at the air-soil interface	$[m \cdot d^{-1}]$	**Equation 70**

The maximum value for the penetration depth (*dp*) is set to 1 metre for all three soil types on the regional scale. The minimum depth is set to the default soil depth (**Table 10**).

Water-air interface

The partial mass transfer coefficients of the air-water interface depend on the windspeed of the system and the molecular weight of the substance:

$$kaw_{air} = 0.01 \cdot (0.3 + 0.2 \cdot WINDSPEED) \cdot (\frac{0.018}{M})^{0.335}$$ **Equation 81**

$$kaw_{water} = 0.01 \cdot (0.0004 + 0.0004 \cdot WINDSPEED^{2}) \cdot (\frac{0.032}{M})^{0.25}$$ **Equation 82**

Explanation of symbols

M	molecular weight of the substance	$[kg_C \cdot mol^{-1}]$
WINDSPEED	average windspeed	$[m \cdot d^{-1}]$
kaw_{air}	partial mass-transfer coefficient at the air side of the air-water interface	$[m \cdot d^{-1}]$
kaw_{water}	partial mass-transfer coefficient at the water side of the air-water interface	$[m \cdot d^{-1}]$

Model parameters for the continental concentration

The continental box covers 15 EU countries and Norway and similar percentages for water and natural, agricultural and industrial/urban soils as given in

Table 12. All other parameters are similar to the ones given in the preceding tables. Emission estimation to this continental box should be based on the EU-wide production volume of the substance.

The resulting concentrations in water and air must be used as background concentrations (i.e. concentrations in water or air that enter the system) in the regional model. When the model is built according to **Figure 1** it is assumed that no inflow of the substance into the continental system takes place.

More recent versions of multimedia models do also contain so-called global scales for different temperature regions, for instance moderate, tropic and arctic (see e.g. Brandes et al., 1996). In this case the continent is embedded in the moderate scale just like the region is embedded in the continent. The size of the total global scale is that of the northern hemisphere. The global scales allow for a more accurate estimation of continental concentrations although this effect tends to be marginal. However, the global scales provide more insight in the ultimate persistence of the chemical.

Table 13: Parameters for continental model

Parameter	Value in continental model
area of the continental system	$3.56 \cdot 10^6$ km^2
area fraction of water	0.03
area fraction of natural soil	0.60
area fraction of agricultural soil	0.27
area fraction of industrial/urban soil	0.10

2.3.8 Summary of PECs derived

In summary, the local estimations yield the following input and output information:

Input

Physico-chemical properties	**section 2.3.2**
Characterisation of the environment	**Table 3**
Emission data	**section 2.3.3.3**
Partition coefficients	**section 2.3.5**
Degradation rates	**section 2.3.6**
Fate in sewage treatment plants	**section 2.3.7**

Output

$PEC_{microorganisms}$	local PEC for microorganisms in the STP	[mg · l^{-1}]	**Equation 41 Equation 39**
$PEC_{local,water}$	local PEC in surface water (dissolved) during episode	[mg · l^{-1}]	**Equation 51**

$PEC_{local,water,ann}$	annual average local PEC in surface water (dissolved)	[mg · l^{-1}]	**Equation 52**
$PEC_{local,sed}$	local PEC in sediment (total)	[mg · kg^{-1}]	**Equation 53**
$PEC_{local, air,ann}$	annual average local PEC in air (total)	[mg · m^{-3}]	**Equation 45**
$PEC_{local, soil}$	local PEC in agricultural soil (total), averaged over 30 days or initial local PEC in agricultural soil (total)	[mg · kg^{-1}]	**Equation 69**
$PEC_{local, agr.soil}$	local PEC in agricultural soil (total), averaged over 180 days	[mg · kg^{-1}]	**Equation 69**
$PEC_{local, grassland}$	local PEC in grassland (total), averaged over 180 days	[mg · kg^{-1}]	**Equation 69**
$PEC_{local, agr.soil,porew}$	local PEC in porewater of agricultural soil	[mg · l^{-1}]	**Equation 70**
$PEC_{local,grassland, porew}$	local PEC in porewater of grassland	[mg · l^{-1}]	**Equation 70**
$PEC_{local, grw}$	local PEC in groundwater under agricultural soil	[mg · l^{-1}]	**Equation 71**

The regional estimations yield the following input and output information:

Input

Physico-chemical properties	**section 2.3.2**
Characterisation of the environment	http://echa.europa.eu/guidance-documents/guidance-on-biocides-legislation/emission-scenario-documents
Parameters of the regional compartments	**Table 9, Table 10, Table 11**
Emission data	**section 2.3.3.3**
Partition coefficients	**section 2.3.5**
Degradation rates	**2.3.6**
Fate in sewage treatment plants	**section 2.3.7**

Output

$PEC_{regional, water}$	regional PEC in surface water (dissolved)	[mg · l^{-1}]	**section 2.3.7.7**
$PEC_{regional,air}$	regional PEC in air (total)	[mg · m^{-3}]	**section 2.3.7.7**
$PEC_{regional, agr.soil}$	regional PEC in agricultural soil (total)	[mg · kg^{-1}]	**section 2.3.7.7**
$PEC_{regional,natural soil}$	regional PEC in natural soil (total)	[mg · kg^{-1}]	**section 2.3.7.7**
$PEC_{regional,agr.soil,porew}$	regional PEC in porewater of agricultural soils	[mg · l^{-1}]	**section 2.3.7.7**
$PEC_{regional,sed}$	regional PEC in sediment (total)	[mg · kg^{-1}]	**section 2.3.7.7**

2.4 Use of measured data

For a number of existing active substances measured data are available for air, fresh- or seawater, sediment, biota and/or soil. These data have to be carefully evaluated for their adequacy and representativeness according to the criteria below. They are used together with calculated environmental concentrations in the interpretation of exposure data.

The evaluation should follow a stepwise procedure:

- reliable and representative data should be selected by evaluation of the sampling and analytical methods employed and the geographic and time scales of the measurement campaigns (**section 2.2.1** of this guidance);
- the data should be assigned to local or regional scenarios by taking into account the sources of exposure and the environmental fate of the substance (**section 2.2.2** of this guidance);
- the measured data should be compared to the corresponding calculated PEC. For naturally occurring substances background concentrations have to be taken into account. For risk characterisation, a representative PEC should be decided upon based on measured data and a calculated PEC (**section 2.5** of this guidance).

2.4.1 Selection of adequate measured data

The available measurements have to be assessed first, before using them in release and exposure estimation. The following aspects should be considered:

- Quality of the sampling and analytical techniques
- Selection of representative data for the environmental compartment of concern
- Outliers
- Treatment of values below the limit of quantification (LOQ)
- Data comparability

Applicants and evaluating authorities should also consider local regulatory requirements where applicable. Local agencies may have specific requirements on how data should be statistically analysed. It is advisable to obtain as much useful information on release and exposure from a data set as possible, but there is inherent danger for inappropriate use of the data for risk assessment purposes. To address this problem, two quality levels for existing data, based on the available contextual information, are given in **Table 14** below (based on OECD, 2000). In recommending this table the OECD stressed "*…these criteria should be applied in a flexible manner. For example, data should not always be discounted because they do not meet the criteria. Risk assessors should make a decision to use the data or not, on a case-by-case basis, according to their experience and expertise and the needs of the risk assessment*". The most important factors to be addressed are the analytical quality and the availability of information necessary to assess the representativeness of the sample.

Table 14: Quality criteria for use of existing data (OECD, 2000k)

Study category		
	1	2
Criteria	Valid without restriction – may be used for measured PEC	Valid with restrictions - May be used to support Exposure Assessment (data interpretation difficult)
What has been analysed? [1)]	x	x
Analytical method [2)]	x	x
Unit specified [3)]	x	x
Limit of quantitation [4)]	x	x
Blank concentration [5)]	x	
Recovery [6)]	x	
Accuracy [7)]	x	
Reproducibility [8)]	x	
Sample collection [9)]	x	
One shot or mean [10)]	x	x
Location [11)]	x	x
Date dd/mm/yy [12)]	x	Minimum is knowledge of year
Compartment characteristics [13)]	x	
Sampling frequency and pattern	x	x
Proximity of discharge points [14)]	x	x

Discharge emission pattern and volume [15)]	x (for local scale)	x (for local scale)
Flow and dilution or application rate	x (for local scale)	x (for local scale)
Explanation of value assigned to non-detects if used in a mean	x	x

Notes on Table 14:

1) Precisely what has been analysed should be made clear. Details of the sample preparation, including for example whether the analysis was of the dissolved fraction, the suspended matter (i.e. adsorbed fraction) or the total (aqueous and adsorbed) should be given.

2) The analytical method should be given in detail or an appropriate reference cited (e.g. the relevant ISO/DIN method or standard operating procedure).

3) Units must be clearly specified and information given whether it has been normalised to e.g. organic carbon, lipid etc.

4) The limit of quantitation and details of possible known interfering substances should be quoted.

5) Concentrations in system blanks should be given.

6) Recovery of standard additions (spikes) should be quoted.

7) Results of analysis of standard "reference samples", containing a known quantity of the substance should be included. Accuracy is connected to the analytical method and the matrix.

8) The degree of confidence (e.g. 95% confidence interval) and standard deviation in the result from repeat analysis should be given. Reproducibility is also connected to the analytical method and the matrix.

9) Whether the sampling frequency and pattern relate to the emission pattern, or whether they allow for effects such as seasonal variations need to be considered.

10) The assessor needs to know how the data have been treated, e.g. are the values reported single values, means, 90-percentile, etc.

11) The monitoring site should be representative of the location and scenario chosen. If data represent temporal means, the time over which concentrations were averaged should be given too.

12) The time, day, month and year may all be important depending upon the release pattern of the chemicals. Time of sampling may be essential for certain discharge/emission patterns and locations. For some modelling and trends analysis, the year of sampling will be the minimum requirements.

13) Compartment characteristics such as lipid content, content of organic carbon and particle size should be specified.

14) For the local aqueous environment, detailed information on the distance of other sources in addition to quantitative information on flow and dilution are needed.

15) It is necessary to consider whether there is a constant and continuous discharge, or whether the chemical under study is released as a discontinuous emission showing variations in both volume and concentration with time.

Quality of the sampling and analytical techniques

The applied techniques of sampling, sample shipping and storage, sample preparation for analysis and analysis must consider the physico-chemical properties of the substance. Measured concentrations that are not representative as indicated by an adequate sampling programme or are of insufficient quality should not be used in the exposure assessment.

The limit of quantification (LOQ) of the analytical method, which is normally defined by the analytical technique being used, should be suitable for the risk assessment and the comparability of the measured data should be carefully evaluated. For example, the concentrations in water may either reflect total concentrations or dissolved concentrations according to the sampling and preparation procedures used. The concentrations in sediment

may significantly depend on the content of organic carbon and particle size of the sampled sediment. The soil and sediment concentrations should preferably be based on concentrations normalised for the particle size (i.e. coarsest particles taken out by sieving). All measurements below the LOQ constitute a special problem and should be considered on a case-by-case basis. One approach that could be considered would be to use a value corresponding to LOQ/2 before estimating a mean or standard deviation (EC, 1999). As this method could heavily influence the mean and standard deviation, other methods may also be considered (e.g. assuming same distribution of data below and above the LOQ).

When a substance is used in materials (e.g. polymers) it may be released to the environment enclosed within the matrix of small particles of the material formed e.g. by weathering or abrasion (see **section 2.3.3.5**). In such cases it would be useful to know if the analytical method used is able to detect also the fraction of substance that is associated with these particles. The availability for analysis can be expected to be reduced for resistant materials and/or large particles. Depending on use pattern, particles may end up in STP sludge/agricultural soil, sediments affected by storm water outflows, industrial/urban soil and indoor dust.

Selection of representative data for the environmental compartment of concern

The representativeness of the monitoring data is related to the objective of the monitoring programme from which they originate. Monitoring programmes may be designed to cover a large spatial area (high number of stations over a large territory), to achieve a high spatial resolution (high number of stations per area unit), or to monitor only one point source release. Monitoring programmes may be designed to assess temporal trends (high sampling frequency), or to monitor the status of a site at a given time.

There are two distinct aspects to consider:

- The level of confidence in the result, i.e. the number of samples, how far apart and how frequently they were taken. The sampling frequency and pattern should be sufficient to adequately represent the concentration at the selected site.
- Whether the sampling site(s) represent a local or regional scenario. Samples taken at sites directly influenced by an emission should be used to describe the local scenario, while samples taken at larger distances may represent the regional concentrations and would not be appropriate for a local assessment.

For example, when evaluating the representativeness of discharges from a wastewater treatment plant, the number of samples and the sampling frequency should be adapted *inter alia* to the type of treatment process (including retention time), environmental significance and nature of the substance and effluent variability. Effluent quality and quantity vary over time in terms of volumes discharged and constituent concentrations. Variations occur due to a number of factors, including changes in human activity, changes in production cycles, variation performance of wastewater treatment systems in particular in responses to influent changes and changes in climate. Even in industries that operate continuous processes, maintenance operations, such as back-washing of filters, cause peaks in effluent constituent concentrations and volumes (US-EPA, 1991).

Data from a prolonged monitoring programme, where seasonal fluctuations are already included, are of special interest. However, too old data may not be representative of the risk management measures and operating conditions described in the exposure scenario. Indeed, pollution may have been reduced or increased by the implementation of risk management measures or of operation conditions, by new releases or change in release pattern.

If available, the distribution of the measured data could be considered for each monitored site, to allow all the information in the distribution function to be used. For regional PEC assessment, a further distribution function covering several sites could be constructed from single site statistics (for example, median, or 90^{th} percentile if the distribution function has only one mode), and the required 90^{th} percentile values, mean or median values of this distribution could be used in the PEC prediction. The mean of the 90^{th} percentiles of the

individual sites within one region is recommended for regional PEC determination. Care should be taken that data from several sites obtained with different sampling frequencies should not be combined, without appropriate consideration of the number of data available from each site.

If individual measurements are not available then results expressed as means and giving standard deviation will be of particular relevance. A 90th percentile concentration may also be calculated. In most instances a log-normal distribution of concentrations can be assumed. If only maximum concentrations are reported, they should be considered as a worst-case assumption, providing they do not correspond to an accident or spillage. However, use of only the mean concentrations can result in an underestimation of the existing risk, because temporal and/or spatial average concentrations do not reflect periods and/or locations of high exposure.

For intermittent release scenarios, even the 90-percentile values may not properly address release episodes of short duration but of high concentration discharge. In these cases, mainly for PEClocal calculations, a more realistic picture of the release pattern can be obtained from the highest value of average concentrations during release episodes.

When considering data about dilution, it should be taken into account that flow rates of receiving waters are typically highly fluctuating. In this case, the 10th percentile, corresponding to the low flow rate, should always be used. If only time averaged flow rates are available, the flow rate for dilution purposes should be estimated as one third of the average.

When releases of a substance from waste treatment or disposal stages are significant, measured data may be important along with model calculations in the assessment of the release of the substance from the waste life stage. Besides measured data on concentrations in leachate and landfill gases it is important that flows of water and, when appropriate, gases and solids, from principal treatment or disposal processes and facilities are measured to obtain flow-weighted concentrations. As a surrogate and complement, average time trend data on real runoff or landfill gas production data can also be used to extend flux measures to long-term estimates. Release data of higher quality may be available in the European Pollutant Release and Transfer Register (E-PRTR)[18].

However, for release scenarios from waste disposal operations including landfills, the measured concentration may underestimate the environmental concentration that might occur once a substance has passed through all the life-cycle stages including the possible time lags. In selecting representative data for waste related releases, consideration should be given to the question whether or not production/import of the substance is in steady state with the occurrence of substance in the waste streams and/or releases from waste treatment and/or releases from landfills.

In a similar manner, if the amount of a substance in use in the society in long-life articles has not reached steady state and the accumulation is ongoing, only a calculated PEC will represent a non-steady-state. Representative and reliable measured data from monitoring programmes or from literature should be compiled as tables and annexed to the risk assessment report. The measured data should be presented with the relevant contextual information in the following manner:

Table 15: Table for presenting data

Location	Substance	Concentration	Period	Remark	Reference
Country – location	substance or metabolite	Units: [µg/L], [ng/L] [mg/kg], etc Data - mean	month, year	limit of quantitation (LOQ) relevant information	Literature reference

[18] http://prtr.ec.europa.eu/

		- average - range - percentile - daily - weekly - monthly - annual - etc.		on analytical method analytical quality control	

Concentrations can be measured in the receiving environment or in the release. If the reported concentration has been measured directly in the release, this should be clearly indicated in the reporting table.

Outliers

Outliers can be defined as unexpectedly high or low values. Outliers may reflect:

- sampling or analytical flaws;
- other errors (e.g. in data capture or treatment);
- random variability;
- accidental, increased or new release, a recent change in release pattern or a newly discovered occurrence in a specific environmental compartment.

Sampling or analytical errors could potentially be demonstrated after quality check of the sampling and analytical methodologies (see previous section). Data with evident mistakes (e.g. wrong units, errors in data capture, etc.) should be discarded or corrected. Measured concentrations caused by an accidental release should not be considered in the exposure estimation.

Outliers are, by definition, infrequent and implausible measurements, i.e. unlikely to be explained by the random variability of the data alone. The probability of deviation of a measurement from the rest of the measurements due to random variability of the data can be quantified assuming a statistical distribution of the data (e.g. using the Grubbs' test (Grubbs, 1969)). But simpler empirical criteria may also be applied to detect outliers[19] (EC, 1999; USEPA (2006)).

Where outliers have been identified their inclusion/exclusion should be discussed and justified. The data should be critically examined with regard to the possible explanations listed above. Extreme values may reflect an actual sudden increase of releases, discharges or losses of the substance, and this should of course be considered in the assessment.

Treatment of measurements below the limit of quantification

A commonly encountered problem when working with monitoring data is the use of concentrations below the LOQ of the analytical method. At very low concentration levels, random fluctuations become preponderant and the uncertainty of the measurement is significantly high. Clearly at concentrations approaching the LOQ of an analytical method, percentage errors will be greater than at higher concentrations.

All measurements below the LOQ constitute a special problem and should be considered on a case-by-case basis. It should be checked first that the matrix analysed is the most appropriate (e.g. hydrophobic substances should be analysed in sediment or biota rather than in water) and that the analytical technique being used is suitable and sensitive enough (EC, 2009a). In the absence of adequate method of analysis for the substance or in case of substances that are toxic in extremely low concentrations, one approach that could be considered would be to use a value corresponding to LOQ/2 (EC, 2009b). As this method could heavily influence the assessment (e.g. when calculating a mean or a standard

[19] For example the following approach may be used: $log(X_i) > log(p_{75}) + K(log(p_{75}) - log(p_{25}))$ Where X_i is the concentration, above which a measured value may be considered an outlier, pi is the value of the ith percentile of the statistic and K is a scaling factor. This filtering of data with a scaling K = 1.5 is used in most statistical packages, but this factor can be subject dependent.

deviation), other methods may also be considered (e.g. assuming same distribution of data below and above the LOQ) (EC, 1999).

Data comparability

Another important point to check is the comparability of the data. For example, the concentrations in water may either reflect total concentrations or dissolved concentrations according to the sampling and preparation procedures used. The concentrations in sediment may significantly depend on the content of organic carbon and particle size of the sampled sediment. The soil and sediment concentrations should preferably be based on concentrations normalised for the particle size (i.e. coarsest particles taken out by sieving).

Samples of living organisms (= biota) may be used for environmental monitoring. They can provide a number of advantages compared to conventional water and sediment sampling especially with respect to sampling at large distances from a release source or on a regional scale. Furthermore they can provide a PEC_{biota} and consequently an estimation of the body burden to be considered in the food chain. But concentrations in biota can vary depending on species (mainly because of different feeding habits and different metabolic pathways) and on other factors such as age, size, lipid content, sex, season etc. These pieces of information should be considered carefully before comparing or aggregating measured concentrations in biota. For instance, normalisation for the lipid content is a common practice when working with monitoring data in biota. Please refer also to the Commision's Guidance on chemical monitoring of sediment and biota under the Water Framework Directive[20] available at http://ec.europa.eu/environment/water/water-framework/facts_figures/guidance_docs_en.htm (Guidance document No 25).

2.4.2 Allocation of the measured data to a local or regional scale

Concentrations measured in the receiving environment should be allocated to a local or regional scale in order to define the nature of the environmental concentration that is derived. If there is no spatial proximity between the sampling site and point sources of release (e.g. from rural regions), the data represent a regional concentration (PECregional) that has to be added to the calculated PEClocal. If the measured concentrations reflect the releases into the environment through point sources, they are of a PEClocal-type. In a PEClocal based on measured concentrations, the regional concentration (i.e. PECregional) is by definition already included.

2.5 Decision on the environmental concentration used for risk characterisation

When PECs have been derived from both measured data and calculation, they are compared. If they are not of the same order of magnitude, analysis and critical discussion of divergences are important steps for developing an environmental risk assessment. The following cases can be distinguished:

- Calculated PEC ≈ PEC based on measured concentrations

  The result indicates that the most relevant sources of exposure were taken into account. For risk characterisation, the value with the highest confidence should be used;

- Calculated PEC > PEC based on measured concentrations

  This result might indicate that relevant elimination processes were not considered in the PEC calculation or that the employed model was not suitable to simulate the real environmental conditions for the regarded substance. On the other hand measured data may not be reliable or represent only the background concentration or PECregional in the regarded environmental compartment. If the PEC based on

[20] Directive 2000/60/EC of the European Parliament and of the Council of 23 October 2000 establishing a framework for Community action in the field of water policy.

measured data has been derived from a sufficient number of representative samples then they should override the model predictions. However if it cannot be demonstrated for the calculated PEC that the scenario is not unrealistically worst-case, the calculated PEC should be preferred;

- Calculated PEC < PEC based on measured concentrations

  This relation between calculated PEC and PEC based on measured concentrations can be caused by the fact that relevant sources of emission were not taken into account when calculating the PEC, or that the used models were not suitable. Similarly, an overestimation of degradation of the compound may be the explanation. Alternative causes may be spillage, a recent change in use pattern or emission reducing measures that are not yet reflected in the samples.

If it is confirmed that the PEC based on measured concentrations is still representative for the exposure situation of the substance further work is needed to elucidate the exposure situation. Other reasons might cause the described divergence:

- there is a transboundary influx;
- a natural source exists;
- the compound represents a metabolite of another substance;
- a retarded remobilisation results from a pool present in other environmental compartments (e.g. from scrap or waste materials or former applications).

If the measured values have passed the procedure of critical statistical and geographical evaluation, a high degree of confidence can be attributed to those data and they must overwrite the calculated PECs. It is necessary to consider all environmental compartments when the measurements and predictions are made otherwise the possibility of chance agreement may be overlooked.

2.6 Marine exposure risk assessment

2.6.1 Introduction

While the approaches to the exposure assessment for the marine compartment must conform to EC requirements for assessment under the Directive 67/548, the REACH Regulation and the BPR, they must also recognise the objectives established by OSPAR policy. The approaches will be guided and implemented, therefore, in accordance with the EU policy under the above legislation as well as taking into account the OSPAR Strategy on Hazardous Substances. With respect to the OSPAR strategy the assessment should specifically contribute to the identification of the sources of release for a chemical and their relative significance in order to facilitate the eventual preparation of measures that substantially, effectively and proportionately reduce the exposure.

The concepts and methodologies for the inland environment have largely been developed with the local and regional spatial scales in mind, rather than the potential for global impact. There are, therefore, additional concerns for the assessment of the marine environment, which may not be adequately addressed by the methodologies used for the inland environmental risk assessment. These are:

a. the concern that hazardous substances may accumulate in parts of the marine environment and that:

   (i) the effects of such accumulation are unpredictable in the long-term;

   (ii) that such accumulation would be practically difficult to reverse;

b. the concern that remote areas of the oceans should remain untouched by hazardous substances resulting from human activity, and that the intrinsic value of pristine environments should be protected.

Of these additional concerns above, the concern stated under "a" may be seen as the main

concern. This is characterised by a spatial and temporal scale not covered by the inland risk assessment approach. It is a concern that chemical substances which can be shown both to persist for long periods and bioaccumulate in biota, can give rise to toxic effects after a greater time and at a greater distance than chemicals without these properties. While this is also true for the freshwater environment, the additional concern in the marine environment is that once the chemical has entered the open seas, any cessation of emission will not necessarily result in a reduction in chemical concentration and hence any effects become difficult to reverse. Equally, because of the long-term exposures and long-life-cycle of many important marine species, effects may be difficult to detect at an early stage.

To meet these concerns, which principally relate to substances that are considered as PBT, or have other properties which give rise to a similar level of concern, an assessment approach will be detailed that will give special consideration to this new protection goal. In this context, the assessment of risk fulfils specifically the purpose of determining what are the sources, routes and pathways to the marine environment. This assessment will facilitate in the subsequent risk management decisions on which measures are the most effective in order to reduce the levels.

2.6.2 Measured data

Guidance on the use of measured data in inland environment also applies to the marine environment. Please refer to **section 2.4** of this guidance.

2.6.3 Partition coeffitients

Specific information on the derivation of the partitioning processes between air-aerosol, air-water, and solids-water in the various compartments can be found in **section 2.3.5** of this guidance. This section only highlights some specific issues related to the marine environmental conditions.

Measured partition coefficients between water and a second compartment, if available, are usually derived from studies using non-saline water (freshwater or distilled/deionised water). In the absence of measured data, the relevant partition coefficients must be extrapolated from the primary data listed in **section 2.3.2** of this guidance. However, the techniques that allow such an extrapolation are also largely based on freshwater data sets. Therefore, to assess the distribution of chemicals in the marine environment, it is necessary to consider the extent to which partition coefficients may differ between seawater and freshwater.

The ionic strength, composition, and pH of seawater, compared with freshwater, have potential effects on the partitioning of a chemical with other compartments. To a large extent, these effects are associated with differences in water solubility and/or speciation of the chemical, compared with freshwater. The relatively high levels of dissolved inorganic salts in seawater generally decrease the solubility of a chemical (referred to as 'salting-out'), by about 10-50% for non-polar organic compounds but by a smaller fraction for more polar compounds (Schwarzenbach et al., 1993). A recent review found a typical reduction factor of 1.36 (Xie et al., 1997).

For non-ionisable organic substances, the decreased solubility in seawater, compared with freshwater, is expected to result in proportional increases in the partition coefficients between water and octanol, organic carbon and air. However, considering the uncertainty in measured partition values and the uncertainty associated with the frequent need to predict some or all of the partition coefficients, the differences attributable to the seawater environment (less than a factor of 2) are unlikely to be significant in risk assessment. Thus, unless measured seawater data of equal reliability are available, freshwater data can be used for non-ionisable organic compounds without adjustment for the marine environment.

For ionisable organic compounds, as for freshwater, the pH of the environment will affect the water solubility and partitioning of the substance. There is some evidence that the degree of dissociation may also be directly affected by the ionic strength of seawater (Esser and Moser, 1982). However, the resulting shift in the dissociation curve is relatively small

compared with that which can occur due to pH for substances with dissociation constants close to the marine water pH. It may, therefore, be preferable to obtain realistic measurements by use of seawater instead of deionised water. Another option is to measure the log K_{ow} dependency of the pH directly (cf. the new draft OECD guideline 122 "Log K_{ow} pH-metric method for ionisable substances" (OECD, 2000g). Because the pH of seawater (approximately 8) tends to be more constant than that of freshwater, the procedure to correct partition coefficients for ionisable substances, as described in **section 4.5.3** of this Guidance, may however be considered sufficiently reliable for marine conditions.

For inorganic chemicals such as metals, the form or speciation of the substance can be directly affected by the ionic composition of seawater, which may have a considerable influence on both solubility and partitioning. On a case-by-case basis, there may be sufficient information available to allow the relevant partition coefficient in seawater to be calculated from the freshwater data; otherwise, measurements under marine conditions may be necessary.

2.6.4 Marine degradation

2.6.4.1 Abiotic degradation

Abiotic degradation (i.e. hydrolysis and photolysis) in marine environments should be assessed in a similar manner to abiotic degradation in freshwater environments except that the different physico-chemical conditions in marine environments should be taken into account. In particular the stable pH of about 8 and the generally lower temperature of in average 9 °C (282 K) should be considered.

2.6.4.2 Biotic degradation

The rate of biodegradation in the various marine environments depends primarily on the presence of competent degraders, the concentration and the intrinsic properties of the chemical in question, the concentration of nutrients and organic matter and the presence of molecular oxygen. These factors vary significantly between various marine environments.

In estuarine environments, the supply of xenobiotics, nutrients and organic matter is much higher than in more distant marine environments. These factors enhance the probability that biodegradation of xenobiotics occurs with a greater rate in estuaries than is the case in more distant marine environments. Furthermore, estuarine and coastal environments are often turbulent and characterised by a constant sedimentation and re-suspension of sediment particles including microorganisms and nutrients, which increase the biodegradation potential in these environments compared to marine environments with a greater water depth. The presence of suspended particles and surfaces for attachment may favour the degradation of xenobiotics in estuarine environments.

ECETOC (1993) reviewed existing biodegradation data for the marine environments. They showed that the biodegradation in estuaries was approximately a factor 4 lower than in freshwater environments for a variety of substances: Linear Alkylbenzene-Sulfonates, Linear Alkyl-Ethoxylates, m-cresol, chlorobenzenes, p-nitrophenol glutamate, hexadecane, and methylparathion. However, for substances known to be very rapidly biodegradable (such as sodium acetate, sodium benzoate and sodium dodecylsulphate), the rates were similar in estuarine and freshwater environments. In this section the average degradation potential in estuarine environments is assumed to be similar to the degradation potential in freshwater environments.

Further away from the land-based sources of xenobiotics and allochthonous material the conditions for microorganisms are less favourable than close to land. The adaptation pressure is low due to much lower concentrations of xenobiotics as a result of degradation and dilution. Moreover, the environment can in general be characterised as oligotrophic, and the concentrations of nutrients and organic matter are lower than in marine environments closer to land. Because of their low concentrations, the xenobiotics are hardly degraded as primary substrates, and due to the relatively low microbial activity, the degradation of

xenobiotics as secondary substrates is assumed to be limited. This implies that the degradation potential in distant marine environments is anticipated to be much lower than the degradation potential in estuaries.

A special case is areas with offshore-based sources as, e.g., oil platforms. It may be assumed that the microorganisms associated with the sediment may be more or less adapted to degradation of chemicals that are continuously emitted from these sources. However, several factors, like e.g. nutrient limitation, may limit the biodegradation potential compared to the situation close to land. Furthermore, microorganisms in the water column will to a large extent drift with the currents and, therefore, a development of stable communities of competent degraders is impeded.

Most marine sediments are anaerobic below the upper 0-5 mm. The assessment of the biodegradation in marine sediments should ideally be based on results from investigations simulating these conditions. If not available, other approaches may be used, e.g.:

- an approach similar to the one used for freshwater sediments could be used, i.e. to use a scenario consisting of a 30 mm thick sediment layer of which the upper 3 mm are considered aerobic and the remaining part anaerobic. If separate degradation rates are available for aerobic and anaerobic sediment, these could be used for estimating the half-life. If only data on aerobic degradation in sediment (or soil) is available, no degradation in the anaerobic compartment should be assumed and consequently, a 10 times longer half-life than the half-life in aerobic sediment (or soil) should be used.
- anaerobic screening tests may be performed using a sediment inoculum (Horowitz et al., 1982; Madsen et al., 1995), and the observed biodegradability may then be used as an indication of the potential biodegradability of the substance in anaerobic sediment. Degradation rates should be derived by expert judgement.

if no degradation data from studies with sediment or soil are available, the use of data on degradation in water could be considered. The degradation potential in the upper aerobic sediment layer is generally assumed to be similar to the degradation potential in the overlying water. However, the possible very low bioavailability in the sediment of highly hydrophobic and/or poorly water-soluble substances should be taken into consideration as is done also for freshwater sediments.

2.6.4.3 Marine biodegradation simulation tests

As a general rule, degradation rates or half-lives determined in tests simulating the conditions in the actual aquatic environment should be considered for use whenever available. Expert judgement of the validity and quality of the test data is necessary. The origin (e.g. relevance of sampling site) of the seawater/sediment inoculum must always be evaluated in connection with assessment and use of simulation test results. Biotransformation (identification of metabolisation pathways and major metabolites) and mineralisation data may be derived from one of the standardised simulation tests (OECD 309 or OECD 308) by using samples from the particular environment as inoculum. Nevertheless, data from anaerobic screening tests conducted with digested sewage sludge cannot be used for predicting the degradation potential in sediments.

2.6.4.4 Use of biodegradation screening test data

When only results from marine or freshwater biodegradation screening tests are available, it is recommended to use the default mineralisation half-lives for the pelagic compartment as specified in **Table 16**.

Table 16: Recommended mineralisation half-lives (days) for use in marine risk assessment when only screening test data are available

	Freshwater 1)	Estuaries 4)	Other marine environments 5)
Degradable in marine screening test	not applicable	15	50
Readily degradable [2)]	15	15	50
Readily degradable, but failing 10-d window	50	50	150
Inherently degradable [3)]	150	150	∞
Persistent	∞	∞	∞

Notes on Table 16:

1) Half-lives from **Table 5**

2) Pass level >70% DOC removal or > 60% ThOD in 28 days. Not applicable for freshwater.

3) A half-life of 150 days may be used only for those inherently degradable substances that are quickly mineralised in the MITI II or the Zahn Wellens Test. The half-life of 150 days is not fully scientifically justifiable, but reflects a "guesstimate consensus" between a number of experts.

4) Also including shallow marine water closest to the coastline

5) The half-lives mentioned under this heading are only added for the sake of completeness, they are only to be used in case a regional assessment (coastal model) is conducted as described in **section 2.6.6** of this guidance.

The half-lives for the marine environments that are described in **Table 16** are provisional recommendations, which should be reconsidered, when sufficient data for degradation of different substances in screening tests and simulation tests have been evaluated. The basis for the recommendation is the assumption that the degradation of xenobiotics in freshwater and estuarine waters in general can be described by similar degradation rates, whereas the degradation rates are lower in other marine environments more distant from the coastline (Here the half-life is suggested to be increased by a factor of three relative to estuaries for readily biodegradable substances and even more for more slowly degradable substances, see **Table 16**).

2.6.5 Local assessment

2.6.5.1 Introduction

Usually releases to the environment stem from a point source leading to a locally high environmental concentration of the substance. The highest risk resulting from discharges, emissions and losses of a chemical into the environment is expected to be at this local scale close to the point of emission. It should be recognised that this might not always be the case and that other local high concentrations can arise some distance from the point of an emission due to marine currents, transport and deposition of sediments etc. Where this is considered possible for a local emission, specific modelling or measurements may be necessary. Since the aquatic concentrations are highest at the point of emission, risks may be adequately assessed, at this local scale, using the existing methodologies.

In addition to the inland sources of emission, there may also be direct discharges to the marine environment. Thus, releases can occur from point sources:

- to estuaries, either by direct discharges or from inland sources via riverine inputs (or both);
- to coastal areas;
- to harbour areas from port activity and shipping;
- to open sea e.g. from offshore oil and gas installations and from ships;

- atmospheric deposition.

2.6.5.2 Calculation of PEClocal for the aquatic compartment

In the current procedure of inland environmental risk assessment, the use of marine exposure scenarios had become necessary whenever site-specific assessments were performed for a large number of industrial sites, of which some actually discharge directly to the sea. A risk assessment for the marine environment on a local scale was therefore only performed for specific sites identified as releasing directly into the sea. In the context of a dedicated methodology for marine risk assessment, a more generic exposure assessment for any given use is necessary.

While in some countries with long coastlines, the number of industrial sites discharging wastewater to the sea is low compared with the overall number of sites (e.g. 5 – 10% in France; IFEN, 1997), it can be very high in others (e.g. 58 % in Sweden; SCB, 2000). It is therefore assumed that for all uses of a given chemical substance, potential local releases to the marine environment can occur and, hence, it is necessary to perform a generic local exposure assessment for the local marine environment.

As for inland risk assessment, the calculation of the PEClocal depends mainly on two parameters: dilution and the presence (or absence) of a STP. Both of these parameters have large influences on the local concentration ($C_{local, seawater}$).

Regarding the presence or absence of a STP, conflicting information is available. Experience with the risk assessment of substances has shown that for chemical processing sites located on the coast, the probability that the effluents are treated in a biological treatment plant is much lower than for sites situated in land (see e.g., risk assessment reports for acrylonitrile, cyclohexane or methylene dianiline). This is confirmed by a survey performed by HELCOM (1998). While most industrial effluents from sites located on the Baltic Sea coast were treated (up to 98 %), the report did not contain detailed information on the treatment used from all contracting parties of HELCOM.

However, from the data compiled in Sweden it appears that less than 50% of the industrial wastewater discharged passes a biological treatment step. On the other hand, statistics regarding treatment of municipal wastewater show that the treatment rate of municipal wastewater from coastal municipalities is not different from overall treatment rates (e.g. IFEN, 1997; HELCOM, 1998). On the other hand, four EU Member States have applied Article 6 of Directive 91/271 allowing them to declare marine areas non sensitive to urban wastewater meaning that they don't have to treat the wastewater biologically but only mechanically.

It is therefore proposed, for a default assessment, that in a local setting, industrial effluents (which may have been subject to some treatment on-site) are not treated in a municipal biological STP. It is recognised though that the situation regarding the treatment of industrial effluents is evolving rapidly and the present scenario could be revised in the near future. When there is specific information available for a certain site that specific treatment facilities are available this information needs to be assessed and can be used to override the default assumption. In practice this information is often available for production and/or large processing sites. It may also be possible to assume the presence of connection to an STP for certain industry and/or use categories if appropriate justification about the general connection frequency to the STP for that specific industry is provided. For releases to municipal wastewater of substances that are used for private or public use (substances belonging to IC5 and IC6, **Appendix 6**), however, it can be assumed that the degree of treatment in a biological STP corresponds to the inland scenario (see **section 2.3.7.1** of this guidance).

For discharges to a coastal zone, local dilution will be greater than in a freshwater river. First, initial dilution may occur if the density between the effluent and the saline receiving medium differs (Lewis, 1997). The initial dilution factor is usually around 10. Further dilution due to currents can also be assumed, particularly if the point of release is subject to tidal influences. In the Baltic or the Mediterranean sea, where there are almost no tidal

influences compared to the Atlantic Ocean or the North Sea, only initial dilution may occur on calm days, but normally, further dilution due to currents is probable. Dilution factors of more than 500 have been determined from model simulations (based on current measurements) in the North Sea, 200 m away from the discharge point (e.g. Pedersen et al., 1994).

A dilution factor for discharges to a coastal zone of 100 may then tentatively be assumed, which seems to be representative of a realistic worst case. The same estimation method as for inland exposure assessment can then be used to obtain the local concentration in seawater ($C_{local,\ seawater}$, see **section 2.3.7.3**; **Equation 46 –Equation 50** of this guidance).

In certain circumstances, it may be possible to identify specific emission points which would allow the use of more precise information regarding the available distribution and fate processes. Such "site-specific" assessments should only be used when it is known that all the emissions emanating from the particular point in the life-cycle, e.g. manufacture, arise from a limited number of specific and identifiable points. In these circumstances each specific point of release will need to be assessed individually. If it is not possible to make this judgement, then the default assumptions should be applied. In "site-specific" assessments, due account can be taken of the true dilution available to the given emission as well as the impact of degradation, volatilisation, etc. in the derivation of the PEC. Normally, only dilution and adsorption to suspended sediment need be considered but site-specific conditions may indicate that valid local distribution models can be used.

For estuaries, which are influenced by currents and tidal movements, it is assumed as a first approach that they are covered by either the inland or the marine risk assessment. Thus, no specific assessment is proposed. Then, the local concentration in seawater can be obtained with:

$$Clocal_{seawater} = \frac{Clocal_{eff}}{(1 + Kp_{susp} \cdot SUSP_{water} \cdot 10^{-6}) \cdot DILUTION}$$

Equation 83

Explanation of symbols

$C_{local,\ eff}$	concentration of the substance in the STP effluent	[mg · l^{-1}]	**Equation 36**
$K_{p,\ susp}$	solids-water partition coefficient of suspended matter	[l · kg^{-1}]	**Equation 26**
$SUSP_{water}$	concentration of suspended matter in the seawater	[mg · l^{-1}]	15
DILUTION	dilution factor	[-]	100
$C_{local,\ seawater}$	local concentration in seawater during emission episode	[mg · l^{-1}]	

$K_{p,\ susp}$ is derived as for inland risk assessment. For a specific estimation of the partitioning behaviour of substances in seawater environments see **section 2.6.3** of this guidance.

It is recognised that the dilution available to a discharge will also be related to the actual volume of that discharge. In the freshwater scenario, this discharge volume is standardised to a volume of 2,000 m^3/day i.e. the outflow from a standard STP. It is therefore proposed that the discharge volume to the marine environment is also normalised at 2,000 m^3/day such that the quantity of the substance discharged (in kg/day) is assumed, for modelling purposes, to be diluted into this volume prior to discharge.

For indirect human exposure and secondary poisoning, an annual average concentration in seawater is calculated:

$$Clocal_{seawater,ann} = Clocal_{seawater} \cdot \frac{Temission}{365}$$ **Equation 84**

Explanation of symbols

$C_{local,\ seawater}$	local concentration in seawater during emission episode	[mg · l^{-1}]	**Equation 82**
$T_{emission}$	number of days per year that the emission takes place	[d · yr^{-1}]	
$C_{local,\ seawater,ann}$	annual average local concentration in seawater	[mg · l^{-1}]	

The concentration at the regional scale ($PECregional_{,seawater}$) is used as background concentration for the local scale, if the exposure assessment is preformed using the tonnage based approach. Therefore, these concentrations are summed:

$$PEClocal_{seawater} = Clocal_{seawater} + PECregional_{seawater}$$ **Equation 85**

$$PEClocal_{seawater,ann} = Clocal_{seawater,ann} + PECregional_{seawater}$$ **Equation 86**

Explanation of symbols

$Clocal_{,\ seawater}$	local concentration in seawater during episode	[mg · l^{-1}]	**Equation 82**
$Clocal_{,\ seawater,ann}$	annual average concentration in seawater	[mg · l^{-1}]	**Equation 83**
$PECregional_{,seawater}$	regional concentration in seawater	[mg · l^{-1}]	
$PEClocal_{,seawater}$	predicted environmental concentration during episode	[mg · l^{-1}]	
$PEClocal_{,seawater,ann}$	annual average predicted environmental concentration	[mg · l^{-1}]	

If relevant site-specific information is available, it can be used to improve the assessment. Some significantly different exposure situations need to be reviewed though:

- substances released from offshore platforms. A harmonised mandatory control system for the use and reduction of the discharge of offshore chemicals is already agreed within OSPAR (OSPAR, 2000a; 2000b). For this specific exposure situation within the EU legislation, the methodology proposed by OSPAR can be taken into consideration[21];
- substances released from harbours, marinas, fish farms and dry-docks. Specific scenarios will have to be developed for these situations, which are most relevant for biocides.

2.6.5.3 Calculation of PEClocal for the sediment compartment

The concentration in freshly deposited sediment is taken as the PEC for sediment; therefore the properties of suspended matter are used. The concentration in bulk sediment can be derived from the corresponding water body concentration, assuming a thermo-dynamic

[21] The methodology for assessing releases from platforms (e.g. CHARM-model) that has been developed in the context of these OSPAR decisions was not re-discussed in the context of the development of the present guidance document for marine risk assessment.

partitioning equilibrium (Di Toro et al., 1991):

$$PEClocal_{sed} = \frac{K_{susp-water}}{RHO_{susp}} \cdot PEClocal_{seawater} \cdot 1000$$ Equation 87

Explanation of symbols

$PEClocal_{seawater}$	concentration in seawater during emission episode	[mg · l^{-1}]	
$K_{susp-water}$	suspended matter-water partition coefficient	[m^3 · m^{-3}]	**Equation 27**
RHO_{susp}	bulk density of suspended matter	[kg · m^{-3}]	**Equation 20**
$PEClocal_{sed}$	predicted environmental concentration in sediment	[mg · kg^{-1}]	

Highly adsorptive substances may not be considered adequately with the approach described above, as they are often not in equilibrium distribution between water and suspended matter because of their cohesion to suspended matter; however they may be desorbed after ingestion by benthic organisms.

Suspended matter exposed to local releases can subsequently be transported over long distances and deposited to sediment in distant areas. Therefore, it is possible that areas unrelated to local settings are exposed to the same sediment concentrations as would be expected only in the immediate vicinity of the releases. This has especially to be taken into account when comparing measured concentrations to estimated concentrations.

2.6.6 Regional assessment

For the release estimation of substances, a distinction is usually made between substances that are emitted through point sources to which specific locations can be assigned, and substances that enter the environment through diffuse releases.

Point source releases may have a major impact on the environmental concentration on a local scale (PEClocal) and contribute to the environmental concentrations on a larger scale (PECregional). Like with the freshwater environment for the marine situation it is necessary to evaluate the impact of substances that are released from point and diffuse sources over a wider area. The PECregional is supposed to take into account the further distribution and fate of a chemical upon release. The resulting PECregional is assumed to be a steady-state concentration of the substance.

The regional system for the freshwater environment is a relatively large area of 200 by 200 km which consists of 97% of soil and 3% of water. This system is surrounded by a larger area of the size of Europe, called the continent (see **section 2.3.7.7**). If for the marine region an area of similar size would be chosen where the water of the freshwater region would enter into, the resulting concentrations would be around 0.1% of the freshwater concentrations, mainly due to the dilution of the freshwater in the much larger seawater region.

To assess the potential impacts of multiple points and diffuse sources of substances on the marine environment a river plume in coastal seawater is considered as a marine regional generic environment as follows: An area of coastal sea that receives all the water from the rivers from the regional system.

This seawater compartment is exchanging chemical with the continental seawater compartment by dispersion and advection (a current of seawater flowing in a certain direction). The size of the coastal compartment is 40 km long, 10 km wide and 10 m deep. In addition to the input from the regional river water it receives 1% of the direct emissions from the inland sources which is supposed to represent a relevant fraction of the sources

that are located near the sea and also have direct emissions into the sea compartment.

Most of the relevant characteristics of the coastal compartment are similar to the freshwater compartment apart from the suspended matter concentration that is set to 5 mg/l. In the absence of specific information (e.g. from marine simulation tests) it is assumed that the biodegradation rate in the water column is approximately three times lower than in freshwater. This scenario is shown in **Figure 15** below.

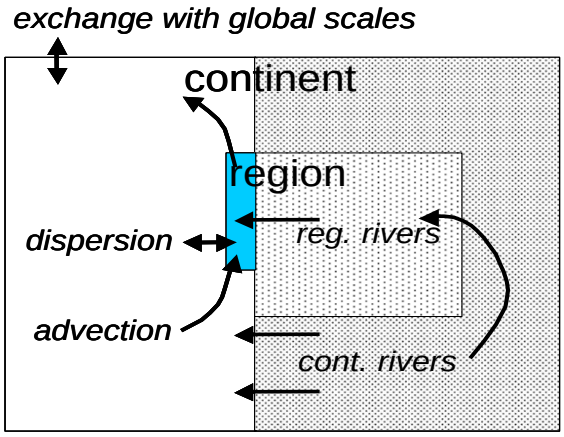

Figure 15: Coastal sea scenario

This scenario can be modelled with the multi-media fate model that is used for the freshwater PEC calculations, modified to allow dispersive exchange between the coastal zoneand the continental seawater. By default, mixing of river water into the coastal sea gives a dilution factor of approximately 10. As a result concentrations in coastal seawater are expected to be a factor of 10 (for conservative chemicals) or more (for chemicals that react, volatilize or sediment) lower than in river water. The extent of degradation, volatilization, etc. in this coastal sea scenario is adequately modeled using the multi-media model.

More details on the features of these models can be found in the section on calculation of PECregional for the freshwater environment (**section 2.3.7.7** of this guidance.)[22].

The calculation of PECregional according to this scenario provides the results for the risk assessment that is necessary for the evaluation for active substances. Sufficient information on sources and emissions and site-specific information on the suspended matter concentration, the flow rate and the dispersion velocity may be available so the generic

[22] A default length: width ratio of the coastal marine compartment has been set at 4:1. Assuming that this reflects the plume shape in the generic assessment situation, this implies a ratio between the advective sea current along the coast and the dispersive transport velocity perpendicular to that. If, in addition to the compartment dimensions, a value is chosen for the sea current, the value of the lateral dispersion coefficient follows, or *vice versa*. If then a value for the freshwater discharge into the coastal marine compartment is set too, mixing of freshwater with coastal seawater is determined completely. In the generic regional model the river discharges approximately 1000 m^3/s into the continental model. With the dimensions of the sea compartment set to 40,000 m·10,000 m·10 m, and a suggested default value for the sea current of 0.03 m/s, taking into account the necessary dispersion coefficient of 50 m^2/s, the freshwater content of the seawater inside the selected box would become approximately 10%.

It should be noted that river water plumes in coastal waters vary greatly with local conditions (river flow, sea current, tide, depth, etc.). Prediction of site-specific dilution of river water into coastal seawater requires site-specific knowledge of flows and salinity distributions. Rhine and Meuse waters (2,000 m^3/s) are known to mix with a sea current of 0.035 m/s in the southern North Sea, yielding a very long-streched plume with approximately 20% river water in the first 10 km of the coast. A dispersion coefficient of 20 m^2/s adequately describes this situation. The Amazon River is known for its great plume.

assessment can be made more site-specific by overriding some of the default parameters or even can be replaced by site-specific models. The dispersion velocity greatly affects all calculated concentrations, while in addition the suspended matter content further affects the dissolved concentration in seawater for chemicals with high log K_{ow}. For the marine environment, models are available that can be used to assess the concentrations in certain specific compartments (bays, estuaries, regions) of the marine environment to which specific industrial sites discharge wastewater.

3. Effects and hazard assessment

3.1 Introduction

The environmental effect and hazard assessment is a required step in the risk assessment. It is based on information to be submitted as detailed in *Guidance on the Biocidal Product Regulation: Volume IV Environment, Part A Information Requirements* on:

- physical and chemical data;
- fate and behaviour in the environment (including degradation and mobility);
- effects on aquatic organisms (including sediment-dwellers);
- effects on terrestrial organisms (including mammals and birds).

Using the data above, a PNEC has to be derived for all relevant environmental protection targets as listed in **Table 1**.

A PNEC is regarded as a concentration below which an unacceptable effect will, most likely, not occur.

For the different compartments and organims, a PNEC is derived that, if not exceeded, ensures protection of the environment represented by that compartment. Certain assumptions are made concerning the aquatic and terrestrial environment which allow for an extrapolation from single-species toxicity data to potential effects on the ecosystem. It is assumed that:

- ecosystem sensitivity depends on the most sensitive species groups, and;
- protecting ecosystem structure protects community function.

These two assumptions have important consequences. By establishing which species are the most sensitive to the toxic effects of a chemical in the laboratory, extrapolation can subsequently be based on the data from those species. Furthermore, the functioning of any ecosystem in which those species exist is protected provided the structure is not sufficiently distorted as to cause an imbalance. It is generally accepted that protection of the most sensitive species groups should protect structure, and hence function.

For most substances, the pool of data from which to predict ecosystem effects is limited as, in general, only single species laboratory toxicity data are available. In these circumstances, it is recognised that, while not having a strong scientific validity, empirically derived assessment factors must be used. Assessment factors have also been proposed by the US EPA and OECD (1992d). In applying such factors, the intention is to predict a concentration below which an unacceptable effect will most likely not occur. It is not intended to be a level below which the chemical is considered to be safe. However, again, it is likely that an unacceptable effect will not occur.

In establishing the size of these assessment factors, a number of uncertainties must be addressed to extrapolate from single-species laboratory data to a multi-species ecosystem. These areas have been adequately discussed in other papers, and may best be summarised under the following headings:

- intra- and inter-laboratory variation of toxicity data;
- intra- and inter-species variations (biological variance);

- short-term to long-term toxicity extrapolation;
- laboratory data to field impact extrapolation.

The size of the assessment factor depends on the confidence with which a PNEC can be derived from the available data. This confidence increases if data are available on the toxicity to organisms at a number of trophic levels, taxonomic groups and with lifestyles representing various feeding strategies. Thus lower assessment factors can be used when larger and more relevant datasets than the core data set are available. The PNECs derivation with the use of assessment factors is described in the sections below.

If a large data set from long-term tests for different taxonomic groups is available statistical extrapolation methods may be used to derive a PNEC. In general, it is assumed that sufficient test data for use of statistical extrapolation methods will only be available for relatively few substances and that these data will be primarily fresh water and in rare cases terrestrial toxicity data. Therefore, the use of statistical extrapolation methods is only described for these two environments but in case enough data are available, they may be used also for other environments.

For futher information when assigning of organisms to trophic levels see **Appendix 1**.

The following Table provides and overview of toxicity test endpoints that can be used for deriving PNEC values. In principle, the PNEC is calculated by dividing the lowest short term L(E)C50 or long term EC10/NOEC value by an appropriate assessment factor.

Short-term studies:

If a test report does not indicate the $L(E)C_{50}$ values but the raw data are presented, the $L(E)C_{50}$ should be calculated, for example by Probit analysis. If only one toxicity value lies between the $L(E)C_{0}$ and the $L(E)C_{100}$, the $L(E)C_{50}$ cannot be calculated by Probit analysis. Instead, the $L(E)C_{50}$ may be estimated by, e.g., linear regression.

If results are presented as $>L(E)C_{10}$ and $<L(E)C_{50}$, they can be rated as $L(E)C_{50}$ while results clearly above a $L(E)C_{50}$ can only be used as an indication of the short-term toxicity of the chemical considered.

Long-term studies:

The NOEC (no observed effect concentration) is defined as "the highest concentration tested at which the measured parameter shows no significant inhibition" (OECD 201, 1984a) or the test concentration immediately below the LOEC (OECD 210, 1984g). There has to be a concentration-effect relationship. The NOEC is determined directly from the concentration-effect curve by consideration of the deviation of the control (e.g. 10%) or derived on the basis of ANOVA (analysis of variance) and a subordinate test (e.g. Dunett's). An EC_{10} for a long-term test which is obtained by extrapolation using appropriate statistics (e.g. Probit analysis) can be considered as a NOEC. The choice between the NOEC or EC_x point estimates is subject of continuing debate. OECD (1998) favours the use of an EC_x. Extensive information on the implications of either choice for test set-up and statistical evaluation is given by OECD (2006). A LOEC (lowest observed effect concentration) stands for the lowest concentration where an effect has been observed. It may therefore not be used as a $NOEC/EC_{10}$. In case only a LOEC is given in the report, it can be used to derive a $NOEC/EC_{10}$ with the following procedures:

- LOEC > 10 and < 20% effect: NOEC can be calculated as LOEC/2.
- LOEC ≥ 20% effect and a distinct effect relationship: the EC_{10} is calculated or extrapolated and regarded as the NOEC.

If the effect percentage of the LOEC is unknown no NOEC can be derived. MATC (maximal acceptable toxicant concentration): In aquatic toxicity the MATC may be calculated. This is the geometric mean of the NOEC and the LOEC. If in the test report only the MATC is presented, the MATC can be divided by √2 to derive a NOEC. It should be noted that in the case of algae studies, which are actually multigeneration studies, it is generally accepted that a 72-hour (results from shorter or longer test can be used provided that all validity criteria are met) EC_{50} value may be considered as equivalent to a short-term result and that a 72-hour (or longer) $NOEC/EC_{10}$ value can be considered as a long-term result.

The assessment factor is an expression of the degree of uncertainty when extrapolating from test data to the real environment. Assessment factors applied for long term tests are smaller as the uncertainty of the extrapolation from laboratory data to the natural environment is reduced. For this reason long term data are preferred to short term data. Results from field tests or mesocosm studies can also be used to derive a PNEC on a case by case basis (**Appendix 7**).

In specific cases where it is not possible to establish a PNEC, a qualitative estimate has to be made.

If, during the transformation of the substance, relevant metabolites/transformation products are formed (see **Info-box 1**), an effect assessment for the concerned compartments will have to be carried out.

The effects and hazard assessment comprises the following steps:

- hazard identification: The aim of the hazard identification is to identify the effects of concern in the different species of each environmental compartment. For active substances and substances of concern, the aim is also to re-assess the classification and labelling of the substance. For new active substance the classification and labelling is still to be etablished;
- dose (concentration) - response (effect) assessment: The aim is to calculate the values for each endpoint tested. At this step the predicted no effect concentration (PNEC), must, where possible, be determined.
- As a new requirement under the BPR, there is need to assess if an active substance fulfills the exclusion criteria according to Article 5(1) of the BPR. PBT/vPvB criteria and endocrine disrupting properties need to be evaluated for the assessment of the exclusion criteria (see **section 3.11** of this guidance).

For the different steps of the effects assessment it is of high importance to evaluate the data with regard to their adequacy and completeness. The evaluation of adequacy must address the quality and relevance of data (see **section 3.2** of this guidance). The evaluation of data is of particular importance where non standard organisms and/or non-standardised methods are used. It is suitable to start the effects assessment process with the evaluation of the available ecotoxicological data.

The environmental compartments considered for the inland environment are the aquatic and terrestrial ecosystem, predators, microbial activity in a STP, and the atmosphere. This means that for each of these compartments a PNEC has to be derived, except for the air compartment because no standardised biotic testing systems are available at present.

In the case of the aquatic environment, a detailed description on deriving a $PNEC_{water}$ is described in **section 3.3** of this guidance. For an intermittent release of substances, aquatic organisms may be exposed for only a short period. In these cases, short-term $L(E)C_{50}$ values are considered sufficient to derive a $PNEC_{water\text{-}intermittent}$. This is described in **section 3.3.2**.

The microbial activity in domestic and industrial STPs may be affected. Assessment factors to derive a $PNEC_{stp}$ are given in **section 3.4**.

For the sediment compartment, the equilibrium partitioning method is proposed as a screening method for derivation of a $PNEC_{sediment}$. If sediment test results are available, the $PNEC_{sediment}$ is derived from these data by applying assessment factors (see **section 3.5** of this guidance).

When assessing the soil compartment, if test data are lacking, also the equilibrium partitioning method can be used to derive a $PNEC_{soil}$. If soil test results are available, the $PNEC_{soil}$ is derived from these data by applying assessment factors (see **section 3.6** of this Guidance).

Biotic and abiotic effects, such as acidification, are addressed for the atmosphere. In view of the lack of suitable data and the fact that no adequate methods are available yet to assess both types of effects, a provisional strategy is described in **section 3.7** of this guidance.

Standard assays of ecotoxicological effects usually provide information about the direct toxic effects of a substance. Chemicals showing bioaccumulation and biomagnification may pose an additional threat due to exposure of organisms higher in the food chain, e.g. top predators. This phenomenon is called 'secondary poisoning' and has to be addressed if an active substance fulfils several criteria, e.g. indication of a bioaccumulation potential. If this is the case, the oral intake of a chemical via fish or worms ($PEC_{oral,\ fish}$ and $PEC_{oral\ worm}$) is compared to a PNEC for fish- or worm-eating mammals or birds. This approach is described in **section 3.8** of this guidance.

In addition to the secondary poisoning described in the paragraph above, primary as well as secondary poisoning is also relevant for rodenticides and some insecticides via consumption of baits contaminated target organisms. For further information please refer to the PT-specific ESDs (http://echa.europa.eu/guidance-documents/guidance-on-biocides-legislation/emission-scenario-documents) and to **Appendix 5** of this guidance.

The methods presented make it possible to identify if the compartment under consideration is possibly "of concern" and whether further data, e.g. testing on relevant organisms for that compartment, should be obtained.

The environmental part of the risk assessment should contain some general reflection on the mode of action of the active substance. Cross-reference to relevant sections in the human health part may be important. For example when a chemical is found to have effects on gonad development in fish and similar effects have been observed in laboratory mammals. Identification of similarities in the nature, intensity and time scale of effects between species, as well as in the susceptibilities of different receptors, will allow a better understanding of the actual risk to these organisms to be obtained and help in the identification of issues of concern (IPCS, 2000).

3.2 Evaluation of data

3.2.1 Ecotoxicity data

As mentioned previously, during the effect and hazard assessment, it is required to evaluate data with regard to their adequacy and completeness. Details on the evaluation of completeness and adequacy of ecotoxicity data is provided in *Guidance on the Biocidal Product Regulation: Volume IV Environment, Part A Information Requirements* available at http://echa.europa.eu/web/guest/guidance-documents/guidance-on-biocides-legislation.

Info-box 6: Derivation of PNEC values

Derivation of PNEC values from studies with no effects at the highest test concentration
When there are no effects at the highest test concentration, a "≥" symbol should be used for expressing the NOEC-value. If at the highest test concentration <50% effect is observed, a ">" sign should be used to express the LC/EC50. If a PNEC value is to be derived from such a value, the assessment factor (AF) is applied to that value and the PNEC presented with the > sign. Example: LC50 >100 mg/L, and an assessment factor of 1000 gives a PNEC >0.1 mg/L. Combining this with a PEC of (e.g.) 1 mg/L, the risk quotient is represented as RQ <10. Note that in some cases it may be possible to derive an LC/EC10 from the data, which may be used for PNEC derivation instead of a NOEC.

Use of efficacy data on target species to derive a PNEC value
Information from efficacy tests can be used to define the potentially most sensitive taxonomic group, which may trigger a need for additional information. However, ecotoxicological data can only be complemented with results from efficacy tests if these fulfil the design criteria for ecotoxicity tests like those described in OECD guidelines.

3.2.2 Quantitative Structure-Activity Relationships (QSAR)

Means of obtaining reliable QSAR estimates for fish, aquatic invertebrate and algal toxicity are available for most organic chemicals. These estimates can be used to assist in data evaluation and/or to contribute to the process of deciding whether further testing is necessary to clarify an endpoint of concern and if so, to optimise the testing strategy, where appropriate. It is also a valuable tool when assessing metabolites, impurities and degradation products where no laboratory tests are available. For more details please consult *Guidance on information requirements and chemical safety assessment, Chapter R.6: QSARs and grouping of chemicals* (http://echa.europa.eu/guidance-documents/guidance-on-information-requirements-and-chemical-safety-assessment) which provides information on the use of QSAR estimates within the testing strategy for:

- predicting the toxicity of chemicals; and
- predicting long-term fish toxicity.

3.3 Effects assessment for the freshwater compartment

3.3.1 Calculation of PNEC

For the description of the PNEC derivation please see **section 3.1**.

3.3.1.1 Calculation of PNEC using assessment factors

The proposed assessment factors are presented in **Table 18**.

When only short-term toxicity data are available, an assessment factor of 1000 will be applied on the lowest L(E)C_{50} of the relevant available toxicity data, irrespective of whether or not the species tested is a standard test organism (see notes on **Table 18**). A lower assessment factor will be applied on the lowest NOEC/EC_{10} derived in long-term tests with a relevant test organism.

When for a species multiple data are available for the same endpoint, obtained in tests with similar duration, life stage and testing conditions, the endpoints rated as reliable or reliable with restrictions (Ri 1 or 2) are used to derive an aggregated endpoint per species. If they are more than one order of magnitude apart, it is necessary to look into more detail at the study reports to see whether a specific reason could explain the difference between test results. If no explanation can be found and the results are for the same species and endpoints, they can be aggregated into a geometric mean. This applies to short term test results (EC50, LC50) as well as long term test results (NOEC, EC10). Detailed guidance on the treatment of multiple data per species can be found in the Technical Guidance for deriving Environmental Quality Standards (EC, 2011; Annex 1, section A1.3.6.1).

The algal growth inhibition test of the core data set is in principle a multigeneration test. However, for the purposes of applying the appropriate assessment factors, the EC_{50} is treated as a short-term toxicity value. The NOEC/EC_{10} from this test may be used as an additional NOEC/EC_{10} when other long-term data are available. In general, an algal NOEC/EC_{10} should not be used unsupported by long-term NOEC/EC_{10} of species of other trophic levels. However, if the short-term algal toxicity test is the most sensitive of the short-term tests, the NOEC/EC_{10} from this test should be supported by the result of a test on a second species of algae. Blue-green algae should be counted among the primary producers due to their autotrophic nutrition.

The assessment factors presented in **Table 18** below should be considered as general factors that under certain circumstances may be changed. In general, justification for changing the assessment factor could include one or more of the following:

- evidence from structurally similar compounds (evidence from a closely related compound may demonstrate that a higher or lower factor may be appropriate);

- knowledge of the mode of action including endocrine disrupting effects (some substances, by virtue of their structure, may be known to act in a non-specific manner);
- the availability of test data from a wide selection of species covering additional taxonomic groups other than those represented by the core data set species;
- the availability of test data from a variety of species covering the taxonomic groups of the core data set species. In such a case the assessment factors may only be lowered if these multiple data points are available for the most sensitive taxonomic group.

Specific comments on the use of assessment factors in relation to the available data set are given in the notes on **Table 18**.

Table 18: Assessment factors to derive a PNECwater

Available data	Assessment factor
At least one short-term L(E)C$_{50}$ from each of three trophic levels (fish, aquatic invertebrate and algae)	1000 [a)]
One long-term NOEC (either fish or aquatic invertebrate)	100 [b)]
Two long-term NOECs from species representing two trophic levels (fish and/or aquatic invertebrate and/or algae)	50 [c)]
Long-term NOECs from at least three species (normally fish, aquatic invertebrate and algae) representing three trophic levels	10 [d)]
Species sensitivity distribution (SSD) method	5-1 (to be fully justified case by case) [e)]
Field data or model ecosystems	Reviewed on a case by case basis [f)]

Notes on Table 18:

a) The use of a factor of 1000 on short-term toxicity data is a conservative and protective factor and is designed to ensure that substances with the potential to cause adverse effects are identified in the effects assessment. It assumes that each of the uncertainties identified above makes a significant contribution to the overall uncertainty. For any given substance there may be evidence that this is not so, or that one particular component of the uncertainty is more important than any other. In these circumstances it may be necessary to vary this factor. This variation may lead to a raised or lowered assessment factor depending on the available evidence. A factor lower than 100 should not be used in deriving a PNEC$_{water}$ from short-term toxicity data except for substances with intermittent release (see s**ection 3.3.1.1** of this guidance).

Variation from a factor of 1000 should not be regarded as normal and should be fully supported by accompanying evidence.

b) An assessment factor of 100 applies to a single long-term NOEC (fish[25] or aquatic invertebrate) if this NOEC was generated for the trophic level showing the lowest L(E)C$_{50}$ in the short-term tests. It is further assumed that no NOEC/EC$_{10}$ for algae is available.

If the only available long-term NOEC/EC$_{10}$ is from a species (standard or non-standard organism) which does not have the lowest L(E)C$_{50}$ from the short-term tests, it cannot be regarded as protective of other more sensitive species using the assessment factors available. Thus the effects assessment is based on the short-term data with an assessment factor of 1000. However, the resulting PNEC based on short-term data may not be higher than the PNEC based on the long-term NOEC/EC$_{10}$ available.

An assessment factor of 100 applies also to the lowest of two long-term NOECs/EC$_{10}$ covering two trophic levels when such NOECs/EC$_{10}$ have not been generated from that showing the lowest L(E)C$_{50}$ of the short-term tests. This should, however, not apply in cases where the acutely most sensitive species has an L(E)C$_{50}$ value lower than the lowest NOEC value. In such cases the PNEC

might be derived by using an assessment factor of 100 to the lowest L(E)C 50 of the short-term tests.

c) An assessment factor of 50 applies to the lowest of two NOECs/EC 10 covering two trophic levels when such NOECs/EC 10 have been generated covering that level showing the lowest L(E)C 50 in the short-term tests. It also applies to the lowest of three NOECs/EC 10 covering three trophic levels when such NOECs/EC 10 have not been generated from that trophic level showing the lowest L(E)C 50 in the short-term tests. This should however not apply in cases where the acutely most sensitive species has an L(E)C 50 value lower than the lowest NOEC/EC 10 value. In such cases the PNEC might be derived by using an assessment factor of 100 to the lowest L(E)C 50 of the short-term tests.

d) An assessment factor of 10 will normally only be applied when long-term toxicity NOECs/EC 10 are available from at least three species across three trophic levels (e.g. fish[23], aquatic invertebrate, and algae or a non-standard organism instead of a standard organism).

When examining the results of long-term toxicity studies, the $PNEC_{water}$ should be calculated from the lowest available NOEC/EC 10. Extrapolation to the ecosystem effects can be made with much greater confidence, and thus a reduction of the assessment factor to 10 is possible. This is only sufficient, however, if the species tested can be considered to represent one of the more sensitive groups. This would normally only be possible to determine if data were available on at least three species across three trophic levels.

It may sometimes be possible to determine with high probability that the most sensitive species has been examined, i.e. that a further long-term NOEC/EC 10 from a different taxonomic group would not be lower than the data already available. In those circumstances, a factor of 10 applied to the lowest NOEC/EC 10 from only two species would also be appropriate. This is particularly important if the substance does not have a potential to bioaccumulate. If it is not possible to make this judgement, then an assessment factor of 50 should be applied to take into account any interspecies variation in sensitivity. A factor of 10 cannot be decreased on the basis of laboratory studies.

e) AFs of 1-2 should not normally be applied, as it will not be possible to prove that there are no remaining uncertainties (see also basic considerations and minimum requirements outlined in **section 3.3.1.2** of this guidance).

f) The assessment factor to be used on mesocosm studies or (semi-) field data will need to be reviewed on a case-by-case basis. Further information on the use of mesocosms for biocides can be found in **Appendix 7** of this guidance.

For compounds with a high log K_{ow} no short-term toxicity may be found. In these cases it may indeed be difficult to maintain the exposure concentration in the test system due to the partitioning of test substance in the test system. This may be the case also in long-term tests in which the steady state may not be reached. In fish tests for non-polar narcotics, this can be substantiated by the use of long-term QSARs (see **section 3.2.2** of this guidance and *Guidance on information requirements and chemical safety assessment Chapter R.6: QSARs and grouping of chemicals*. Use of a higher assessment factor can be considered in such cases where steady state does not seem to have been reached.

A long-term test has to be carried out for substances showing no toxicity in short-term tests if the log K_{ow} > 3 (or BCF > 100) and if the PEClocal is > 1/100th of the water solubility. The long-term toxicity test should normally be an aquatic invertabrate test to avoid unnecessary vertebrate testing. The NOEC from this test can then be used with an assessment factor of 100. If in addition to the required long-term test a NOEC is determined from an algal test of the core data set, an assessment factor of 50 is applied.

3.3.1.2 Calculation of PNEC using statistical extrapolation techniques

The effect assessment performed with assessment factors can be supported by a statistical extrapolation method if the database on SSDs is sufficient for its application. If a large data set from long-term tests for different taxonomic groups is available (OECD, 1992d),

[23] Derived from a fish early life stage (FELS) test or fish full life cycle (FFLCT) test. Under certain conditions also a fish juvenile growth test (for substances with a log K_{ow} < 5) or a fish short-term toxcitiy test on embryo and sac fry stages (for substances wit a log K_{ow} < 4) can cover long-term toxicity to fish.

statistical extrapolation methods may be used to derive a PNEC. The main underlying assumptions of the statistical extrapolation methods are as follows (OECD, 1992d):

- the distribution of species sensitivities follows a theoretical distribution function;
- the group of species tested in the laboratory is a random sample of this distribution.

In general, the methods work as follows: long-term toxicity data are log transformed and fitted according to the distribution function and a prescribed percentile of that distribution is used as criterion. Several distribution functions have been proposed. The US EPA (1985) assumes a log-triangular function, Kooijman (1987) and Van Straalen and Denneman (1989) a log-logistic function, and Wagner and Løkke (1991) a log-normal function. Aldenberg and Slob (1993) refined the way to estimate the uncertainty of the 95th percentile by introducing confidence levels.

The statistical extrapolation for regulatory purposes is still under debate and needs further validation. An advantage of these methods is that they use the whole sensitivity distribution of species in an ecosystem to derive a PNEC instead of taking always the lowest long-term NOEC. However, such methods could also be criticised. Among the most common drawbacks, the reasons put forward are: the lack of transparency by using this method compared to the standard approach, the question of representativity of the selected test species, the comparability of different endpoints, the arbitrary choice of a specific percentile and a statistical confidence level etc.

In response to these concerns it has been seen as necessary to provide some guidance on when and how to use such methods. What is proposed below has been discussed during an Expert Consultation Workshop on Statistical Extrapolation Techniques for Environmental Effects Assessments, in London on 17-18th January 2001 (EC, 2001). Although the primary objective of this workshop was focused on how statistical extrapolation techniques might be used to derive PNECs in the assessments of metals and their compounds, the general principles outlined here should be also applicable for other substances.

Input data

The methods should be applied on all reliable available NOECs or preferably EC10 from chronic/long-term studies, preferably on full life-cycle or multi-generation studies. NOECs and preferably EC10 are derived according to previous considerations (**Table 17**).

Which taxonomic groups?

It is important to include all available information on the mode of action of the chemical, in order to evaluate the need to include possible other (sensitive) taxonomic groups or exclude possible over-representation of certain taxonomic groups, realising that the mode of action may differ between short-term effects and long-term effects and between taxonomic groups. The minimum species requirements when using the SSD method are:

- fish (species frequently tested include salmonids, minnows, bluegill sunfish, channel catfish, etc.);
- a second family in the phylum Chordata (fish, amphibian, etc.);
- a crustacean (e.g. cladoceran, copepod, ostracod, isopod, amphipod, crayfish etc.);
- an insect (e.g. mayfly, dragonfly, damselfly, stonefly, caddisfly, mosquito, midge, etc.);
- a family in a phylum other than Arthropoda or Chordata (e.g. Rotifera, Annelida, Mollusca, etc.);
- a family in any order of insect or any phylum not already represented;
- algae;
- higher plants.

It is recognised that for some of the taxa mentioned above, no internationally standardised test guidelines for long-term tests are currently available. The applicability of existing test

data and the fulfilment of the above requirements thus need to be assessed on a case-by-case basis. There is a need to evaluate additional information in order to assess how relevant and representative the list of taxonomic groups is to the risk assessment scenario being investigated.

Minimal sample size (number of data)

Confidence can be associated with a PNEC derived by statistical extrapolation if the database contains at least 10 NOECs (preferably more than 15) for different species covering at least 8 taxonomic groups.

Deviations from these recommendations can be made, on a case-by-case basis, through consideration of sensitive endpoints, sensitive species, mode of toxic action and/or knowledge from structure-activity considerations.

According to Brock et al. (2011), measurement parameters, from which endpoints are calculated, should preferably be sensitive/responsive in the range of tested concentrations such that SSDs avoid the use of greater- or lower-than values. In general, it is not recommended to include unbound values (greater-than or lower-than values) in the SSD. There are situations, however, where ignoring those data would lead to a loss of valuable information. When a lower-than value is lower than the lowest toxicity endpoint, this means that the other data do not cover the whole range of sensitivities. Leaving out this information might lead to a lower limit, median and upper limit hazardous concentration to 5% of the species (HC5) that is underprotective.

How to deal with multiple data for one species?

Where appropriate and possible, a pre-selection of the data should be performed in relation to realistic environmental parameters for Europe (e.g. hardness of water, pH, organic matter and/or temperature). The full database should be carefully evaluated to extract information (e.g., on sensitive endpoints), which may be lost when "averaging" the data to a single value.

The test data applicable to the most sensitive endpoint should be taken as representative for the species. In this context, demographic parameters can be used as endpoints, as can bio-markers if they are toxicologically relevant in terms of population dynamics.

Multiple values for the same endpoint with the same species should be investigated on a case-by-case basis, looking for reasons for differences between the results. For instance, particular attention should be given to the conditions which may justify the differences in the obtained results: e.g concentrations tested in the various studies, different life stages of the species tested in different tests, different exposure durations, etc., which may justify the differences in the results obtained. For equivalent data on the same end-point and species, the geometric mean should be used as the input value for the calculation. If this is not possible, perhaps because valid results are considered to be too variable, then grouping and combining the values, e.g. by pH ranges, and using reduced numbers of values should be considered. The effects that these different treatments have on the derived value (and on the resulting risk characterisation) should be investigated and discussed.

Where it is considered that the results are limited to certain conditions (e.g. not appropriate for low pH conditions) then these limitations should be explained. The values derived from different treatments of the data may be useful to indicate sensitive regions.

Fit to a distribution

Logistic and log normal distributions are most often used, because they require less data than distribution-free methods and are relatively easy to fit with standard statistical software (Aldenberg and Jaworska, 2000; Aldenberg et al., 2002; Van Vlaardingen et al., 2004). However, while it is typically assumed that SSDs follow a lognormal distribution, significant deviation from normality (whether log transformed or not) should be a trigger for

trying other distributions, (e.g. Burr type III, Weibull) that may provide a better goodness of fit. Techniques such as bootstrapping have been avoided, since they do not meet the assumption of normality, but if sample size is sufficiently large then (non-) parametric bootstrapping methods may provide point estimates and confidence intervals that are fit for purpose. Please note that there are many ways of calculating 5th percentiles, but the methods presented by Aldenberg and Jaworska (2000), Aldenberg et al. (2002) and Van Vlaardingen et al. (2004) provide 5th percentiles taking into account the sample size and also allowing the calculation of the uncertainty around the calculated 5th percentile.

Whatever the fit to a distribution, results should be discussed in regards to the graphical representation of the species distribution and the different p values that were obtained with each test. Finally, any choice of a specific distribution function should be clearly explained.

If the data do not fit any distribution, the left tail of the distribution (the lowest effect concentrations) should be analysed more carefully. If a subgroup of species can be identified as particularly sensitive and if the number of data on this subgroup is sufficient, the distribution can be fit to this subgroup. In case of lack of fit, the SSD method should not be used.

Estimated parameter

For pragmatic reasons it has been decided that the concentration corresponding with the point in the SSD profile below which 5 % of the species occur should be derived as an intermediate value in the determination of a PNEC. A 50 % confidence interval (CI) associated with this concentration should also be derived.

Estimation of the PNEC

The PNEC is calculated as:

$$PNEC = \frac{5\ \%\ SSD(50\ \%\ CI)}{AF}$$ **Equation 88**

The choice of assessment factor should follow the general principles that are described in **section 3.1** of this guidance. In particular, the following aspects should be considered:

1. AFs should always be natural numbers.
2. Lowering the AF below 5 on the basis of increased confidence needs to be fully justified. The exact value of the AF must depend on an evaluation of the uncertainties around the derivation of the 5th percentile. As a minimum, the following points have to be considered when determining the size of the assessment factor:
   - the overall quality of the database and the endpoints covered, e.g., if all the data are generated from "true" chronic studies (e.g., covering all sensitive life stages);
   - the diversity and representativity of the taxonomic groups covered by the database, and the extent to which differences in the life forms, feeding strategies and trophic levels of the organisms are represented;
   - relevance of routes of uptake other than those applied in the tests (for example for adsorptive chemicals the dietary route of uptake may become important solely or in addition to uptake from water phase)
   - knowledge on presumed mode of action of the chemical (covering also long-term exposure); Details on justification could be referenced from structurally similar substances with well-known mode of action
   - statistical uncertainties around the 5th percentile estimate, e.g., reflected in the goodness of fit or the size of confidence interval around the 5th percentile, and consideration of different levels of confidence (e.g. by a comparison between the 5 % of the SSD (50 %) with the 5 % of the SSD (95 %));

- comparisons between field and mesocosm studies (see **Appendix 7**), where available, and the 5th percentile and mesocosm/field studies to evaluate the laboratory to field extrapolation. Even if communities in micro-/mesocosm studies would be, on the whole, representative of the range of possible communities existing in surface waters, the sensitivity distribution of communities in individual micro-/mesocosm studies may not fully represent the distribution of sensitivity of communities in real surface waters

3. Since it will not be possible to prove that there are no remaining uncertainities, an AF = 1 should not normally be applied. Only in very specific cases the use of an AF of 1 may be justified. Besides the uncertainties mentioned above, certain effects of ecological significance such as delayed and trans-generational effects, overlooked species of unknown ecological importance, reduced competitive ability or interaction with other pollutants and environmental stressors, may not be revealed by single species laboratory testing nor by mesocosm.

For metals and other naturally occurring compounds the derived PNEC should be further evaluated in relation to natural background concentrations (see **section 4.5.1.3** on effects assessment of metals,metal compounds and other naturally occurring compounds.

A full justification should be given for the method used to determine the PNEC.

Further recommendations

NOEC values below the 5 % of the SSD need to be discussed in the risk assessment report. For example if all such NOECs are from one trophic level, then this could be an indication that a particular sensitive group exists, implying that some of the underlying assumptions for applying the statistical extrapolation method may not be met;

The deterministic PNEC should be derived by applying the "standard" Assessment Factor Approach on the same database;

If mesocosm studies are available, they should also be evaluated (see **Appendix 7**); in any case a PNEC should also be derived according to the standard method (deterministic approach) The various estimates of PNEC should be compared and discussed and the final choice of a PNEC be based on this comparison.

3.3.2 Effects assessment for substances with intermittent release

For substances subject to intermittent release (see **section 2.3.3.4** of this guidance for the definition of intermittent release) a single exposure event may be of only short duration. At least for dynamic systems such as rivers, the likelihood of long-term effects arising from such exposure is low, the principal risk being that of short-term toxic effects. Thus, the risk assessment should be based on a no-effect-concentration for intermittent release. In extrapolating to such a $PNEC_{water\text{-}intermittent}$, therefore, generally only short-term studies need to be considered. It is therefore proposed that, to derive a $PNEC_{water\text{-}intermittent}$ for such situations, an assessment factor of 100 be normally applied to the lowest $L(E)C_{50}$ of at least three short-term tests from three trophic levels. The assessment factor is designed to take account of the uncertainty that exists in extrapolating from the results of short-term laboratory toxicity tests to short-term effects that can be anticipated in the ecosystems.

In undertaking such an extrapolation, due account is taken of the biological variables of intra- and inter-species toxicity, as well as the general uncertainties in predicting ecosystem effects from laboratory data. This extrapolation should be carried out with care. Some substances may be taken up rapidly by aquatic organisms and this can lead to delayed effects even after exposure has ceased. This will generally be taken into account by the assessment factor of 100 but there may be occasions when a higher or lower factor would be appropriate. For substances with a potential to bioaccumulate the lowered assessment factor of 100 may not always be sufficient to provide adequate protection. For substances with a known non-specific mode of action, inter-species variations may be low. In such cases, a lower factor may be appropriate. In no case should a factor lower than 10 be applied to a short-term $L(E)C_{50}$ value.

3.4 Effect assessment for microorganisms in sewage treatment plants (STP)

Since chemicals may cause adverse effects on microbial activity in STPs it is necessary to derive a $PNEC_{stp}$. The $PNEC_{stp}$ will be used for the calculation of the PEC/PNEC ratio concerning microbial activity in STPs.

Current test systems for measuring the effect of chemicals on microbial activity have different endpoints and different levels of sensitivity. A number of internationally accepted test systems exist (cf. **Table 19**). Available data (e.g. UBA, 1993; Reynolds et al., 1987) suggest the following order of increasing sensitivities among particular test systems: respiration inhibition test (EU Annex V C.11; OECD 209, 1984f) < inhibition control in base-set tests < growth inhibition test with P. putida < inhibition of nitrification.

In general, short-term measurements in the order of hours (e.g. 10 h) are preferred, in accordance with the retention time in a STP. Information available on the toxicity for microorganisms has also to be relevant for the endpoint considered, i.e. microbial degradation activity in a STP. Test systems such as the respiration inhibition test and the nitrification inhibition test can be used. Respiration tests using a mixed inoculum are considered more relevant than respiration inhibition tests using a single-species inoculum.

The assumption that the substance under investigation is not inhibitory to the microorganisms when dosed in the test system is implicit in ready biodegradability testing (i.e., EU Annex V C.4A-F, OECD 301A-F, 1992f). Reynolds et al. (1987) report that microbial EC_{50} values determined for test substances using a variety of tests (EU Annex V C.11, OECD 209, 1984f, EU Annex V C.4F, Closed Bottle Test, Growth Inhibition) were found to be inhibitory in ready biodegradability tests (EU Annex V C.4C,F,E,B; OECD 301B,C,D,E, 1992f). No-effect or EC_0 values were 1.5 to 10 times lower than the corresponding EC_{50} values. Therefore, the authors recommend as a provisional rule that biodegradation testing should therefore be conducted at one-tenth of the EC_{50} concentration to ensure that a "probable non-inhibitory level" is employed in biodegradation testing. It would, therefore, seem appropriate to consider the test concentration from a positive ready biodegradability test to be an acceptable alternative to a NOEC obtained from a microbial toxicity test for the purposes of determining a $PNEC_{stp}$. This is particularly the case if domestic sludge is used as the source of microorganisms and if there is no indication of toxicity for the test concentration, e.g. due to other available test results. Similarly, data from inherent biodegradability testing may also prove useful. However, some additional issues have to be considered:

Only Ready Biodegradability Tests (RBT) relying on continuous monitoring, i.e. the MITI I test (EU Annex V C.4F; OECD 301C, 1992f) and the Manometric Respirometry test (EU Annex V C.4D; OECD 301F, 1992f), are considered reliable for observing the effects of a chemical on the inoculum, i.e. activated sludge diluted by factors ranging from ca. 100 to 1000. In parallel to the test itself, a toxicity control is run in extra bottles containing both the test chemical and a reference chemical that is easily degraded in the system. If for that purpose sodium acetate is used, the toxic effect is most often manifest as a delayed mineralisation of the substance. However, even if the vast majority of microorganisms are initially killed in the test system, such a delay may only be in the order of a few hours or days before rapid mineralisation of sodium acetate takes place. If measurements are carried out only weekly, which is the case in most RBT's, a delay in mineralisation of sodium acetate of only a few days may not be detected, leading erroneously to the conclusion that the test chemical is not inhibitory. Sodium benzoate may provide an acceptable alternative to sodium acetate when an inhibitory control test (i.e. the official term, not 'toxicity test') is performed with an RBT method that is not based on continuous monitoring, because mineralisation of benzoate occurs at a much slower rate.

Subject to expert judgement, consideration of data from biodegradation/removal studies using the laboratory/pilot scale Activated Sludge Simulation, Continuous Activated Sludge or Aerobic Sewage Treatment Coupled-Units tests (OECD 303A, 2001b; ISO-11733) may also prove useful in any consideration of $PNEC_{stp}$. These tests are laboratory scale models for

simulation of activated sludge, representing realistic approximation to actual conditions within full scale STPs. A NOEC from well-conducted simulation studies using domestic activated sludge would correspond to the concentration of the chemical substance that does not perturb the proper functioning of the Continuous Activated Sludge unit with regard to performance parameters such as:

- test substance elimination;
- COD removal;
- nitrification;
- denitrification;
- phosphorus removal;
- effluent quality etc.

when compared to a parallel non-dosed control.

Additionally, the results from tests with ciliated protozoa can be used for deriving a $PNEC_{stp}$. In this case Protozoa have to be regarded as additional species, not as an additional trophic layer. Ciliated protozoa, constituting the most important class of protozoa in STPs, are, except for certain industrial plants, important for their functioning. The toxicity data for ciliates are considered to be supplementary to the data for activated sludge or specific bacteria, i.e. no correlation exists between activated sludge and ciliate test results, neither are ciliates consistently more sensitive. The data from one ciliate species are representative for other ciliates, i.e. test data from species not dominant or not present in STPs can serve as basis for the PNEC-derivation. The function of the protozoa in STP is correlated to their growth. Therefore, values from ciliate growth inhibition tests, preferably with *Tetrahymena* (cf. OECD, 1998a), are relevant for the risk assessment for STPs. Tests using other characteristics (e.g. ciliary motion, cell movement, etc.) should not serve as a basis for the PNEC-derivation.

Often information may also be present on individual bacterial species such as from tests with *Vibrio fischeri* (used in the MICROTOX® test), *Pseudomonas putida*, *Pseudomonas fluorescens* and even *Escherichia coli*. These tests must be considered as less relevant. The tests with *P. fluorescence* and *E. coli* (Bringmann and Kühn, 1960) cannot be used for determination of the $PNEC_{stp}$ as they use glucose as a substrate. Likewise, the MICROTOX® test cannot be used as it uses a saltwater species. Results of the cell multiplication inhibition test with *P. putida* (Bringmann and Kühn, 1980) should only be used for calculation of the $PNEC_{stp}$ in cases where no other test results employing mixed inocula are available.

In general, the aim of the assessment is the protection of the degradation and nitrification functions and process performance and efficiency of domestic and industrial STPs – as also influenced by protozoan populations. The toxicity of a substance to microorganisms in a STP is assessed by comparing the concentration of a substance in STP aeration tank with the microbial effect concentration data for that substance (see also **section 2.3.7.1** of this guidance). If the substance under consideration is relevant for industrial and municipal STPs the toxicity assessment should be conducted for both kinds of STPs separately. A $PNEC_{stp}$ should be obtained as a first step in the effects assessment for microorganisms in both domestic and industrial sewage treatment plants.

The $PNEC_{stp}$ is usually derived from results obtained in the most sensitive test system available, regardless of whether this is a test with activated sludge, relevant bacteria or ciliated protozoa:

- the $PNEC_{stp}$ is set equal to a NOEC from a test performed with 'specific bacterial populations' like nitrifying bacteria or *P. putida* or from a growth inhibition test performed with ciliated protozoa, the Shk1 Assay (activated sludge bacterial luminescence inhibition assay). An EC_{50} from this test is divided by an assessment factor of 10;

- An assessment factor (AF) of 10 is to be applied to the NOEC of a sludge respiration test, reflecting the lower sensitivity of this endpoint as compared to nitrification, as well as the short duration of the test. The corresponding AF is 100 when based on the EC_{50};
- the lowest value is selected as the $PNEC_{stp}$.
- If no standard microbial inhibition test data are available, the $PNEC_{stp}$ can also be derived from available ready biodegradation tests. An assessment factor of 10 is applied to the test concentration at which no toxicity to the inoculum was observed. This approach can also be used for inherent biodegradability tests.
- From an activated sludge simulation study, a $PNEC_{stp}$ can be derived based on the PEC_{stp} or $PEC_{influent}$. The AF of 1 can be used in case there is no impact on nitrification and BOC/COD (biological oxygen demand/chemical oxygen demand) removal performance (NB: if sludge from an industrial WWTP was used for the test, the $PNEC_{stp}$ can not be used for the extrapolation to a domestic STP).
- No AF is needed to derive a $PNEC_{stp}$ based on good quality field data as this has to be assessed by expert judgement.

There may be cases in which the lowest $PNEC_{stp}$ does not correspond to the effect value of the most sensitive test system because different AF (100 or 10) are applied to the different test systems. In these cases expert judgement should be used to decide which effect value is appropriate for the calculation of the $PNEC_{stp}$. Usually the effect value of the most sensitive test system should be used as a basis for the calculation of $PNEC_{stp}$ employing the appropriate AF.

Table 19 on the next page provides a complete listing of the test systems mentioned above, effect concentrations that are determined using them and the corresponding assessment factors.

Table 19: Test systems for derivation of PNECstp

Test	Available value	Assessment factor
Respiration inhibition tests **EU Annex V C.11; OECD 209 (1984f)** ISO 8192 (1986)	NOEC or EC_{10}	10
	EC_{50}	100
Inhibition control in standardised biodegradation tests - Ready biodegradability tests EU Annex V C.4 A-F; OECD 301A-F (1992f) 92/69/EEC C4 (1992) ISO-7827 (1994), -9439 (1999), -10707 (1994), -9408 (1999) - Inherent biodegradability tests EU Annex V C.9; OECD 302 B-C (1981d-1992g) 88/302/EEC (1988) ISO-9888 (1999)	The tested concentration at which toxicity to the inoculum can be ruled out with sufficient reliability (cf. corresponding text section above) could be considered as a NOEC for the toxicity to microorganisms of a STP	10
Inhibition of nitrification ISO-9509 (1989)	NOEC or EC_{10}	1
	EC_{50}	10
Ciliate growth inhibition tests (preferably with Tetrahymena, cf. OECD, 1998a) [1)]	NOEC or EC_{10}	1
	EC_{50}	10
Activated sludge growth inhibition tests ISO-15522	NOEC or EC_{10}	10
	EC_{50}	100
Pilot scale activated sludge simulation tests **OECD 303A (2001b)** ISO-11733	Based on case-by-case expert judgement, the tested concentration not impairing proper functioning of the CAS [2)] unit could be considered as NOEC for microorganisms in STPs	Case by case: 10 down to 1 (for a well executed and documented test)*
Growth inhibition test with *Pseudomonas putida* NF EN ISO 10712 (1995) (Bringmann and Kühn, 1980)	NOEC or EC_{10}	1
	EC_{50}	10
	To be used if no other tests are available	
Pseudomonas fluorescens (Bringmann and Kühn, 1960)	Not usable as it uses glucose as substrate	
Escherichia coli (Bringmann and Kühn, 1960)	Not usable as it uses glucose as substrate	
***Vibrio fischeri* (MICROTOX®)** NF EN ISO 11348-1, -2, -3 (1999)	Not relevant for STP as the bacterium is a seawater species	

*A higher AF (i.e. 10) can be applied in case of badly executed tests

Notes on Table 19:

1) Ciliate testing would be required as the guideline becomes available
2) CAS: Continuous Activated Sludge

If on the basis of the $PNEC_{stp}$ derived using the procedures described above the PEC/PNEC ratio for industrial / domestic sewage treatment plants is above 1, the following procedure is proposed for refining the $PNEC_{stp}$:

- If on the basis of a test with nitrifying bacteria, a PEC/PNEC ratio above 1 is derived for a specific industrial STP, a revised $PNEC_{stp}$ for this specific site can be derived from a nitrification inhibition test using sludge from this site's STP. The revised $PNEC_{stp}$ for a specific industrial STP is derived from this test using the assessment factors described for nitrifying bacteria. For domestic STPs a revision of the PNEC is not possible in this way - sludge from one STP can not be regarded as being representative (in comparison with the single species test) of all domestic STPs with respect to the nitrifying activity;
- If on the basis of a respiration inhibition test, a PEC/PNEC ratio above 1 is derived for a specific industrial STP, a revised $PNEC_{stp}$ for this specific STP can be derived from a respiration inhibition test using sludge from this site's STP (the result from such a test is sometimes already available). A revised $PNEC_{stp}$ for a specific industrial STP is derived from these tests using the assessment factors described above for respiration inhibition tests. A $PNEC_{stp}$ for domestic STPs can not be derived on the basis of results from respiration tests that use industrial sludge as the source of inoculum;
- If on the basis of a respiration inhibition test, a standardised biodegradation test or an activated sludge growth inhibition or simulation test, a PEC/PNEC ratio above 1 is derived for a specific industrial sewage treatment plant, a revised PNECstp for this site can be derived from an appropriate pilot scale simulation test using activated sludge from the site's STP as a source of inoculum;
- If on the basis of a single species test with ciliated protozoa a PEC/PNEC ratio above 1 is derived for municipal or industrial sewage treatment plants, a test reflecting the integrity of the native ciliate population in (industrial or domestic) sewage sludge is necessary. The exception to this is where it can be shown that for the industrial STP under consideration protozoa are not relevant. The ability of the protozoan community to eliminate external bacterial food supply should be considered as a possible endpoint in this test. At present a standard protocol for a test based on ciliated protozoa which can be used to provide data for revising a $PNEC_{stp}$ is not available.

Info-box 7: Derivation of $PNEC_{stp}$ for active substances where the $NOEC/EC_{50}$ values exceed the water solubility

If significant inhibition is observed in the test, when concentrations higher than the water solubility are used, the test result (EC50) is used to derive a PNECstp by applying the appropriate AF from Table 19 to the test result.

If no inhibition is observed at the highest test concentration, the NOEC is set equal to the water solubility which is subsequently used to derive the PNECstp by applying the appropriate AF from Table 19 to the NOEC value. If then a risk is indicated the assessment should be refined.

Info-box 8: PNECstp derivation when both the EC50 and the NOEC from a respiration inhibition test are available

When a NOEC/EC10 and an EC50 from study compliant with OECD 209 are available and both values are derived from the same study, the $PNEC_{stp}$ should be derived by dividing the NOEC/EC10 by an AF of 10. The use of the EC50 with an assessment factor of 100 should still remain as an option when the NOEC/EC10 derived from OECD 209 test is not reliable.

Special attention should be paid to the reliability of the statistical analysis performed to derive the NOEC. Not enough replicates, substantial variance within the response of the

replicates or a poor statistical fit may result in a less reliable NOEC due to a lack of statistical power. In that case a study can only deliver an EC50/EC10 which should then be used with an AF of 100/10.

3.5 Effects assessment for the sediment

3.5.1 Introduction

Sediments may act as both a sink for chemicals through sorption of contaminants to particulate matter, and a source of chemicals through resuspension. Sediments integrate the effects of surface water contamination over time and space, and may thus present a hazard to aquatic communities (both pelagic and benthic) which is not directly predictable from concentrations in the water column. Effects on benthic organisms are of concern because they constitute an important link in aquatic food chain and play an important role in the recycling of detritus material. Due to the lack of standardised test methods on, e.g. the role of microorganisms in recycling of detritus material and nutrients, further tests needs to be developed and to be added for guidance in future.

Statistical extrapolation methods for calculation of PNEC for sediment organisms could be used when sufficient data are available (see **section 3.3.1.2** of this guidance). Further guidance needs to be developed in future.

General recommendations on the risk assessment for sediment compartment are available at the Proceedings of the ECHA Topical Scientific Workshop on Risk Assessment for the Sediment Compartment (http://echa.europa.eu/view-article/-/journal_content/title/topical-scientific-workshop-on-risk-assessment-for-the-sediment-compartme-1).

3.5.2 Strategy for effects assessment for sediment organisms

Substances that are potentially capable of depositing on or sorbing to sediments to a significant extent have to be assessed for toxicity to sediment-dwelling organisms.

In general, substances with a Koc < 500 – 1000 L/kg are not likely sorbed to sediment (SETAC, 1993). To avoid extensive testing of chemicals a log Koc or log Kow of ≥ 3 can be used as a trigger value for sediment effects assessment. Nevertheless, for certain product types such as product-type 21 antifouling products, sediment effects assessment must always be conducted (product-type specific data requirement according to Guidance on the BPR: Vol IV Part A: Information requirements). Effects assessment for marine sediment organisms is further described in **section 3.9.2**.

For most chemicals the number of toxicity data on sediment organisms will be limited. For the initial risk assessment, normally no effect data from tests with sediment organisms will be available. Therefore, the equilibrium partitioning method is proposed as a screening approach to compensate for this lack of toxicity data. This approach is based on the assumption that sediment-associated organisms are only exposed via pore water and are equally sensitive to the toxic action of the substance as pelagic aquatic organisms. Results from this screening can be used as a trigger for determining whether tests with benthic organisms should be conducted or not. The test results will enable a more realistic risk assessment of the sediment compartment to be carried out.

The EPM can be used for neutral organic substances but may not normally be used for substances that are poorly water soluble and for which no effects are observed in acute and/or chronic aquatic studies or for substances with a high adsorption or binding behaviour that is not driven by lipophilicity (e.g. ionisable substances, surface active substances, substances forming covalent bound with sediment particles such as aromatic amines). Note that in situations where it is valid to apply the EPM approach, it is not necessary to formally apply the method to assess sediment risks when the predicted environmental concentrations have been obtained from application of an exposure model that has used the same Koc (or log Kow) value as that used to predict the sediment PNEC. The reason is that

for substances with a log Kow up to 5 the EPM screening assessment results in the same risk characterisation ratio for sediment as for the pelagic compartment, as both $PEC_{sediment}$ and $PNEC_{sediment}$ screening are modelled from the corresponding pelagic data using the same partition coefficients and model assumptions. In such cases no quantitative risk characterisation for the sediment compartment need be performed since under these circumstances the assessment conducted for the aquatic compartment will also be protective of the sediment compartment. Note that due to the limitations of the equilibrium partitioning approach to account for additional exposure via sediment ingestion, this is only true for chemicals with a log Kow up to 5. For substances with a log Kow ≥ 5 an additional safety factor of 10 is applied to the PNECsediment. The additional factor takes into account the possible additional uptake via sediment ingestion. It has to be borne in mind that even this factor may be insufficient to achieve an appropriate level of protection in case of, for example, ionisable substances.

Even in situations where it is valid to apply the EPM approach but no quantitative assessment is needed because risks to the sediment compartment are addressed by read across to the aquatic compartment, care should be taken to ensure that any refinements or risk mitigation arguments applied to the aquatic risk assessment would not compromise the read across to the sediment phase. For example, mitigating factors such as degradation in the aquatic compartment and/or the absence of chronic effects data for pelagic species would not necessarily be directly applicable to the sediment compartment. As highlighted above sediments integrate the effects of surface water contamination over time and space, and may thus present a hazard to aquatic communities (both pelagic and benthic) which may not be directly predictable from concentrations in the water column. The EPM approach should therefore be used with care, taking into account all available information on sediment partitioning, persistence and toxicity to sediment dwelling organisms.

With regard to testing on sediment organisms, sediment assessment has been traditionally limited to sediment invertebrates, but other taxonomic groups and sediment functions may be also relevant. Getting a proper coverage of species is particularly relevant for some biocides, which have specific modes of action frequently leading to high sensitivity for certain taxonomic groups. Current OECD Test Guidelines mostly cover sediment dwelling invertebrates, although other taxonomic groups are covered by other standard guidelines. The OECD Guideline 239 is designed to assess the toxicity of chemicals on the growth of the rooted aquatic plants (*Myriophyllum spicatum*) growing in water-sediment system.

Regarding the invertebrate community, and especially infaunal species (i.e. living in the sediment, rather than on the sediment surface), it is important that different functional groups are represented: detritivores, filter-feeders and predators. Each group represents different energy pathways and different trophic levels in aquatic food webs, and hence may express different responses to chemical exposures. In addition, there are many pelagic organisms feeding on sediment and deposited materials.

If the information available confirms that invertebrates are expected to be among the most sensitive group, an assessment focusing on this group with the AFs indicated in Table 22 is sufficient. The selection of species/taxa and of feeding behaviour and traits should also consider the biocidal mode of action and fate and behaviour. In general, tests with spiked sediment should be conducted following the recommendations (e.g. OECD TG 218 and 225) for ensuring that dietary exposure is properly covered during the test.

For substances that bind or adsorb strongly to sediment or particulate matter (i.e. substances with a log Kow > 5, or with a corresponding adsorption or binding behaviour not triggered by the lipophilicity (i.e. log Kow) of the substance but by other mechanisms), ingested food or sediment are often neglected routes of uptake during the ecotoxicity testing. Available sediment tests should be carefuly evaluated (see Guidance on the BPR: Vol IV Part A: Information requirements). Special attention should be given to the pathways through which the test organisms are exposed to the chemical and their feeding behaviour as feeding with unspiked food could potentially reduce the exposure via sediment or food ingestion by the organism, for example, *Chironomus riparius* is known to feed selectively on added food (spiked or unspiked), (Åkerblom, N. and W. Goedkoop). Test organisms should

be fed with spiked food or the food should be added to the sediment before application of the test substance (for example via the procedure described in OECD Guideline 233). Test data for strongly adsorbing or binding substances should include sediment eating species (e.g. Lumbriculus spp., Tubifex spp.) if Chironomus spp. are not expected to be amongst the most sensitive species or the test method for Chironomus spp. is not feasible. If such test data are not available the possible additional uptake via spiked food should be accounted for by an additional assessment factor (see **section 3.5.4** of this guidance).

In some cases, exposure via food is not always contributing to the toxicity of an active substance that bind or adsorb strongly to sediment or particulate matter.
In order to determine if exposure via food is significantly contributing to the toxicity, results from a study with spiked food could be compared with the results from a study with unspiked food with the relevant test organism. Further guidance needs to be developed and to be added in this guidance in future. When pore water is the leading route for toxicity, standard tests (with unspiked food) with Chironomus are preferred and the additional assessment factor of 10 is not warranted in this case.

Three situations can be distinguished for deriving a $PNEC_{sed}$:

- When no toxicity test results are available for sediment organisms, the equilibrium partitioning method is applied to identify a potential risk to sediment organisms. For substances that bind or adsorb strongly to sediment or particulate matter, the possible additional uptake via sediment ingestion is accounted for by an extra assessment factor as explained above. This method is regarded as "screening approach" and is explained in **section 3.5.3** of this guidance;
- when only acute toxicity test results for benthic organisms are available (at least one) the risk assessment is performed both on the basis of the test result of the most sensitive species using an assessment factor of 1000 and on the basis of the equilibrium partitioning method. The lowest $PNEC_{sed}$ is then used for the risk characterisation;
- when long-term toxicity test data are available for benthic organisms the $PNEC_{sed}$ is calculated using assessment factors for long-term tests and this result should prevail in the risk assessment. This approach is explained in **section 3.5.4** of this guidance.

Table 20: Requirements for performing a risk characterisation for sediment

Available measured data: PECsed	Available measured data: PNECsed	Risk characterisation
$C_{pore\ water}$	none	$\frac{C_{pore\ water}}{PNEC_{water}}$
C_{bulk}	none	$\frac{C_{bulk} RHO_{susp}}{K_{susp-water} PNEC_{water} \cdot 1000}$
none	$PNEC_{sed}$	$\frac{K_{susp-water} PEC_{water} \cdot 1000}{PNEC_{sed}\ RHO_{susp}}$
$C_{pore\ water}$	$PNEC_{sed}$	$\frac{K_{susp-water} C_{pore\ water} \cdot 1000}{PNEC_{sed}\ RHO_{susp}}$

Available measured data: PECsed	Available measured data: PNECsed	Risk characterisation
C_{bulk}	$PNEC_{sed}$	$\frac{C_{bulk}}{PNEC_{sed}}$

where:

$C_{pore\ water}$	concentration in sediment pore water	$[mg \cdot l^{-1}]$	
C_{bulk}	concentration in whole sediment	$[mg \cdot kg_{sed}^{-1}]$	
$K_{susp\ water}$	suspended matter-water partition coefficient	$[m^3 \cdot m^{-3}]$	
RHO_{susp}	bulk density of dry suspended matter	$[kg \cdot m^{-3}]$	**Equation 20**

Info-box 9: Use of dry weight exposure and effect concentrations and normalisation to default organic matter for freshly deposited sediment

Use of dry weight concentrations

When toxicity tests with sediment dwelling organisms are available, the test results should be reported in dry weight sediment concentrations (as recommended by e.g. OECD TG 218) and consequently the PNEC will be expressed in dry weight. This means no correction procedure would be needed on the effects endpoint. Then the PEC should be converted to dry weight by:

a) Replacing the RHOss (wet) of 1150 kg wwt/m³ with RHOss (dry) 250 kg dwt/m³ in the formula for the PEC_{sed} (**Equation 53**).

b) Keeping RHOss (wet) to calculate a PEC wet weight and then convert it to dry weight using the default conversion factor of 4.6 kgwwt/kgdwt.

Normalisation to default organic carbon content

When ecotoxicity test endpoints are available for sediment, they relate to the specific test conditions, including organic carbon content, used in the study. For example, the OECD 218 Guideline states that organic carbon content of the test sediment should be 2% (±0.5 %). For non-ionic organic compounds it is assumed that bioavailability is determined by the organic carbon content only. In such cases, in order to facilitate meaningful comparison with exposure values, the effect endpoint should be corrected to reflect the organic carbon concentration assumed for the purposes of PEC calculations. For the local assessment the PEC is calculated assuming the properties of suspended sediment (i.e. the fraction organic carbon in standard suspended matter, Foc_{susp} – see **Table 3**) should be set to 0.1 $kg_{oc}\ kg_{solid}^{-1}$ i.e. 10% organic carbon. Accordingly the study result should be corrected to reflect this according to the following formula:

$$NOEC/EC10 \text{ and } L(E)C_{50(standard)} = NOEC/EC10 \text{ and } L(E)C_{50(experiment)} \cdot \frac{Foc_{susp}}{Foc_{susp\,(experiment)}}$$

Info-box 10: Sediment assessment for metabolites

Metabolites tend to be generally less hydrophobic as compared to the parent substance. As a result, the metabolites exhibit a lower adsorption potential. Therefore, the degradation products in the sediment compartment are usually less relevant than the parent compound. Nevertheless, the same basic triggers and approaches can be applied to parent compounds and metabolites. Furthermore, it should be noted that the degradation of parent substances with a low bioavailability, due to a very high Kow / Koc, might result in metabolites with an increased bioavailablility.

3.5.3 Calculation of PNEC using equilibrium partitioning

In the absence of any ecotoxicological data for sediment-dwelling organisms, the $PNEC_{sed}$ may be provisionally calculated using the equilibrium partitioning method (EPM). This method uses the $PNEC_{water}$ for aquatic organisms and the sediment/water partition coefficient as inputs (OECD, 1992b; Di Toro et al., 1991).

It has to be considered that the EPM may result both in an overestimation or underestimation of the toxicity to benthic organisms (Di Toro et al. 2005). Therefore this method can only be used as rough screening to decide whether sediment toxicity tests with benthic organisms are required.

In the EPM, it is assumed that the:

- sediment-dwelling organisms and water column organisms are equally sensitive to the chemical;
- concentration of the substance in sediment, interstitial water and benthic organisms are at thermodynamic equilibrium: the concentration in any of these phases can be predicted using the appropriate partition coefficients;
- sediment/water partition coefficients can either be measured or derived on the basis of a generic partition method from separately measurable characteristics of the sediment and the properties of the chemical. (For the derivation of the sediment-water partition coefficient and the limits of the calculation methods see **section 2.3.5** of this guidance).

The following formula, which is based on equilibrium partitioning theory, is applied:

$$PNEC_{sed} = \frac{K_{susp-water}}{RHO_{susp}} \cdot PNEC_{water} \cdot 1000$$ **Equation 89**

Explanation of symbols

$PNEC_{water}$	Predicted No Effect Concentration in water	$[mg \cdot l^{-1}]$	
RHO_{susp}	bulk density of sediment	$[kg \cdot m^{-3}]$	**Equation 20**
$K_{susp\ water}$	partition coefficient suspended matter water	$[m^3 \cdot m^{-3}]$	**Equation 27**
$PNEC_{sed}$	Predicted No Effect Concentration in sediment	$[mg \cdot kg^{-1}]$	

Concentrations in soil and sediment are total concentrations, and therefore expressed on a wet-weight basis (see **Equation 18** and **Equation 19**). Optionally, intermediate results can be presented and changed on dry-weight basis. The conversion factors for sediment are derived from the compartment definition in phases.

The following qualifying comments apply regardless of whether the $K_{susp\ water}$ is measured or estimated:

- the formula only considers uptake via the water phase. However, uptake may also occur via other exposure pathways like ingestion of sediment and direct contact with sediment. This may become important, especially for adsorbing chemicals, for example those with a log K_{ow} greater than 3. For these compounds the total uptake may be underestimated;

  for compounds with a log K_{ow} greater than 5 or with a corresponding adsorption or binding behaviour not triggered by the lipophilicity (e.g. log K_{ow}) of the substance but by other mechanisms (e.g. ionisable substances, surface active substances,

substances forming covalent bound to sediment, components like e.g. aromatic amines) a modified equilibrium method is used.

It should be noted that this approach is considered only as a screen for assessing the level of risk to sediment dwelling organisms. If with this method a PEC/PNEC ratio > 1 is derived, then tests with benthic organisms using spiked sediment have to be conducted to support a refined risk assessment for the sediment compartment.

3.5.4 Calculation of PNEC using assessment factor

The $PNEC_{sed}$ is derived from the lowest available NOEC/EC_{10} obtained in long-term tests by application of the following assessment factors:

Table 21: Assessment factors for derivation of PNECsed

Available test result	Assessment factor
One long-term test (NOEC or EC_{10})	100
Two long-term tests (NOEC or EC_{10}) with species representing different living and feeding conditions	50
Three long-term tests (NOEC or EC_{10}) with species representing different living and feeding conditions	10
Species sensitivity distribution (SSD) method	5-1[a] (to be fully justified case by case)

a) In case a large data set from long-term tests is available, statistical extrapolation methods may be used to derive a PNEC for sediment compartment. AFs of 1-2 should not normally be applied, as it will not be possible to prove that there are no remaining uncertainties (see also basic considerations and minimum requirements outlined in section 3.3.1.2 of this guidance).

For substances with a log Kow > 5, or with a corresponding adsorption or binding behaviour not triggered by the lipophilicity (e.g. log Kow) of the substance but by other mechanisms, the assessment factor for the PNEC derivation for the sediment compartment may be increased by a factor of 10 as mentioned in **section 3.5.2** above).

If other taxonomic groups or environmental functions are expected to be of higher sensitivity, a case-by-case assessment is needed, and a comparison with a PNEC based on equilibrium partitioning may be considered as part of a whole evidence approach to assess the sediment compartment. Mesocosms studies may offer adequate coverage if the relevant endpoints are measured. Further guidance on the use of mesocosm studies for biocides can be found in **Appendix 7**.

3.6 Effects assessment for the terrestrial compartment

3.6.1 Introduction

Chemicals can reach the soil via several routes: application of sewage sludge in agriculture, manure application, direct application of chemicals by means of spraying, leaching and deposition from the atmosphere. Consequently the possibility of adverse effects has to be assessed. The proposed strategy in this section is based on assessing the effects of chemicals on soil organisms. At the moment no strategy is available to assess possible effects on soil functions such as filtration, buffering capacity and metabolic capacity.

As mentioned in the introduction, the substances discharged into the soil can not only affect the soil organisms but also can influence soil functions. Substances that are hydrophilic and that are readily eluted with the rainwater into the groundwater as well as those that geo-accumulate and those that are poorly degradable in soil should be considered with special care. If the substance is a biocide directly applied/emitted to soil, then the methodology

referred in the *Guidance on the Biocidal Product Regulation: Volume IV Environment, Part A Information requirements* applies.

The terrestrial ecosystem comprises of an above-ground community, a soil community and a groundwater community. In this section only effects on soil organisms exposed directly via pore water and/or soil are addressed. It is recognised that the strategy described here must therefore be regarded as provisional. However, reference is made to the strategy for the air compartment (**section 3.7** of this guidance) and for bioaccumulation and secondary poisoning of birds and mammals (**section 3.8** of this guidance).

The strategy described below is based on several documents relating to terrestrial effects assessment: OECD (1989), Stavola (1990), Samsøe-Petersen and Pedersen (1994), UBA (1993) and Römbke et al. (1993).

3.6.2 Strategy for effects assessment for soil organisms

Standardised methods exist for the soil compartment and toxicity tests with terrestrial organisms may be required for biocides depending on product-type and expected use.

When no toxicity data are available for soil organisms or if experimental data are missing for the potentially most sensitive species group, the equilibrium partitioning method can be applied to aquatic data to identify a PNEC for soil organisms. However, this method cannot replace required core toxicity data for soil organisms and should only be considered as a "screening approach" for identifying substances requiring further testing.

In common with the aquatic compartment, the objective of the assessment is to identify substances that present an immediate or delayed danger to the soil communities.

Soil is a complex and heterogeneous medium in which biological processes are occurring. Microorganisms play an important role in degradation processes and the mineralisation of organic matter, allowing nutrients to be re-cycled in the ecosystem. Soil invertebrates are contributing to the recycling of elements and play a significant part in creating and maintaining a good soil structure. Finally, plants are primary producers and provide food for all other heterotrophic organisms. Consequently, the protection of the soil community requires protection of all organisms playing a leading role in establishing and maintaining the structure and the functioning of the ecosystem. The use of results from tests that represent different and significant ecological functions in the soil ecosystem is therefore suggested.

A suite of soil tests should therefore ideally be designed to obtain data relevant to:

- primary producers (plants);
- consumers (for example invertebrates that represent an important group in the soil compartment);
- decomposers (comprising microorganisms that play an important role in foodwebs and nutrients cycling).

Info-box 11: Significant deviation (decrease or increase) from the control in a soil nitrification inhibition/carbon transformation tests

Any significant deviation (decrease or increase) from the control in a soil nitrification inhibition/carbon transformation test should be considered as a relevant effect for the derivation of PNEC for biocides in general. There are no exemptions to the interpretation that any significant deviation (decrease or increase) from the control in a soil nitrification inhibition/carbon transformation tests is a relevant effect for the derivation of PNEC for biocides.

Natural soils used in ecotoxicological tests differ in characteristics such as organic matter and clay content, soil pH and soil moisture content. The bioavailability of the test compound, and therefore the toxicity observed, may be influenced by the soil properties.

This means that results from different test soils may not be compared directly. As far as possible, toxicity tests should be conducted in conditions (as regards the nature of the soil, its organic content and any other parameter that could influence the bioavailability of the substance) where the test substance is bioavailable to the tests organism(s). However, if possible data should be normalized using relationships that describe the bioavailability of chemicals in soils. Results are converted to a standard soil, which is defined as a soil with an organic matter content of 3.4 % (see section 2.3.4 of this guidance).

For non-ionic organic compounds it is assumed that bioavailability is determined by the organic carbon content only. NOECs and L(E)C_{50}s are corrected according to the formula:

$$NOEC\ or\ L(E)C_{50(standard)} = NOEC\ or\ L(E)C_{50(exp)} \cdot \frac{Foc_{soil(standrd)}}{Foc_{soil(exp)}}$$ **Equation 90**

Explanation of symbols

NOEC or L(E)$C_{50, exp}$	NOEC or L(E)C_{50} in experiment	[mg·kg^{-1}]	
$F_{oc, soil(standard)}$	fraction organic carbon in standard soil	[kg·kg^{-1}]	**Table 3**
$F_{oc, soil(exp)}$	fraction organic carbon in experimental soil	[kg·kg^{-1}]	
NOEC or L(E)$C_{50, standard}$	NOEC or L(E)C_{50} in standard soil	[mg·kg^{-1}]	

All effect concentrations from terrestrial plants and terrestrial organisms should be converted to the standard organic matter as described in **Info-box 9**: for the sediment compartment. It should be noted that this recommended normalisation is only appropriate when it can be assumed that the binding behaviour of a non-ionic organic substance in question is predominantly driven by its log K_{ow}, and that organisms are exposed predominantly via pore water.

Three situations can be distinguished for deriving a $PNEC_{soil}$:

- terrestrial toxicity data are a product-type specific information requirement for some of the PT. However, when no toxicity data are available for soil organisms, or if experimental data are missing for the potentially most sensitive species group, the equilibrium partitioning method is applied to identify a potential risk to soil organisms. This method is regarded as a "screening approach" and is explained in **section 3.6.2.1** of this guidance (see also **section 3.5.2** of this guidance);
- when toxicity data are available for a producer, a consumer and/or a decomposer the $PNEC_{soil}$ is calculated using assessment factors as presented in **section 3.6.2.2** of this guidance; provided that the potentially most sensitive taxon is not included in the test species; the previous bullet point still applies.
- When only test results for a single soil dwelling species are available the risk assessment is performed both on the basis of this result using assessment factors and on the basis of the EPM. From both $PEC_{soil}/PNEC_{soil}$ ratios the highest one is chosen for the risk characterisation.

3.6.2.1 Calculation of PNEC using equilibrium partitioning

The EPM is based on the assumption that soil toxicity expressed in terms of the freely-dissolved substance concentration in the pore water is the same as aquatic toxicity. The pore water concentration is correlated with the bioavailable fraction. Although Di Toro *et al.* (1991) based their analysis on sediment partitioning the rationale can also be applied to soils. However the applicability of the equilibrium partitioning method has been evaluated less for soil than for sediment-dwelling organisms. Van Gestel and Ma (1993) have shown

the model to be valid for short-term toxicity of several chlorophenols, chlorobenzenes and chloroanilines to earthworms.

The equilibrium partitioning method may not be suitable for highly lipophilic substances or substances with a specific mode of action nor for organisms that are exposed primarily through food (Van Gestel, 1992). However, for Collembola and Oribatid mites, there are indications that direct exposure to soil may be of much greater importance for uptake than is exposure via the food (Løkke and van Gestel, 1998).

It should be recognised that substitution of terrestrial toxicity data by aquatic toxicity data should be used with caution. This is because the effects on aquatic species can only be considered as effects on soil organisms that are exposed exclusively to the soil pore water and may only be appropriate for organisms with a water-permeable epidermis. Furthermore, studies have shown that the equilibrium partitioning method can give significant over- or underestimations, due to inaccurate partition coefficients or differences in species sensitivities. Therefore, further research is required into the general applicability of the EPM for other organisms.

Therefore, if the $PEC_{soil}/PNEC_{soil}$ ratio calculated using the EPM is greater than 1, tests with soil organisms should be considered as an essential requirement for a refined effects assessment. Alternatively, the PEC could also be refined. The $PNEC_{soil}$ is calculated as follows:

$$PNEC_{soil} = \frac{K_{soil\text{-}water}}{RHO_{soil}} \cdot PNEC_{water} \cdot 1000$$ **Equation 91**

Explanation of symbols

$PNEC_{water}$	Predicted No Effect Concentration in water	$[mg \cdot l^{-1}]$	
RHO_{soil}	bulk density of wet soil	$[kg \cdot m^{-3}]$	**Equation 20**
$K_{soil\text{-}water}$	partition coefficient soil water	$[m^3 \cdot m^{-3}]$	**Equation 27**
$PNEC_{soil}$	Predicted No Effect Concentration in (wet) soil	$[mg \cdot kg^{-1}]$	

Concentrations in soil and sediment are total concentrations, and therefore expressed on a wet-weight basis. Optionally, intermediate results can be presented and changed on dry-weight basis. The conversion factors for soil are derived from the compartment definition in phases. The conversion can be done according to **Equation 102b**.

In order to take uptake by soil ingestion into account the same approach is used as for the derivation of the $PNEC_{sed}$. Thus, $PNEC_{soil}$ is decreased by a factor of 10 for compounds with a log K_{ow} > 5 (or for compounds with a corresponding adsorption or binding behaviour, e.g. ionisable substances).

EPM probably overestimates the actual uptake from soil by soil invertebrates (Jager, 2004). However, this relation is complicated and probably depends on the ability to properly calculate the dissolved concentration in the soil. Therefore it is considered that the possible overestimation of exposure is acceptable when using the equilibrium partitioning method for chemicals with a log K_{ow} between 3 and 6;

In principle, toxicity data for aquatic organisms cannot replace data for soil dwelling organisms. This is because the effects on aquatic species can only be considered as effects on soil organisms that are exposed exclusively to the soil pore water of the soil (Samsøe-Petersen and Pedersen, 1994).

3.6.2.2 Calculation of PNEC using assessment factors

The same assessment factors used for the aquatic compartment (see Table 18) are applied to the terrestrial compartment (see Table 22). The size of the assessment factor therefore again depends on the type of data that are available i.e. short-term or long-term toxicity test, the number of trophic levels tested and the general uncertainties in predicting ecosystem effects from laboratory data. The assessment factors suggested for the soil compartment are not based on comprehensive experience. The choice of taxonomic groups for which toxicity data are necessary (conform to the core data set of algae, invertebrate and fish for the aquatic environment), is a point of discussion. A dataset comprising of toxicity data for primary producers, consumers and decomposers is preferred. The assessment factors for the PNEC determination are reported in Table 22.

Table 22: Assessment factors for derivation of PNECsoil

Information available	Assessment factor
L(E)C$_{50}$ short-term toxicity test(s) (e.g. plants, earthworms, or microorganisms)	1000
NOEC for one long-term toxicity test (e.g. plants)	100
NOEC for additional long-term toxicity tests of two trophic levels	50
NOEC for additional long-term toxicity tests for three species of three trophic levels	10
Species sensitivity distribution (SSD method)	5-1, to be fully justified on a case-by-case basis[a]
Field data/data of model ecosystems	case-by-case

a) In case a large data set from long-term tests is available, statistical extrapolation methods may be used to derive a PNEC for soil compartment. AFs of 1-2 should not normally be applied, as it will not be possible to prove that there are no remaining uncertainties (see also basic considerations and minimum requirements outlined in section 3.3.1.2 of this guidance).

Info-box 12: Clarifications on the assessment factor to derive PNEC$_{soil}$

Test with plants described in OECD TG 208 or OECD TG 227: Can this test be considered as a short or long term test and how does this influence the assessment factor to derive the PNEC$_{soil}$?

Different interpretations exist on whether this test can be considered as a short or a long term study. The study is in principle a short-term study; however, it was decided that it also can be considered a long-term study under certain circumstances, provided that in addition to the EC50 also a NOEC/EC10 was derived from this test. Depending on the sensitivity of plants compared to other taxonomic groups when comparing L(E)C50 values, different assessment factors to derive the PNEC$_{soil}$ must be chosen (for details see "Choice of AF for PNEC$_{soil}$ derivation", below).

Possibility to lower the assessment factor for the derivation of the PNEC$_{soil}$ from 1000 to 100 when the most sensitive species is unknown (e.g. data for micro-organisms and acute data for earthworms are available, but no data for plants).

Application of an assessment factor of 100 instead of 1000 is only possible when effect data for three different species (i.e. micro-organisms, earthworms and plants) are available and therefore the potentially most sensitive species can be established (for details see "Choice of AF for PNEC$_{soil}$ derivation", below).

In specific situations, and on a case by case basis, when the necessary data to establish the most sensitive species is available from a very similar compound as the active

substance under consideration, and can be extrapolated, than these data can be used to lower the assessment factor to 100.

Choice of AF for PNECsoil derivation

If test results are available for:

- Microorganisms (28 days EC_{50} and NOEC/EC_{10})
- Plants (EC_{50} and NOEC/EC_{10} according to e.g OECD 208)
- Earthworms (14 days LC_{50} and 56 days NOEC/EC_{10}),

three different situations can be distinguished with respect to PNEC derivation and the choice of the AF:

1. Acutely, plants are not the potentially most sensitive species ($EC_{50} \geq$ 10 times higher than L(E)C_{50} for microorgansims and/or earthworms): An AF of 10 should be applied to the lowest NOEC/EC_{10} for either microorganisms, plants or earthworms.
2. Acutely, plants are the potentially most sensitive species but the plant EC_{50} is $\geq$ 10 times higher than the NOEC/EC_{10} from either the microorganism or the long-term earthworm study: An AF of 50 should be applied to the lowest NOEC/EC_{10} for earthworm or microorganism.
3. Acutely, plants are the potentially most sensitive species and the plant EC_{50} is significantly* lower than the NOECs/EC_{10} from the microorganism and the long-term earthworm study: An AF of 100 should be applied to the lowest L(E)C_{50} (in analogy to the PNEC derivation for the aquatic compartment).

These assessment factors can be reduced if further testing on chronic toxicity to plants, e.g. according to ISO standard 22030:2005 on determining the inhibition of the growth and reproductive capabilities of higher plants, becomes available.

* Endpoints are considered not to be significantly different when the sensitivity difference is within a factor of less than 10.

Info-box 13: Presentation of recalculations of effect results (e.g. NOEC values) expressed as a.s./ha

Any recalculations necessary for the effects assessment should be explained and performed in the effects assessment section of the Assessment Report. Consequently, conversion of a test result expressed as active substance/ha to for example mg/kg must be presented in Part A/B of Section 2 of the Assessment Report. If information on test conditions (i.e. soil density, structure, type of soil, etc) is available, then this should be used for the recalculation to mg/kg. If no information can be derived from the test, a default soil depth of 10 cm and soil density of 1500 kg/m³ dry soil should be used. The original expression of the study results will be maintained in IUCLID.

Info-box 14: How to deal with studies with terrestrial microorganisms that were performed using the PPP design (2 test concentrations with a control)

Tests using the PSM design (two test concentrations with a control) can be used for the environmental risk assessment of biocides in special circumstances. First, a statistical evaluation (student t-test) of difference of the test concentrations to the control is conducted. If no statistical difference is found in both tested concentrations the highest concentration can be used as NOEC. If a statistical difference is found and the effect is >15% no NOEC can be derived. The test cannot be used for assessment under the BPD/BPR and, if the test is critical for he assessment, a new test using 5 concentrations needs to be requested. If in at least one concentration no statistical difference from the control is found and the effect value is </= 15% the concentration can be considered the

NOEC. The NOEC micro-organisms can be used to derive the $PNEC_{soil}$ by using an AF of 100 even if no other NOEC's for soil organisms are available.

3.6.2.3 Calculation of PNEC using statistical extrapolation techniques

Calculation of a $PNEC_{soil}$ using statistical extrapolation techniques can be considered when sufficient data are available. SSDs can obly be performed when at least 10 NOECs (and preferably 15 NOECs) are available from at least 8 taxonomic groups. For comparable data on the same end-point and species, by default the geometric mean should be used as the input value for the calculation of the species sensitivity distribution. When results are available from tests using different soils and it is likely that the soil characteristics have influence on the results, the effect data should be normalised before further processing. If not possible, the lowest NOEC per end-point and species should be used. Data on microbial mediated processes and single species tests should be considered separately due to fundamental differences between these tests (functional vs. structural test, multi-species vs. single species, adapted indigenous microbe community vs. laboratory test species, variability of test design and different endpoints, etc.). The results should be compared and evaluated on a case-by-case basis in deciding on a final PNEC for the soil compartment.

3.7 Effects assessment for the air compartment

For the risk assessment of the air compartment biotic and abiotic effects are considered.

3.7.1 Biotic effects

The methodology used for effects assessment (and therefore the risk characterisation) of chemicals in water and soil cannot be applied yet in the same manner to the atmosphere. Methods for the determination of effects of chemicals on species arising from atmospheric contamination have not yet been fully developed, except for inhalation studies with mammals.

It is evident that the quantitative characterisation of risk by comparison of the PEC_{air} to $PNEC_{air}$ is not possible at the moment: only a qualitative assessment for air is feasible.

For the air compartment toxicological data on animal species other than mammals are usually not or only scarcely available. For volatile compounds acute or short-term inhalation tests may be present. On the basis of these data there may be indications of adverse effects. Short-term LC_{50} data can be used for a coarse estimation of the risk a chemical poses for animals. However, in most cases, it is unlikely that the atmospheric concentration of a chemical will be high enough to cause short-term toxic effects in the environment, so data on long-term or chronic toxicity should be considered. For example, a chemical may be dangerous for the atmospheric environment at a low concentration, if it is classified for STOT-RE cat. 1 with the hazard statement H372 (Causes damage to organs through prolonged or repeated exposure) or cat. 2 with the hazard statement H373 (May cause damage to organs through prolonged or repeated exposure). Also mutagenic effects and toxic effects on reproduction by a chemical indicate a toxic potential for terrestrial vertebrates.

Fumigation tests on invertebrates are usually not available. For some substances investigations on the toxicity to honey bees (*Apis mellifera*), which are conducted according to guidelines for the testing of plant protection agents, may be available. In these tests, it is sometimes difficult to determine the effective concentration and therefore a $PNEC_{air}$ cannot be derived.

Concerning the toxicity for plants, data from tests where a chemical is applied directly via air (gaseous or deposited) are normally scarce. When toxicity data are available or information is available that plants might be affected this information must be carefully screened and if necessary further plant toxicity testing can be requested. When no specific information on toxicity to plants is available for the substance and considerable air emissions and exposure are expected the information on related compounds (e.g. toxicity,

phys.chem. properties) should be screened and a decision should be made whether there is reason for concern and whether actual plant testing should be considered.

Some experience has been obtained over the last years on substances for which actual plant testing has been requested and performed (e.g. risk assessment reports on tetrachloroethylene and dibutylphthalate, ECB, 2001). The test protocols have been developed on a case-by-case basis and varied from relatively simple laboratory test designs that can be considered as screening tests, to very extensive long-term open-top chambers with a large variety of species. Further discussion is needed before these test designs can be standardised and inserted in a more rigid testing strategy for plants.

How the results of the available toxicity test should be used in the actual setting of a PNEC for plants has yet to be decided on a case-by-case basis. Like with the effects assessments for the other compartments it is expected that an assessment factor is expected applied to the available effects data. The selection of this factor should take into account factors such as:

- the type of tests that have been performed;
- the duration of these tests;
- the variety of species tested;
- the type and severity of the effects observed.

3.7.2 Abiotic effects

For the evaluation of an atmospheric risk, the following abiotic effects of a chemical on the atmosphere have to be considered:

- global warming;
- ozone depletion in the stratosphere;
- ozone formation in the troposphere;
- acidification.

If for a chemical there are indications that one or several of these effects occur, expert knowledge should be consulted. Please see also Annex I and II of Regulation (EC) No 1005/2009 of the European Parliament and of the Council of 16 September 2009 on substances that deplete the ozone layer. A first quantitative approach is described in De Leeuw (1993):

Global warming

The impact of a substance on global warming depends on its IR absorption characteristics and its atmospheric lifetime. A potential greenhouse gas shows absorption bands in the so-called atmospheric window (800-1,200 nm).

Stratospheric ozone

A substance may have an effect on stratospheric ozone if;

- the atmospheric lifetime is long enough to allow for transport to the stratosphere, and;
- it contains one or more Cl, Br or F substituents.

In general, ozone depletion potential values approach zero for molecules with atmospheric lifetimes less than one year.

Tropospheric ozone

The generation of tropospheric ozone depends on a number of factors:

- the reactivity of the substance and the degradation pathway;

- the meteorological conditions. The highest ozone concentrations are expected at high temperatures, high levels of solar radiation and low wind speeds;
- the concentration of other air pollutants. The concentration of nitrogen oxides has to exceed several ppb.

Highly reactive compounds (e.g. xylene, olefins or aldehydes) contribute significantly to the ozone peak values. Species with a low reactivity (e.g. CO, CH_4) are important for ozone formation in the free troposphere and therefore for the long-term ozone concentrations. However, all studies showed significant variability in the tropospheric ozone building potential values assigned to each organic component. It has to be concluded that at present there is no procedure available to estimate the effect on tropospheric ozone if only the basic characteristics of a substance are known.

Acidification

During the oxidation of substances containing Cl, F, N or S substituents, acidifying components (e.g. HCl, HF, NO_2 and HNO_3, SO_2 and H_2SO_4) may be formed. After deposition, these oxidation products will lead to acidification of the receiving soil or surface water.

3.8 Assessment of secondary poisoning[24]

3.8.1 Introduction

Bioconcentration and bioaccumulation may be of concern for lipophilic organic chemicals and some metal compounds as both direct and indirect toxic effects may be observed upon long-term exposure. For metals guidance is given in **section 4.5.1** of this guidance. Bioconcentration is defined as the net result of the uptake, distribution and elimination of a substance in an organism due to water-borne exposure, whereas bioaccumulation includes all routes, i.e. air, water, soil and food. Biomagnification is defined as accumulation and transfer of chemicals via the food chain, resulting in an increase of the internal concentration in organisms at higher levels in the trophic chain. Secondary poisoning is concerned with toxic effects in the higher members of the food chain, either living in the aquatic or terrestrial environment, which result from ingestion of organisms from lower trophic levels that contain accumulated substances.

For many hydrophobic chemicals, accumulation through the food chain follows many different pathways along different trophic levels. A good risk estimation of this complex process is hampered when only limited data from laboratory studies are available. One way to assess a chemicals risk for bioaccumulation in aquatic species is to measure the bioconcentration factor (BCF). The BCF at any time during the uptake phase of this accumulation test is the concentration of test substance in/on the fish or specified tissues thereof (Cf as mg/kg) divided by the concentration of the chemical in the surrounding medium (Cw as mg/L). BCF is expressed in l/kg-1. Please note that corrections for growth and/or a standard lipid content are not accounted for. The steady-state bioconcentration factor (BCF_{SS}) does not change significantly over a prolonged period of time, the concentration of the test substance in the surrounding medium being constant during this period. The kinetic bioconcentration factor (BCF_K) is the ratio of the uptake rate constant, k_1, to the depuration rate constant, k_2 (i.e. k_1/k_2 – see corresponding definitions in Annex 1 of the OECD TG 305). In principle the value should be comparable to the BCF_{SS} (see definition above), but deviations may occur if steady-state was uncertain or if corrections for growth have been applied to the kinetic BCF. The lipid normalised kinetic bioconcentration factor (BCF_{KL}) is normalised to a fish with a 5 % lipid content. The lipid normalised, growth corrected kinetic bioconcentration factor (BCF_{KgL}) is normalised to a fish with a 5 % lipid content and corrected for growth during the study period as described in Annex 5 of the OECD TG 305. The dynamic bioconcentration factor can be calculated as follows:

[24] Please note: in the ESD for PT18 (household and professional uses), the term secondary poisoning has a different definition.

$$BCF_{fish} = \frac{C_{fish}}{C_{water}} \quad or \quad \frac{k_1}{k_2}$$ Equation 92

Explanation of symbols

C_{fish}	concentration in fish	[mg·kg$_{ww}^{-1}$]
C_{water}	concentration in water	[mg·l^{-1}]
k_1	uptake rate constant from water	[l·kg$_{ww}^{-1}$·d^{-1}]
k_2	elimination rate constant	[d^{-1}]
BCF_{fish}	bioconcentration factor	[l·kg$_{ww}^{-1}$]

At the core data level the available physico-chemical and (eco-)toxicological information can be used to decide whether or not there are indications for a potential for bioaccumulation and/or indirect effects. This estimation is used as a first step in the testing strategy for bioaccumulation and secondary poisoning (see **section 3.8.3** of this guidance). For the terrestrial ecosystem a similar strategy is used (see **section 3.8.3.7** of this guidance).

3.8.2 Indication of bioaccumulation potential

The simplest way to estimate the potential of a substance to bioaccumulate in aquatic species is by experimental measurement of the BCF. But also results from bioaccumulation studies in aquatic species can be used. Determination of the BCF alone, however, only gives a partial picture of the potential of bioaccumulation,results from a bioaccumulation study in terrestrial species, data from scientific analysis of human body fluids or tissues, such as blood, milk, or fat; detection of elevated levels in biota, in particular in endangered species or in vulnerable populations, compared to levels in their surrounding environment; results from a chronic toxicity study on animals; assessment of the toxicokinetic behaviour of the substance; information on the ability of the substance to biomagnify in the food chain, where possible expressed by biomagnification factors (BMF) or trophic magnification factors (TMF) can be used to assess the bioaccumulation potential in addition to experimental measurements of the BCF or BMF. Such data will rarely be available and the potential for bioaccumulation will usually need to be determined using simple physico-chemical and structural evidence (OECD, 2001c).

The most important and widely accepted indication of bioaccumulation potential is a high value of the *n*-octanol/water partition coefficient. In addition, if a substance belongs to a class of chemicals, which are known to accumulate in living organisms, it may have a potential to bioaccumulate. However, some properties of a substance may preclude high accumulation levels even though the substance has a high log K_{ow} or has a structural similarity to other substances likely to bioaccumulate. Alternatively there are properties, which may indicate a higher bioaccumulation potential than that suggested by a substance's low log K_{ow} value. A survey of these factors is given below.

***n*-Octanol/water partition coefficient**

At the core data set level, the potential for bioaccumulation can be estimated from the value of the *n*-octanol/water partition coefficient, log K_{ow}, this parameter should be determined experimentally. If the test cannot be performed for the physico-chemical properties of the substance, then, a calculated value for log P as well as details of the calculation method must be provided. For further information please consult *Guidance on information requirements and chemical safety assessment, Chapter R.7a: Endpoint specific guidance* (c 7.1.8) available at https://echa.europa.eu/guidance-documents/guidance-on-information-requirements-and-chemical-safety-assessment.

It is accepted that values of log K_{ow} greater than or equal to 3 indicate that the substance may bioaccumulate. For certain types of chemicals, e.g. surface-active agents and those which ionise in water, log K_{ow} values may not be suitable for calculation of a BCF value.

There are, however, a number of factors that are not taken into consideration when BCF is estimated only on the basis of log K_{ow} values. These are:

- phenomena of active transport;
- metabolism in organisms and the accumulation potential of any metabolites;
- affinity due to specific interactions with tissue components;
- special structural properties (e.g. amphiphilic substances or dissociating substances that may lead to multiple equilibrium processes);
- uptake and depuration kinetics (leading for instance to a remaining concentration plateau in the organism after depuration).

n-Octanol only simulates the lipid fraction in organisms and therefore does not simulate other possibilities for storage and accumulation of substances and their metabolites in living organisms.

Adsorption

Adsorption onto biological surfaces, such as gills or skin, may also lead to bioaccumulation and an uptake via the food chain. Hence, high adsorptive properties may indicate a potential for both bioaccumulation and biomagnification. For certain chemicals, for which the octanol/water partition coefficient cannot be measured properly, a high adsorptive capacity (of which log K_p > 3 may be an indication) can be additional evidence of bioaccumulation potential.

Hydrolysis

The effect of hydrolysis may be a significant factor for substances discharged mainly to the aquatic environment: the concentration of a substance in water is reduced by hydrolysis so the extent of bioconcentration in aquatic organisms would also be reduced. Where the half-life, at environmentally relevant pH values (4-9) and temperature, is less than 12 hours, it can be assumed that the rate of hydrolysis is greater than that for uptake by the exposed organisms. Hence, the likelihood of bioaccumulation is greatly reduced. In these cases, it may sometimes be appropriate to perform a BCF test on the hydrolysis products, if identified, instead of the parent substance. However, it should be noted that, in most cases hydrolysis products are more hydrophilic and as a consequence will have a lower potential for bioaccumulation.

Degradation

Both biotic and abiotic degradation may lead to relatively low concentrations of a substance in the aquatic environment and thus to low concentrations in aquatic organisms. However, the uptake rate may still be greater than the rate of the degradation processes, leading to high BCF values even for readily biodegradable substances. Therefore ready biodegradability does not preclude a bioaccumulation potential, but for most readily biodegradable substances concentrations will be low in aquatic organisms.

If persistent metabolites are formed in substantial amounts the bioaccumulation potential of these substances should also be assessed. However, for most substances information will be scarce. From experiments with mammals information may be obtained on the formation of possible metabolites, although extrapolation of results should be treated with care.

Molecular mass

Certain classes of substances with a molecular mass greater than 700 are not readily taken up by fish, because of possible steric hindrance at passage of gill membranes or cell membranes of respiratory organs, but molecular weight alone is insufficient to demonstrate limited bioaccumulation potential. These substances are unlikely to bioconcentrate significantly (regardless of the log K_{ow}-value).

Summary of indications of bioaccumulation potential

Taking the factors mentioned above into account will indicate whether or not there is potential for bioaccumulation. In summary, if a substance:

- has a log $K_{ow} \geq 3$; or;
- has a BCF ≥ 100 L/kg_{ww}; or;
- has a BAF ≥ 100 L/kg_{ww}; or;
- has a BMF >1; or;
- is highly adsorptive; or;
- belongs to a class of substances known to have a potential to accumulate in living organisms; or;
- there are indications from structural features;
- and there is no mitigating property such as hydrolysis (half-life less than 12 hours);

there is an indication of bioaccumulation potential. It is noted that, in addition to the list above, there may be other factors affecting the bioaccumulation potential as well as further information sources to be taken into account in the overall assessment of bioaccumulation potential (e.g. molecular size, degradability, and information from mammalian toxicokinetic studies).

Reference is made to the OECD guidelines and to the guidance document on environmental hazard classification (OECD, 2001c) in relation to interpretation of bioaccumulation studies and measurements of log K_{ow}. The test guidelines also contain information on the suitability of the various log K_{ow} determination methods depending on the type of substance concerned. Further information on octanol-waterpartition coefficient and in bioaccumulation can also be found in the *Guidance on information requirements and chemical safety assessment, Endpoint specific guidance* Chapter R.7a (section 7.1.8) and Chapter R.7c (sections R.7.10) and R.11 available at https://echa.europa.eu/guidance-documents/guidance-on-information-requirements-and-chemical-safety-assessment.

3.8.3 Effects assessment for bioaccumulation and secondary poisoning

3.8.3.1 General approach

The assessment of the potential impact of substances on top predators is based on the accumulation of hydrophobic chemicals through the food chains which may follow many different pathways along different trophic levels. This accumulation may result in toxic concentrations in predatory birds or mammals ingesting biota containing the chemical. This effect is called secondary poisoning and should in principle be assessed by comparing the measured or estimated concentrations in the tissues and organs of the top predators with the no-effect concentrations for these predators expressed as the internal dose. In practice, however, data on internal concentrations in wildlife animals are hardly ever available and most no-effect levels are expressed in term of concentrations of the food that the organisms consume (i.e. in $mg \cdot kg^{-1}$ food). Therefore, the actual assessment (see below) is normally based on a comparison of the (predicted) concentration in the food of the top predator and the (predicted) no-effect concentration which is based on studies with laboratory animals. A distinction is made between the methodology used to assess the effects of substances whose effects can be related directly to bioconcentration (direct uptake via water) and those where also indirect uptake via the food may contribute significantly to the bioaccumulation. Bioaccumulation of metallic species is not considered explicitly in this section.

For substances with a log $K_{ow} < 4.5$ the primary uptake route is direct uptake from the water phase. In the absence of data on other uptake routes, it is assumed that the direct uptake accounts for 100 % of the intake. For substances with a log $K_{ow} \geq 4.5$, other uptake routes such as intake of contaminated food or sediment may become increasingly

important. Especially the uptake through the food chains eventually leading to secondary poisoning should be considered and a strategy for the assessment of secondary poisoning has been developed. This strategy takes account of the $PEC_{aquatic}$, the direct uptake and resulting concentration in food of aquatic organisms and the mammalian and avian toxicity of the chemical. On this basis, possible effects are estimated on birds and mammals in the environment via uptake through the food-chain water → aquatic organisms → fish → fish-eating mammal or fish-eating bird (Romijn et al., 1993). Due to the lack of experience with this approach the assessment is considered as provisional.

For some chemicals results from field measurements and monitoring data are available. Although interpretation is often difficult, these results can be used to support the assessment of risks due to secondary poisoning (Ma, 1994).

The first step in the assessment strategy is to consider whether there are indications for bioaccumulation potential. These indications have been discussed in the previous section. Subsequently, it is necessary to consider whether the substance has a potential to cause toxic effects if accumulated in higher organisms. This assessment is based on classifications on the basis of mammalian toxicity data, i.e. for substances:

- classified for acute toxicity cat. 1-4 – oral (H300, H301 and H302), dermal (H310, H311 and H312) and inhalation (H330, H331 and H332);
- classified for STOT-SE 1-2 (H370, H371), STOT-RE 1-2 (H372, H373);
- classified as presenting an aspiration hazard (H304);
- classified for reproductive toxicity cat. 1A-1B (H360) and cat. 2 (H361);
- classified for reproductive toxicity in a separate hazard category: effects on or via lactation (H362)[25].

Here it is assumed that the available mammalian toxicity data can give an indication on the possible risks of the chemical to higher organisms in the environment.

The current, either qualitative or quantitative, approach in the human health risk assessment for genotoxic carcinogens is not practicable in the environmental part. Tumor incidence rates for a genotoxic carcinogen and subsequent cancer risks are related to individual risks in man and it is in most cases difficult to link those effects to populations. Endangoured species might be an exception, particularly those characterized by long-life-cycles where individuals may need to be protected to support survival of the species. It is not unlikely, however, that the conservative approach followed in the risk assessment for man indirectly exposed via the environment for genotoxic substances, will also be protective for individual top predators.

If a substance is classified accordingly or if there are other indications (e.g. endocrine disruption), an assessment of secondary poisoning is performed.

A schematic view of the assessment scheme for the exposure route water → aquatic organisms → fish → fish-eating mammal or fish-eating bird described above is given below:

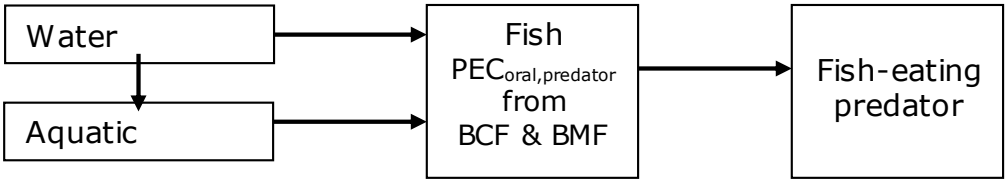

Figure 15: Assessment of secondary poisoning

No specific assessment of the risk to fish as a result of the combined intake of contaminants

[25] The translation between DSD and CLp classification needs to be checked.

from water and contaminated food (aquatic organism) is considered necessary as this is assumed to be covered by the aquatic risk assessment and the risk assessment for secondary poisoning of fish-eating predators.

The risk to the fish-eating predators (mammals and/or birds) is calculated as the ratio between the concentration in their food ($PEC_{oral,\ predator}$) and the no-effect-concentration for oral intake ($PNEC_{oral}$). The concentration in fish is a result of uptake from the aqueous phase and intake of contaminated food (aquatic organisms). Thus, $PEC_{oral,\ predator}$ is calculated from the bioconcentration factor (BCF) and a biomagnification factor (BMF). Note that $PEC_{oral,\ predator}$ could also be calculated for other relevant species that are part of the food of predators.

The details of the individual assessment steps are described in the following sections.

3.8.3.2 Calculation of BCF from log K_{ow}

If measured BCF values are not available, the BCF for fish can be predicted from the relationship between K_{ow} and BCF. Various methods are available to calculate K_{ow}, such as:

- Quantitative structure-activity relationships (QSARs);
- Expert systems; and
- Grouping approaches (including read-across, structure-activity relationships (SARs) and chemical categories).

Often a large variation is found in the K_{ow} values of a chemical by using different methods. Therefore the K_{ow}-value must have been evaluated by an expert. For substances with a log K_{ow} of 2-6 the following linear relationship can be used as developed by Veith et al. (1979).

$$\log BCF_{fish} = 0.85 \cdot \log Kow - 0.70$$ **Equation 93**

Explanation of symbols

K_{ow}	octanol-water partition coefficient	[-]
BCF_{fish}	bioconcentration factor for fish on wet weight basis	[l·$kg_{wet\ fish}$]

For substances with a log K_{ow} higher than 6 a parabolic equation can be used.

$$\log BCF_{fish} = -0.20 \cdot logKow^2 + 2.74 \cdot \log Kow - 4.72$$ **Equation 94**

Explanation of symbols

K_{ow}	octanol-water partition coefficient	[-]
BCF_{fish}	bioconcentration factor for fish on wet weight basis	[l·$kg_{wet\ fish}$]

It should be noted that due to experimental difficulties in determining BCF values for such substances this mathematical relationship has a higher degree of uncertainty than the linear one. Both relationships apply to compounds with a molecular weight less than 700.

3.8.3.3 Experimentally derived BCF

Traditionally, bioconcentration potential has been assessed using laboratory experiments that expose fish to the substance dissolved in water. In most cases preference should be given to experimentally determined BCF values, especially if the test is conducted according to EU Annex V C.13 and OECD guideline 305 (OECD, 2012). Dietary bioaccumulation tests might be better considered for adsorptive and poorly water-soluble substances (when it is

technically not feasible to test), than the OECD 305 guideline, because a higher and more constant exposure to the substance can be administered via the diet than via water. A further advantage is that multiple substances, including mixtures, can be investigated in a single test.

The following parameters may be of importance when considering the results of testing:

- BCF (bioconcentration factor);
- CT_{50} (clearance time, elimination or depuration expressed as half-life);
- metabolism/ transformation;
- organ-specific accumulation (reversible/ irreversible);
- incomplete elimination (bound residues);
- substance bioavailability.

Past work has shown that tests with substances with a high log K_{ow} value result in high bioaccumulation factors if the chemical is carefully tested within the limit of its water solubility, i.e. without enhancement of solubility by the use of solubilisers. Also, the test duration is very important because for highly hydrophobic chemicals it may take a very long time before a true steady-state situation between water and organism has been reached. In addition, such lipophilic substances may be adsorbed onto biological surfaces such as gills, skin etc. which may lead to toxic effects in higher organisms after biomagnification.

For a more detailed guidance on interpretation of bioaccumulation test data, the OECD guidance document on environmental hazard classification (OECD, 2001c) or the *Guidance on information requirements and chemical safety assessment,* Chapter R.11 (PBT Assessment) may be consulted.

3.8.3.4 Calculation of a predicted environmental concentration in food

The concentration of contaminant in food (fish) of fish-eating predators ($PEC_{oral,\ predator}$) is calculated from the PEC for surface water, the measured or estimated BCF for fish and the biomagnification factor (BMF):

$$PEC_{oral,predator} = PEC_{water} \cdot BCF_{fish} \cdot BMF$$ **Equation 95**

Explanation of symbols

$PEC_{oral,predator}$	Predicted Environmental Concentration in food	$[mg \cdot kg_{wet\ fish}^{-1}]$
PEC_{water}	Predicted Environmental Concentration in water	$[mg \cdot l^{-1}]$
BCF_{fish}	bioconcentration factor for fish on wet weight basis	$[l \cdot kg_{wet\ fish}^{-1}]$
BMF	biomagnification factor in fish	[-]

The BMF is defined as the relative concentration in a predatory animal compared to the concentration in its prey ($BMF = C_{predator}/C_{prey}$). The concentrations used to derive and report BMF values should, where possible, be lipid normalised.

An appropriate PEC_{water} reflecting the foraging area of fish-eating mammals and birds should be used for the estimate. The foraging area will of course differ between different predators which makes it difficult to decide on an appropriate scale. For example use of PEClocal may lead to an overestimation of the risk as fish-eating birds or mammals do also forage on fish from other sites than the area around the point of discharge. Also, biodegradation in surface water is not taken into account using PEClocal. However, using PECregional may have the opposite effect, as there may be large areas in the 200 x 200 km region with higher

concentrations. It has therefore been decided that a scenario where 50 % of the diet comes from a local area (represented by the PEClocal) and 50 % of the diet comes from a regional area (represented by the PECregional) is the most appropriate for the assessment.

The biomagnification factor (BMF) should ideally be based on measured data. However, the availability of such data is at present very limited and therefore, the default values given in **Table 23** should be used. By establishing these factors it is assumed that a relationship exists between the BMF, the BCF and the log K_{ow} (for further explanation, see **section 2.6** of this guidance on marine risk assessment). The recommended BCF triggers take into account more realistically the potential for metabolism in biota. Due to this the use of measured BCF values as a trigger would take precedence over a trigger based on log K_{ow}.

Table 23: Default BMF values for organic substances

log Kow of substance	BCF (fish)	BMF
<4.5	< 2,000	1
4.5 - <5	2,000-5,000	2
5 – 8	> 5,000	10
>8 – 9	2,000-5,000	3
>9	< 2,000	1

3.8.3.5 Calculation of the predicted no-effect concentration ($PNEC_{oral}$)

Only toxicity studies reporting on dietary and oral exposure are relevant because the pathway for secondary poisoning is referring exclusively to the uptake through the food chain. Secondary poisoning effects on bird and mammal populations rarely become manifested in short-term studies. Therefore, results from long-term studies are strongly preferred, such as NOECs for mortality, reproduction or growth. If no adequate toxicity data for mammals or birds are available, an assessment of secondary poisoning cannot be made.

The results of mammalian repeated-dose toxicity tests and data for birds (e.g. OECD test 205 (1984h): LC_{50}, 5-day acute avian dietary study or OECD test 206 (1984i): chronic) are used to assess secondary poisoning effects. Extrapolation from such test results gives a predicted no-effect concentration in food ($PNEC_{oral}$) that should be protective to other mammalian and avian species. Nevertheless, it should be considered that information from the dietary toxicity tests could be used on a case-by-case basis in higher-tier assessments when appropriate. This risk assessment scheme does not routinely use output from the LC_{50} study (EFSA 2008, Risk Assessment for Birds and Mammals).

Acute lethal doses LD_{50} (rat, bird) are not acceptable for extrapolation to chronic toxicity, as these are not dietary tests. Acute effect concentrations (e.g. OECD 205 (1984h)) for birds are acceptable for extrapolation. The results of the available mammalian or avian tests may be expressed as a concentration in the food ($mg \cdot kg_{food}^{-1}$) or a dose ($mg \cdot kg_{bw} \cdot day^{-1}$) causing no effect. For the assessment of secondary poisoning, the results always have to be expressed as the concentration in food. In case toxicity data are given as NOAEL only, these NOAELs can be converted to NOECs with the following two formulae:

$$NOEC_{bird} = NOAEL_{bird} \cdot CONV_{bird}$$ **Equation 96**

$$NOEC_{mammal,food\_chr} = NOAEL_{mammal,oral\_chr} \cdot CONV_{mammal}$$ **Equation 97**

Explanation of symbols

$NOEC_{bird}$	NOEC for birds	$(kg \cdot kg_{food}^{-1})$	
$NOEC_{mammal,\ food\ chr}$	NOEC for mammals	$(kg \cdot kg_{food}^{-1})$	
$NOAEL_{bird}$	NOAEL for birds	$(kg \cdot kg_{bw} \cdot d^{-1})$	
$NOAEL_{mammal,\ oral\ chr}$	NOAEL for mammals	$(kg \cdot kg_{bw} \cdot d^{-1})$	
$CONV_{bird}$	conversion factor from NOAEL to NOEC	$(kg_{bw} \cdot d \cdot kg_{food}^{-1})$	**Table 24**
$CONV_{mammal}$	conversion factor from NOAEL to NOEC	$(kg_{bw} \cdot d \cdot kg_{food}^{-1})$	**Table 24**

Conversion factors (body weight/daily food intake ratio) for laboratory animals are presented in Table 24. For further information, please see **Appendix 2**.

Table 24: Conversion factors from NOAEL to NOEC for several mammalian and one bird species

Species	Conversion factor (BW/DFI*)
Canis domesticus	40
Macaca sp.	20
Microtus spp.	8.3
Mus musculus	8.3
Oryctolagus cuniculus	33.3
Rattus norvegicus (> 6 weeks)	20
Rattus norvegicus (≤ 6 weeks)	10
Gallus domesticus	8

* BW = body weight (g); DFI: daily food intake (g/day)

NOECs converted from NOAELs have the same priority as direct NOECs.

The $PNEC_{oral}$ is ultimately derived from the toxicity data (food basis) applying an assessment factor. In formula:

$$PNEC_{oral} = \frac{TOX_{oral}}{AF_{oral}}$$ **Equation 98**

Explanation of symbols

$PNEC_{oral}$	PNEC for secondary poisoning of birds and mammals	[in $kg \cdot kg_{food}^{-1}$]	
AF_{oral}	assessment factor applied in extrapolation of PNEC	[-]	**Table 25**
TOX_{oral}	either $LC_{50\ bird}$, $NOEC_{bird}$ or $NOEC_{mammal,\ food,\ chr}$	[in $kg \cdot kg_{food}^{-1}$]	

The assessment factor (AF_{oral}) takes into account interspecies variation, acute/subchronic to chronic extrapolation and laboratory data to field impact extrapolation. Some specific considerations need to be made for the use of the assessment factor for predators.

CCME (1998) contains wildlife data on body weight and daily food ingestion rates for 27 bird and 10 mammalian species. In addition, Schudoma et al. (1999) derived the mean body weight and daily food intake for the otter. The currently available set on wildlife BW/DFI

ratios ranges from 1.1 to 9 for birds and from 3.9 to 10 for mammalian species. Comparison of these wildlife conversion factors with the values given in **.**
Table 24 for laboratory species (8.3 – 40) shows that the wildlife species often have a lower BW/DFI ratio than laboratory animals. The difference can be up to a factor 8 for birds and 10 for mammals. This difference is in theory accounted for in the use of the interspecies variation factor that is part of the standard assessment factor. The interspecies variation, however, should comprise more than just the BW/DFI differences between species, e.g. the differences in intrinsic sensitivity. The protective value of the "normal" interspecies variation factor may therefore be questionable in case of predators. On top of that, many predator species are characterised by typical metabolic stages in their life-cycle that could make them extra sensitive to contaminants in comparison with laboratory animals (e.g. hibernation or migration). Similar to the BW/DFI differences, also this aspect goes beyond the "normal" interspecies variation.

The AF_{oral} should compensate for the above-mentioned specific aspects in the effects assessment of predators. A factor of 30, accounting for both interspecies variation and lab-to-field extrapolation, is considered to be appropriate for this purpose. Aditionally, acute/subchronic to chronic extrapolation needs to be taken into account. The resulting assessment factors are given in **Table 25**.

Table 25: Assessment factors for extrapolation of mammalian and bird toxicity data

TOXoral	Duration of test	AForal
$LC_{50\ bird}$	5 days	3,000
$NOEC_{bird}$	chronic	30
$NOEC_{mammal,\ food,chr}$	28 days 90 days chronic	300 90 30

If a NOEC for both birds and mammals is given, the lower of the resulting PNECs is used in the risk assessment. It is highly unlikely that sufficient avian toxicity data will be available for any substance to allow a species sensitivity distribution to be developed (i.e. an insufficient number of species will have been tested in long-term tests), so this is not considered further.

3.8.3.6 Assessment of secondary poisoning via the aquatic food chain

It should be recognised that the schematic aquatic food chain water → aquatic organism → fish → fish-eating bird or mammal is a very simplistic scenario as well as the assessment of risks for secondary poisoning based on it. Any other information that may improve the input data or the assessment should therefore be considered as well. For substances where this assessment leads to the conclusion that there is a risk of secondary poisoning, it may be considered to conduct additional laboratory tests (e.g. tests of bioaccumulation in fish or feeding studies with laboratory mammals or birds) in order to obtain better data.

The simplified food chain is only one example of a secondary poisoning pathway. Safe levels for fish-eating animals do not exclude risks for other birds or mammals feeding on other aquatic organisms (e.g. mussels and worms). Therefore it is emphasised that the proposed methodology gives only an indication that secondary poisoning is a critical process in the aquatic risk characterisation of a chemical.

For a more detailed analysis of secondary poisoning, several factors have to be taken into account (US EPA, 1993; Jongbloed et al., 1994):

- differences in metabolic rates between animals in the laboratory and animals in the field;

- normal versus extreme environmental conditions: differences in metabolic rate under normal field conditions and more extreme ones, e.g. breeding period, migration, winter;
- differences in caloric content of different types of food: cereals versus fish, worms or mussels. As the caloric content of fish is lower than cereals birds or mammals in the field must consume more fish compared to cereals for the same amount of energy needed leading to a higher body burden of the pollutant;
- pollutant assimilation efficiency: differences in bioavailability in test animals (surface application of a test compound) and in the field (compound incorporated in food) and/or;
- relative sensitivity of animals for certain chemicals: differences in biotransformation of certain compounds between taxonomic groups of birds or mammals. The US EPA uses a species sensitivity factor (SSF) which ranges from 1 to 0.01.

3.8.3.7 Assessment of secondary poisoning via the terrestrial food chain

Biomagnification may also occur via the terrestrial food chain. A similar approach as for the aquatic route can be used here. The food-chain soil → earthworm → worm-eating birds or mammals is used as has been described by Romijn et al. (1994). The $PNEC_{oral}$ is derived in the same way as for the aquatic route (see **section 3.8.3.5** of this guidance). Since birds and mammals consume worms with their gut contents and the gut of earthworms can contain substantial amounts of soil, the exposure of the predators may be affected by the amount of substance that is in this soil. The $PEC_{oral,\ predator}$ is calculated as:

$$PEC_{oral,predator} = C_{earthworm}$$ **Equation 99**

where $C_{earthworm}$ is the total concentration of the substance in the worm as a result of bioaccumulation in worm tissues and the adsorption of the substance to the soil present in the gut:

$$C_{earthworm} = \frac{BCF_{earthworm} \cdot C_{porewater} \cdot W_{earthworm} + C_{soil} \cdot W_{gut}}{W_{earthworm} + W_{gut}}$$ **Equation 100**

For PEC_{soil} the PEClocal is used in which with respect to sludge application the concentration is averaged over a period of 180 days (see **section 2.3.7.5** of this guidance). The same scenario is used as for the aquatic food chain (see **section 3.8.3.4** of this guidance): i.e. 50 % of the diet comes from PEClocal and 50 % from PECregional. Gut loading of earthworms depends heavily on soil conditions and available food (lower when high quality food like dung is available). Reported values range from 2-20 % (kg dwt gut/kg wwt voided worm), 10 % can therefore be taken as a reasonable value. The total concentration in a full worm can be calculated as the weighted average of the worm's tissues (through BCF and porewater) and gut contents (through soil concentration):

Explanation of symbols

$PEC_{oral,predator}$	Predicted Environmental Concentration in food	$[mg \cdot kg_{wet\ earthworm}^{-1}]$
$BCF_{earthworm}$	bioconcentration factor for earthworms on wet weight basis	$[L \cdot kg_{wet\ earthworm}^{-1}]$
$C_{earthworm}$	concentration in earthworm on wet weight basis	$[mg \cdot kg_{wet\ earthworm}^{-1}]$
$C_{porewater}$	concentration in porewater	$[mg \cdot L^{-1}]$

C_{soil}	concentration in soil	[mg·kg$_{wwt}^{-1}$]
$W_{earthworm}$	weight of earthworm tissue	[kg$_{wwt\ tissue}$]
W_{gut}	weight of gut contents	[kg$_{wwt}$]

The weight of the gut contents can be rewritten using the fraction of gut contents in the total worm where:

$$W_{gut} = W_{earthworm} \cdot F_{gut} \cdot CONV_{soil}$$ **Equation 101a**

$$CONV_{soil} = \frac{RHO_{soil}}{F_{solid} \cdot RHO_{solid}}$$ **Equation 102b**

Explanation of symbols

$CONV_{soil}$	conversion factor for soil concentration wet-dry weight soil	[kg$_{wwt}$·kg$_{dwt}^{-1}$]	
F_{solid}	volume fraction of solids in soil	[m^3·m^{-3}]	**Table 3**
F_{gut}	fraction of gut loading in worm	kg$_{dwt}$·kg$_{wwt}^{-1}$	0.1
RHO_{soil}	bulk density of wet soil	[kg$_{wwt}$·m^{-3}]	**Equation 20**
RHO_{solid}	density of solid phase	[kg$_{dwt}$·m^{-3}]	**Table 3**

The default wet-dry weight conversion factor for soil of **1.13** can be obtained using the default values of RHO_{soil}=1700 [kg$_{wwt}$·m^{-3}], RHO_{solid}=2500 [kg·m^{-3}] and the F_{solid} 0.6 [m^3·m^{-3}]. Using this equation, the concentration in a full worm can be written as:

$$C_{earthworm} = \frac{BCF_{earthworm} \cdot C_{porewater} + C_{soil} \cdot F_{gut} \cdot CONV_{soil}}{1 + F_{gut} \cdot CONV_{soil}}$$ **Equation 103c**

The BCF factors can be inserted in the above equation when measured data on bioconcentration in worms are available. For most substances, however, these data will not be present and BCF will have to be estimated. For organic chemicals, the main route of uptake into earthworms will be via the interstitial water. Bioconcentration can be described as a hydrophobic partitioning between the pore water and the phases inside the organism and can be modelled according to the following equation as described by Jager (1998):

$$BCF_{earthworm} = \left(0.84 + 0.012K_{ow}\right) / RHO_{earthworm}$$ **Equation 104d**

where for $RHO_{earthworm}$ by default a value of 1 (kg$_{wwt}$·L^{-1}) can be assumed.

Jager (1998) has demonstrated that this approach performed very well in describing uptake in experiment with earthworms kept in water. For soil exposure, the scatter is larger and the experimental BCFs are generally somewhat lower than the predictions by the model. The reasons for this discrepancy are unclear but may include experimental difficulties (a

lack of equilibrium or purging method) or an underestimated sorption[26].

Earthworms are also able to take up chemicals from food and it has been hypothesized that this process may affect accumulation at log K_{ow}>5 (Belfroid et al., 1995). The data collected by Jager (1998), however, do not indicate that this exposure route actually leads to higher body residues than expected on the basis of simple partitioning. Care must be taken in situations where the food of earthworms is specifically contaminated (e.g. in case of high concentrations in leaf litter) although reliable models to estimate this route are currently lacking.

The model was supported by data with neutral organic chemicals in soil within the range log K_{ow} 3-8 and in water-only experiments from 1-6. An application range of 1-8 is advised and it is reasonable to assume that extrapolation to lower K_{ow} values is possible. The model could also be used for chlorophenols when the fraction in the neutral form was at least 5 % and when both sorption and BCF are derived from the K_{ow} of the neutral species. The underlying data are however too limited to propose this approach in general for ionised chemicals.

3.9 Effects assessment from the marine compartment

3.9.1 Effects assessment for the marine aquatic compartment

3.9.1.1 Introduction

Marine effects assessment should ideally be based upon data generated using a range of ecologically relevant seawater species (for example algae, invertebrates and fish). However, such data are not always available and, therefore, guidance is given on how marine hazard assessment can be based on available data on both freshwater and seawater organisms.

Usually there are fewer studies available for seawater species than for freshwater ones (as well as fewer test methods available for seawater species).

The sensitivity to narcotic chemicals is considered to be highly comparable between freshwater and seawater species. However, the marine environment contains key/abundant taxa that are not present in freshwater environments (e.g Echinodermata, Ctenophora and Cephalopoda) Given the greater species diversity in the marine environment, compared to freshwaters, including the presence of a number of taxa that occur only in the marine environment, a broader distribution of sensitivities of species, and thus a higher uncertainty in extrapolation is needed. **Table 26** describes the assessment factors for marine hazard assessment, which includes a factor of 10,000 for assessments based on data from tests with the three standard freshwater species.

Historically, the patterns of chemical production and usage resulting from urban and industrial development have led to the freshwater environment being considered to be the hydrosphere most at risk from these substances. Consequently, most regulatory schemes for evaluating the hazards and risks posed by active substances have focussed primarily on the protection of freshwater communities. As a result there is a considerable body of data on the ecotoxicity of chemical substances to freshwater organisms (ECETOC, 1994a)[27].

Where there is a need to assess the potential impact of substances entering estuarine and seawaters, any hazard or risk assessment should ideally be based upon data generated

[26] According to certain studies some soil ingesting organisms may accumulate chemical substances not only from the soil pore water but also directly (possibly by extraction in the digestive tract) from the fraction of the substance adsorbed onto soil particles. This may become important for strongly adsorbing chemicals, e.g. those with a log K_{ow} > 3. For these compounds the total uptake may be underestimated. In other studies however it has been shown that soil digesters virtually only bioaccumulate the substance via the pore water, i.e. bioconcentrate chemical substances from the soil pore water. At present the latter process can be modelled by use of the equilibrium partitioning theory (cf. also Section 3.5).

[27] The ECETOC database consists of 2,203 entries on 361 chemicals, covering 121 species. Data on freshwater species accounted for 1862 entries (84.5%) while data for seawater (estuarine/marine) species accounted for 341 entries (15.5%).

using a range of ecologically relevant seawater species (for example algae, invertebrates and fish). This is particularly important given the greater diversity of species (particularly invertebrates) present in seawaters, relative to freshwaters. There are also circumstances, however, where the special conditions existing in a particular environment such as that existing in the Baltic Sea, give rise to a reduced or limited species diversity and/or specific stresses such as low or variable salinity. In such circumstances of low species diversity, adverse impacts in individual species can have devastating impacts on the specialised ecosystem. Thus, while high species diversity may lead to a wide sensitivity distribution, but also considerable functional overlap, low species diversity may result in a lower sensitivity distribution but increase the ecosystem function dependency on individual keystone species.

Due to these facts, the effects assessment must use, where possible, data relevant to the marine environment. However, compared to the situation for freshwaters, there are relatively few data on the effects of chemical substances on estuarine and marine organisms. Therefore, in practice there will be situations where seawater toxicity data are needed for hazard/risk assessments, but may not be available. In these situations it may be necessary to use freshwater data *in lieu* of data for estuarine/marine species (Schobben et al., 1994; Karman et al., 1998). In using data on freshwater species to characterise the risk in the seawaters, a clear understanding of the comparability of effects data generated on both types of species is necessary. Furthermore, there is some evidence, e.g. for some metals, that species living in brackish water are more susceptible because of the salinity (osmotic) stress they have to endure in contrast to those of the same species living in truly marine conditions. Under these circumstances the applicability of the toxicity data needs to be considered on a case-by-case basis.

3.9.1.2 Evaluation of data

It has been recognised for many years that there is a wider diversity of taxonomic groups (particularly invertebrates) in seawaters compared to freshwaters and that many groups are only found in seawater (see Russell and Yonge, 1928; Tait, 1978). Moss (1988) stated that 56 phyla were present in seawater compared to 41 in freshwaters. No phyla are confined to freshwaters only while 15 phyla are found only in seawater. These differences are partly due to the fact that multicellular animals originated in the seas and they have been well populated since the earliest fossil records.

Nevertheless, an important part of any evaluation of data must involve an assessment of the usefulness of the main body of freshwater ecotoxicity data in predicting effects in the marine environment. Where such data can be used, the focus of further investigation can concentrate on additional factors which specifically characterise the marine conditions. Studies conducted on the comparability of sensitivity of freshwater and marine species have been hampered by the low level of substances for which a comparable dataset has been available. Nevertheless where such data are available, it has tended to show that there is no systematic bias in sensitivity where comparable tests and endpoints are paired. A recent report which collated much of the available data confirmed these findings (ECETOC, 2000). Based on the currently available data, it can be concluded that:

- overall, the data reviewed and current marine risk assessment practice suggest a reasonable correlation between the ecotoxicological responses of freshwater and seawater biota - at least for the usual aquatic taxa (i.e., fish, crustacea, algae). No marked difference in sensitivity between freshwater and seawater biota appears that systematically applies across all three trophic levels considered;
- where evaluated, differences between trophic levels within each medium were generally as significant or even more marked than between media. Such variation is implicitly assumed in the use of assessment factors in current risk assessment practice;
- where differences in the apparent sensitivity of freshwater and marine biota were observed for individual compounds, such differences were consistently within a factor of 10 (<1 log unit) and usually somewhat less;

- average differences in sensitivity for such paired species comparisons were typically within a factor of ~2;

The use of freshwater acute effects data in lieu of or in addition to seawater effects data for risk assessment purposes is not contra-indicated by the empirical data reviewed. No comparison of long-term effects data has been made due to the lack of suitable data but again there are no reasons to believe that a systematic bias to freshwater or marine species would exist. Therefore it is proposed that data on freshwater or marine fish, crustacea and algae be used interchangeably for evaluation of the risks to either compartment. Under such circumstances, PNEC values should be derived from the most sensitive endpoint regardless of the medium. However, the use of pooled data is not recommended if there is data that shows that the species sensitivity between freshwater and marine organisms is above a factor of 10, when considering small datasets. With larger datasets, statistical testing is recommended, showing that there are no major differences in sensitivities amongst freshwater and seawater toxicity tests. Nevertheless, toxicity data for freshwater and seawater species for metals should not be pooled a priori since metal speciation in different environments may greatly influence bioavailability. Only when statistical comparison shows that there is no difference in sensitivity, the datasets for metals may be pooled. Note that this may differ per taxon.

Info-box 15: Use of freshwater data for the derivation of a PNEC for marine systems

For organic compounds, the improvement of ecotoxicity data through the pooling of marine and aquatic freshwater ecotoxicity data is possible for PNECwater and PNECseawater. Pooling of available marine and freshwater ecotoxicity data for derivation of the freshwater PNEC is possible as long as the species sensitivity between freshwater and marine organisms is within a factor of 10. For larger datasets statistical testing showing no major differences in sensitivities amongst freshwater and seawater toxicity tests should if needed to consider the pooling of data.

Note that in the event of pooling of toxicity data, the assessment factor table for the marine water compartment still applies to the pooled dataset.

For inorganic compounds, the datasets for freshwater and seawater may be pooled only when statistical comparison shows that there is no difference in sensitivity, given the effects that different environments may have on the speciation and bioavailability of metal species.

Additional information can be found in the UK Defra funded research project "Addressing interspecific variation in sensitivity and the potential to reduce this in ecotoxicological risk assessments". The project addressed the issue of differences in toxicity between marine and freshwater aquatic invertebrates:

http://randd.defra.gov.uk/Default.aspx?Menu=Menu&Module=More&Location=None&Completed=0&ProjectID=9596#RelatedDocuments

3.9.1.3 Derivation of PNEC

The greater species diversity in the marine environment, compared to freshwaters, including the presence of a number of taxa that occur only in that environment, may mean that the distribution of sensitivities of species is broader. It is necessary to consider, therefore, whether the three-taxon model offers sufficient certainty that sensitive species will be covered using the assessment factors developed for the freshwater systems. Since it is not possible to make a clear judgement on the basis of available data, it is considered prudent to assume that this greater diversity of taxa will produce a broader distribution of species sensitivity. Thus, where only data for freshwater or seawater algae, crustaceans and fish is available a higher assessment factor than that for the derivation of $PNEC_{seawater}$ for freshwaters should be applied, to reflect the greater uncertainty in the extrapolation. Where data is available for additional taxonomic groups, for example rotifers, echinoderms or molluscs the uncertainties in the extrapolation are reduced and the magnitude of the assessment factor applied to a dataset can be lowered. Test protocols for these groups are

available from organisations such as the American Society for Testing and Materials, the International Council for the Exploration of the Seas and the United States Environmental Protection Agency (OECD, 1998a). The assessment factors given are based on current scientific understanding on the species comparability of toxicity between freshwater and seawater species and the issue of differences in diversity in freshwaters and seawaters. These may need to be revisited as additional information becomes available.

It is recognised that the assumption of a greater species sensitivity distribution covering the additional marine taxa is based on limited data and is precautionary. The generation of additional toxicity data on marine species may allow this assumption to be further refined such that lower or higher assessment factors may be considered following a systematic review of accumulating evidence.

The additional assessment factor is also considered sufficient to cover the situations noted above where low species diversity may result in high ecosystem dependency on individual species.

The assessment factors decrease in magnitude from higher values for short-term acute studies from which $L(E)C_{50}$ values have been derived to lower values for long-term chronic studies from which NOECs have been derived. For long-term studies the magnitude of the assessment factors also decreases as information on a wider range of species becomes available. The assessment factors described in **Table 26** are those that would normally be applied to the datasets available. There are some circumstances, however, where expert judgement may be applied to the interpretation of a dataset which may allow a pragmatic approach to the application of the factors and the generation of new data. In each case where expert judgement is so applied, a full justification must be provided.

Even when based on the same set of data, the $PNEC_{seawater}$ may differ from the $PNEC_{water}$.

Where data are available for additional marine taxonomic groups, the uncertainties are reduced and so the magnitude of the AF applied to a data set can be lowered (**Table 26**)

Data from studies with marine test organisms other than algae, crustaceans and fish, and/or having a life form or feeding strategy differing from that of algae, crustaceans or fish can be accepted as additional marine taxonomic groups and will allow a reduction in the AF applied (provided that the toxicity data are reliable and relevant). Marine species from taxa other than algae, crustaceans and fish include:

- Macrophyta. e.g. Sea grass (Zosteraceae)
- Mollusca. e.g. *Mytilus edulis, Mytulis galloprovincialis*.
- Rotifera e.g. *Brachyonus plicatilis*.
- Hydrozoa (Phylum Cnidaria) e.g. *Cordylophora caspia, Eirene viridula*;
- Annelida. e.g. *Neanthes arenaceodentata*.

In addition, marine organisms that belong to the taxa algae, crustaceans or fish but have a different life form or feeding strategy than the representatives in the freshwater toxicity dataset can be considered additional marine taxonomic groups and may also allow a decrease in the AF:

- Macro-algae. e.g. Enteromorpha sp., Fucus sp and Champia sp.
- Crustaceans (including crabs) are found in both freshwater and seawater.

However, crabs, for example, have a life form and feeding strategy very much different from Daphnia sp., which is the test organism which is nearly always present in the freshwater toxicity data set, or other common freshwater crustaceans. Thus, such species can be used to reduce the AF where other crustaceans may not. Examples of crabs used in toxicity tests include *Cancer magister*, *Cancer pagurus*, *Carcinus maenas* and *Cancer anthonyi*.

Table 26: Assessment factors proposed for deriving PNECseawater for different data sets

Data set	Assessment factor
Lowest short-term L(E)C_{50} from freshwater or seawater representatives of three taxonomic groups (algae, crustaceans and fish) of three trophic levels	10,000 [a)]
Lowest short-term L(E)C_{50} from freshwater or seawater representatives of three taxonomic groups (algae, crustaceans and fish) of three trophic levels, + two additional marine taxonomic groups (e.g. echinoderms, molluscs)	1000 [b)]
One long-term NOEC/EC_{10} (from freshwater or seawater crustacean reproduction or fish growth studies)	1000 [b)]
Two long-term NOEC/EC_{10} from freshwater or seawater species representing two trophic levels (algae and/or crustaceans and/or fish)	500 [c)]
Lowest long-term NOEC/EC_{10}s from three freshwater or seawater species (normally algae and/or crustaceans and/or fish) representing three trophic levels	100 [d)]
Two long-term NOEC/EC_{10}s from freshwater or seawater species representing two trophic levels (algae and/or crustaceans and/or fish) + one long-term NOEC from an additional marine taxonomic group (e.g. echinoderms, molluscs)	50
Lowest long-term NOEC/EC_{10}s from three freshwater or seawater species (normally algae and/or crustaceans and/or fish) representing three trophic levels + two long-term NOEC/EC_{10}s from additional marine taxonomic groups (e.g. echinoderms, molluscs)	10

Notes on Table 26:

Evidence for varying the assessment factor should in general include a consideration of the availability of data from a wider selection of species covering additional feeding strategies/ life forms/ taxonomic groups other than those represented by the algal, crustacean and fish species (such as echinoderms or molluscs). This is especially the case, where data are available for additional taxonomic groups representative of marine species. More specific recommendations as with regard to issues to consider in relation to the data available and the size and variation of the assessment factor are indicated below.

When substantiated evidence exists that the substances may be disrupting the endocrine system of mammals, birds, aquatic or other wildlife species, it should be considered whether the assessment factor would also be sufficient to protect against effects caused by such a mode of action, or whether an increase of the factor would be appropriate.

a): The use of a factor of 10,000 on short-term toxicity data is a conservative and protective factor and is designed to ensure that substances with the potential to cause adverse effects are identified in the effects assessment. It assumes that each of the identified uncertainties described above makes a significant contribution to the overall uncertainty.

For any given substance there may be evidence that this is not so, or that one particular component of the uncertainty is more important than any other. In these circumstances it may be necessary to vary this factor. This variation may lead to a raised or lowered assessment factor depending on the evidence available. Except for substances with intermittent release, as defined in **section 2.3.3.4** of this guidance, under no circumstances a factor lower than 1000 should be used in deriving a $PNEC_{seawater}$ from short-term toxicity data.

Evidence for varying the assessment factor could include one or more of the following:

- evidence from structurally similar compounds which may demonstrate that a higher or lower factor may be appropriate;
- knowledge of the mode of action as some substances by virtue of their structure may be known to act in a non-specific manner. A lower factor may therefore be considered. Equally a known specific mode of action may lead to a higher factor;
- the availability of data from a variety of species covering the taxonomic groups across at least three trophic levels. In such a case the assessment factors may only be lowered if multiple data points are available for the most sensitive taxonomic group (i.e. the group showing acute toxicity more than 10 times lower than for the other groups).

Variation from an assessment factor of 10000 should be fully reported with accompanying evidence.

b): An assessment factor of 1000 applies where data from a wider selection of species are available covering additional taxonomic groups (such as echinoderms or molluscs) other than those represented by algal, crustacean and fish species; if at least data are available for two additional taxonomic groups representative of marine species.

An assessment factor of 1000 applies to a single long-term NOEC (freshwater or seawater crustacean or fish) if this NOEC was generated for the taxonomic group showing the lowest L(E)C_{50} in the short-term algal, crustacean or fish tests.

If the only available long-term NOEC/EC_{10} is from a species which does not have the lowest L(E)C_{50} in the short-term tests, it cannot be regarded as protective of other more sensitive species using the assessment factors available. Thus, the effects assessment is based on the short-term data with an assessment factor of 10,000. However, normally the lowest PNEC should prevail.

An assessment factor of 1000 applies also to the lowest of the two long-term NOEC/EC_{10}s covering two trophic levels (freshwater or seawater algae and/or crustacean and/or fish) when such NOECs have not been generated for the species showing the lowest L(E)C_{50} of the short-term tests.

This should not apply in cases where the acutely most sensitive species has an L(E)C_{50}-value lower than the lowest NOEC/EC_{10} value. In such cases the PNEC might be derived by applying an assessment factor of 1000 to the lowest L(E)C_{50} of the short-term tests.

c): An assessment factor of 500 applies to the lowest of two NOEC/EC_{10}s covering two trophic levels (freshwater or seawater algae and/or crustacean and/or fish) when such NOECs have been generated covering those trophic levels showing the lowest L(E)C_{50} in the short-term tests with these species. Consideration can be given to lowering this factor in the following circumstances:

- It may sometimes be possible to determine with a high probability that the most sensitive species covering fish, crustacea and algae has been examined, that is that a further longer-term NOEC/EC_{10} from a third taxonomic group would not be lower than the data already available. In such circumstances an assessment factor of 100 would be justified;
- a reduced assessment factor (to 100 if only one short-term test, to 50 if two short-term tests on marine species are available) applied to the lowest NOEC/EC_{10} from only two species may be appropriate where:
    - short-term tests for additional species representing marine taxonomic groups (for example echinoderms or molluscs) have been carried out and indicate that these are not the most sensitive group, and;
    - it has been determined with a high probability that long-term NOEC/EC_{10}s generated for these marine groups would not be lower than that already obtained. This is particularly important if the substance does not have the potential to bioaccumulate.

An assessment factor of 500 also applies to the lowest of three NOECs covering three trophic levels, when such NOECs have not been generated from the taxonomic group showing the lowest L(E)C_{50} in short-term tests. This should, however, not apply in the case where the acutely most sensitive species has an L(E)C_{50} value lower than the lowest NOEC/EC_{10} value. In such cases the PNEC might be derived by applying an assessment factor of 1000 to the lowest L(E)C_{50} in the short-term tests.

d): An assessment factor of 100 will be applied when longer-term toxicity NOEC/EC10s are available from three freshwater or seawater species (algae, crustaceans and fish) across three trophic levels.

The assessment factor may be reduced to a minimum of 10 in the following situations:

- where short-term tests for additional species representing marine taxonomic groups (for example echinoderms or molluscs) have been carried out and indicate that these are not the most sensitive group, and it has been determined with a high probability that long-term NOEC/EC10s generated for these species would not be lower than that already obtained;
- where short-term tests for additional taxonomic groups (for example echinoderms or molluscs) have indicated that one of these is the most sensitive group acutely and a long-term test has been carried out for that species. This will only apply when it has been determined with a high probability that additional NOECs generated from other taxa will not be lower than the NOECs already available.

A factor of 10 cannot be decreased on the basis of laboratory studies only. For instance, the availability of mesocosm studies or (semi-) field data that reflect the proposed pattern of exposure might be used for decrasing the factor of 10. However, the data needs to be reviewed on a case-by-case basis.

Statistical extrapolation methods for calculation of PNEC for marine organisms could be used when sufficient data are available. More information on these methods and the prerequisites to apply them for risk assessment purposes can be found in **section 3.3.1.2** of this guidance.

Info-box 16: *Americamysis* is not to be considered an additional specifically marine species when deciding on the assessment factor for the marine PNEC

Daphnia and *Americamysis* belong to the same taxonomic group, both are crustaceans. Furthermore they do not have different feeding strategies and/or life forms. *Americamysis* is thus not to be counted as an additional typically marine species.

3.9.2 Effects assessment for the marine sediment compartment

3.9.2.1 Introduction

Substances that are highly hydrophobic may be assessed as of low risk for pelagic fauna but can accumulate in sediments to concentrations at which they might exert significant toxic effects (SETAC, 1993). This may be of concern particular in the marine environment, where the sediment may act as a permanent sink for highly hydrophobic substances that can be accumulated to a large extent. Because seawater sediment constitutes an important compartment of marine ecosystems it may be important to perform an effects assessment for the seawater sediment compartment for those substances.

Several test methods on sediment are developed and used in Member States of the European Union. Most of the tests are used for sediment management purposes; only a few tests are conducted for risk assessment of substances. An inventory of tests with marine organisms for the evaluation of dredged material and sediments has been compiled by the Federal Environment Agency of Germany, UBA (Herbst and Nendza, 2000). It comprises of biotests with various species of marine organisms of different trophic levels on whole sediment, pore water or sediment extracts. In addition, OECD has prepared a detailed review paper on aquatic ecotoxicity tests including seawater sediment test methods (OECD, 1998a). Only whole sediment tests with infaunal and epibentic organisms are considered suitable for being used in a risk assessment of the seawater sediment compartment. From examination of the UBA and OECD inventories it is clear that no fully internationally accepted, standardised test methods for whole sediment are currently available.

Most of the existing whole sediment tests measure acute toxicity; only a few measure long-term, sub-lethal endpoints. Only the latter tests are considered applicable to marine risk assessment because of the long-term exposure of benthic organisms to sediment-bound substances that occur under field conditions.

In **section 3.9.1.2** of this guidance freshwater toxicity data are compared to marine and estuarine data. It is concluded that the use of freshwater acute effects data *in lieu* or together with seawater effects data is acceptable for risk assessment purposes. Although it is not sure that this also applies to sea- and freshwater sediment data, it is nevertheless recommended to use pooled sea- and freshwater sediment toxicity data for effect assessment for the sediment compartment. However, when sufficient data for ecologically relevant seawater species are available lower assessment factors can be applied.

3.9.2.2 Strategy for effects assessment for sediment organisms

In principle, the same strategy as applied to freshwater sediment is recommended (see **3.5** of this guidance) for the effects assessment of seawater sediment). Substances that are potentially capable of depositing on or sorbing to sediments to a significant extent have to be assessed for toxicity to sediment-dwelling organisms. In addition, seawater sediment effects assessment is necessary for substances that are known to be persistent in seawater, and may accumulate in sediments over time. Further information on the exposure related triggers for sediment risk assessment are provided in **section 2.3.7.4** and **Info-box 10**.

For most substances the number of toxicity data on benthic and sediment organisms will be limited. As a screening approach the equilibrium method can be used to compensate for the lack of toxicity data if a PEC_{seased} can be determined on the basis of a measured concentration of the substance in water that is independent of the value of the K_{oc}. If the PEC/PNEC determined using this method is > 1 then the need for testing with benthic organisms using spiked sediment should be considered.

It is not necessary to apply the equilibrium partitioning method to predicted environmental concentrations obtained from application of an exposure model when such a model will have used the same K_{oc} or log K_{ow} value as that used to predict the $PNEC_{seased}$. The reason is that the resulting PEC/PNEC ratio for sediment will have the same value as for the water compartment. In this case no quantitative risk characterisation for seawater sediment should be performed. Under these circumstances the assessment conducted for the aquatic compartment will also cover the sediment compartment for chemicals with a log K_{ow} up to 5. For substances with a log K_{ow} > 5 (or with a corresponding K_{oc}), however, the PEC/PNEC ratio for the aquatic compartment is increased by a factor of 10. The increased factor is justified by the fact that the equilibrium partitioning method considers mainly the exposure via the water phase and does not include that potential additional accumulation via sediment ingestion may occur for certain types of sediment dwelling invertebrates.

Four situations can be distinguished for deriving a $PNEC_{sed}$:

1. where only results from acute tests with benthic freshwater organisms are available (at least one) the risk assessment is performed both on basis of the tests and on the basis of the equilibrium partitioning method. The lowest $PNEC_{seased}$ is then used for the risk characterisation.
2. where, in addition to the tests with freshwater benthic organisms, an acute toxicity test is performed with a marine benthic organism that is preferably representative of the same taxon that is judged to be the most sensitive in the freshwater tests. Under these circumstances an assessment factor of 1000 is applicable. A reduction of the assessment factor is only justified if sufficient long-term tests with sediment-dwelling organisms are available, and, if possible, where other evidence indicates that these tests include sensitive taxonomic groups. Also in this case a comparison with the screening approach has to be made and the lowest $PNEC_{seased}$ should be used for the risk characterisation.
3. where long-term toxicity data are available for benthic freshwater organisms. Under this circumstance the $PNEC_{seased}$ is calculated using assessment factors for long-term tests. This approach is explained in **section 3.9.2.4** of this guidance.
4. where long-term toxicity data are available for benthic freshwater *and* a minimum of two marine organisms. Under these circumstances a $PNEC_{seased}$ is calculated using the

lower assessment factors that are associated with data obtained from long-term tests. A $PNEC_{seased}$ obtained in **section 3.9.2.4** of this guidance.

Table 21 in **section 3.5.2** of this guidance presents an overview of different data configurations and explains how to use them for the risk characterisation for sediment. Attention should be paid to the fact that very often contaminants are not analysed in whole sediment but in a certain fraction of the sediment, for example in the sediment fraction of particles < 63 μm. The organic carbon content of this fraction is typically 15-30 % for seawater sediment while for whole seawater sediments it is generally less than 2 %. It is important, for reasons of comparability of PEC and PNEC values, that the organic carbon content of sediment used for toxicity tests are comparable with those of actual seawater sediments. The methodology to normalise measured PNEC values to the standard organic carbon content of the exposure models is presented in **Info-box 9**. If not there are likely to be concerns regarding the relative bioavailability of a substance in the different sediments.

3.9.2.3 Calculation of PNEC for seawater sediment using equilibrium partitioning

In the absence of any ecotoxicological data for sediment-dwelling organisms, but with measured data to predict the PEC_{seased}, the $PNEC_{seased}$ may provisionally be calculated using the equilibrium partitioning method. This method uses the $PNEC_{seawater}$ for aquatic organisms and the marine suspended matter/water partition coefficient. The assumptions that are made in this method are described in **section 3.5.3** of this guidance. Based on the equilibrium partitioning the following equation is applied:

$$PNECseased = \frac{Ksusp\ water}{RHO_{susp}} \cdot PNEC_{seawater} \cdot 1000$$ **Equation 105**

Explanation of symbols

$PNEC_{seawater}$	Predicted No Effect Concentration in seawater	$[mg \cdot l^{-1}]$	
RHO_{susp}	bulk density of suspended matter	$[kg \cdot m^{-3}]$	**Equation 20**
$K_{susp\ water}$	partition coefficient suspended matter water	$[m^3 \cdot m^{-3}]$	**Equation 27**
$PNEC_{seased}$	Predicted No Effect Concentration in seawater sediment	$[mg \cdot kg^{-1}]$	

In **section 3.5.2** of this guidance a remark is made with respect to the calculation of $PNEC_{seased}$ using the equilibrium partitioning method. The equilibrium partitioning method considers uptake via the water phase, while uptake may also occur via other exposure pathways such as ingestion of sediment or direct contact with sediment. This may be important, especially for chemicals that have a tendency to adsorb to sediment organic matter. Direct uptake from seawater sediment is also observed in studies with marine benthic organisms and may significantly contribute to the uptake of organic contaminants such as PAHs (Kaag, 1998). There is also however evidence from studies in soil and in seawater sediment that the proportion of the total dose taken up through intake of sediment particles remains low for chemicals with a log K_{ow} up to 5. From other studies it is obvious that feeding mode also influences uptake of substances (via water or ingestion of sediment). Furthermore, the absorption of contaminants in the gastrointestinal tract has been found to be increased compared with absorption from the surrounding water (Mayer et al., 1996; Voparil and Mayer, 2000). However, no quantitative conclusions can be drawn from these studies regarding uptake of substances from sediment.

For substances with a log K_{ow} greater than 5 (or with a corresponding $K_{p,\ sed}$) the equilibrium partitioning method is used in a modified way in order to take account of possible uptake via ingestion of sediment. Thus the resulting PEC/PNEC ratio is increased by a factor of 10 for these compounds. It should be borne in mind that this approach is considered as a

screening level assessment of the risk to sediment dwelling organisms. If with this method a PEC/PNEC > 1 is derived then tests, preferably long-term, with benthic organisms using spiked sediment have to be conducted in order for a realistic risk assessment appropriate to the sediment compartment to be carried out.

3.9.2.4 Calculation of PNEC for seawater sediment using assessment factors

If results from whole-sediment tests with benthic organisms are available the $PNEC_{seased}$ has to be derived using assessment factors. In establishing the size of the assessment factors, a number of uncertainties have to be addressed (cf. **section 3.2** of this guidance). **Table 27** describes the assessment factors for seawater sediment hazard assessment when only short-term sediment toxicity tests are available, and defines the assessment factors when at least one long-term sediment toxicity test is available.

Due to the generally long-term exposure of benthic organisms to sediment-bound substances, long-term tests with sub-lethal endpoints like reproduction, growth, emergence, sediment avoidance and burrowing activity are regarded as most relevant.

In contrast to the concept applied to the pelagic marine compartment, it is only necessary to have results from one acute sediment test for the assessment factor of 10000 to apply. Furthermore if only results from short-term tests with freshwater sediment-dwelling organisms are available (at least one) an assessment factor of 10,000 is also applied to the lowest value. The $PNEC_{seased}$ should also be calculated from the $PNEC_{seawater}$ using the equilibrium-partitioning method.

If, in addition to the results of tests with freshwater benthic organisms, a result from an acute toxicity test with a marine benthic organism (preferably representative of the same taxa that is most sensitive in aquatic freshwater or seawater tests) is available then an assessment factor of 1000 is applicable. Once again a $PNEC_{seased}$ should also be calculated from the $PNEC_{seawater}$ using the equilibrium partitioning method. A reduction of the assessment factor is only permitted if results from long-term tests with sediment-dwelling organisms are available.

A $PNEC_{seased}$ is derived by application of the following assessment factors to the lowest LC_{50} value from acute tests:

Table 27: Assessment factors for derivation of $PNEC_{seased}$ from short-term sediment toxicity tests

Available test results	Assessment factor	$PNEC_{seased}$
One acute freshwater or seawater test	10,000	Lowest of LC_{50}/10,000 and equilibrium-partitioning method
Two acute tests including a minimum of one seawater test with an organism of a sensitive taxa	1000	Lowest of LC_{50}/1000 and equilibrium-partitioning method

A $PNEC_{seased}$ is derived by application of the following assessment factors to the lowest $NOEC/EC_{10}$ value from long-term tests:

Table 28: Assessment factors for derivation of $PNEC_{seased}$ from long-term sediment toxicity tests

Available test results	Assessment factor [a)]
One long-term freshwater sediment test	1000
Two long-term freshwater sediment tests with species representing different living and feeding conditions	500

One long-term freshwater and one seawater sediment test representing different living and feeding conditions	100
Three long-term sediment tests with species representing different living and feeding conditions	50
Three long-term tests with species representing different living and feeding conditions including a minimum of two tests with marine species	10

a) The general principles of notes (c) and (d) as applied to data on aquatic organisms must also apply to sediment data. Additionally, where there is convincing evidence that the sensitivity of marine organisms is adequately covered by that available from freshwater species, the assessment factors used for freshwater sediment data may be applied. Such evidence may include data from long-term testing of freshwater and marine aquatic organisms, and must include data on specific marine taxa.

If no results from long-term tests with sediment organisms are available and the PEC/PNEC derived from the results of short-term sediment tests or via the equilibrium partitioning method is a cause for concern then the need for long-term testing with sediment organisms should be considered.

Since there are no chronic seawater sediment test methods that are internationally accepted the results from any tests should always be carefully evaluated. Several factors can contribute to variability in test results. Of major importance to sediment tests are the effects of grain size and organic carbon content of the sediment on the bioavailability of a substance. Sediment grain size can also be an important factor in tests for other reasons. For example, the extent to which bacteria can be adsorbed onto the sediment varies with particle size. Likewise, different species of amphipods prefer sediments with different particle size distributions. No satisfactory solution to the question which reference sediment should be considered appropriate is therefore currently available. One should thus consider the tolerance of a given species with regard to the grain size distribution of the sediments in question. Also spiking techniques have to be optimised because often water is spiked after spiking the sediment. In addition, more insight is needed in the uptake route of sediment bound contaminants in the organisms (exposure assessment).

Next to standardisation and test guidelines, it is necessary to further investigate the sensitivity, reproducibility and inter-laboratory variability of the tests. It must be mentioned that most available data on these facts concern the tests applied on field sediments, and not on spiked sediments.

Examples of sub-chronic and chronic toxicity tests with whole sediment are given in **Table 29**. Most of the tests have been developed for amphipods and polychaetes and some of them are recommended by the OECD (1998a). There is a need for chronic tests to be developed for Mollusca. Early life-stage tests with mussels and oysters are available for testing aqueous phases but no standardised test is available for testing whole seawater sediment samples. Chronic tests that measure effects on community structure are also available but these tests seem to be very insensitive. Functional endpoints tests, e.g. nutrient release rates, have been used to assess the effects of contaminated sediments (Dahllöff et al., 1999).

A final point that should be borne in mind is that single-species toxicity tests do not take account of the interactions between the sediment inhabiting fauna and the fate or behaviour of chemical substances, caused by e.g. bioturbation (Ciarelli et al., 1999; 2000). No procedures are currently available for assessing the significance of such interactions but it is clear that they could be of potential significance, particularly in respect of the bioavailability of a sediment contaminant.

Table 29: Acute and chronic whole sediment toxicity tests

Test organism	Acute or chronic test	Duration [days]	Endpoints	Reference	
AMPHIPODS					
Corophium sp. (*C. volutator* or *C. arenarium*)	chronic	28	survival, growth and reproduction	ASTM (1993), Environment Canada (Burton, 1992), (OECD, 1998a recommended)	Degrader. Organisms can be field collected. Cultivation causes intermediate to high expenses. Organism does not like coarse sediment. Low concern with regard to animal welfare. Ecologically important organisms relevance for exposed ecosystems is high. SOP [1)] available with field-collected organisms. Ringtested.
Leptocheirus plumulosus	chronic	28	survival, growth and reproduction	ASTM (1993), Environment Canada (Burton, 1992), US EPA (1996) EPA 600-R-01-020 (2001) Method for Assessing the Chronic Toxicity of Marine and Estuarine Sediment-associated Contaminants with the Amphipod *Leptocheirus plumulosus.*	Degrader. Grain size has a significant effect on survival, growth and reproduction. Survival is highest between 25 % clay and 75 % sand. Low concern with regard to animal welfare. Ecologically important organisms relevance for exposed ecosystems very high SOP [1)] available with field-collected organisms. Ringtested
POLYCHAETES					
Nereis/Neanthes sp Neanthes arenaceodentatakan cultivated	subacute/ chronic	12 - 28	survival - survival/ growth	ASTM (1994)	Distributed widely throughout the world. Can be cultivated on the laboratory; degrader. Low concern with regard to animal welfare relevance for

Test organism	Acute or chronic test	Duration [days]	Endpoints	Reference	
					exposed ecosystems very high. SOP [1] available, equipment and test species commercially available. Ringtested.
Arenicola marina	chronic	28	Survival	ASTM (1994) (OECD, 1998a recommended)	Degrader, wide tolerance of sediment grain size. Organism is found extensively over the OSPAR and Helsinki conventions area; cultivation is difficult Low concern with regard to animal welfare relevance for exposed ecosystems very high. SOP [1] available, equipment and test species commercially available. Ringtested.
Arenicola marina	subacute	10	Casting rate	Thain and Bifield (2001)	See row above. Changes in feeding rate have consequences for sediment communities. SOP [1] available, equipment and test species commercially available. OSPAR ringtested
ECHINODERMES					
Echinocardium cordatum	acute/ subchronic	14	Survival	Stronkhorst (OECD, 1998a recommended)	Degrader, SOP [1] available with field-collected organisms. Ringtested
MICROCOSM					
Nematodes	chronic	60	community structure	(Austen and Somerfield, 1997)	

1) Standard operating procedure

3.9.3 Assessment of secondary poisoning

3.9.3.1 Introduction

The assessment of the potential impact of substances on top predators in the marine environment can be based, in principle, on the same methodology as that used for a freshwater scenario. As with freshwater ecosystems the accumulation of hydrophobic chemicals through the marine food chains may follow many different pathways along different trophic levels. This accumulation may result in toxic concentrations in predatory birds or mammals ingesting aquatic biota containing the chemical. This effect is called secondary poisoning and should in principle be assessed by comparing the measured or estimated concentrations in the tissues and organs of the top predators with the no-effect concentrations for these predators expressed as the internal dose. In practice, however, data on internal concentrations in wildlife animals are hardly ever available and most no-effect levels are expressed in term of concentrations of the food that the organisms consume (i.e. in $mg \cdot kg^{-1}$ food). Therefore, the actual assessment is normally based on a comparison of the (predicted) concentration in the food of the top predator and the (predicted) no-effect concentration which is based on studies with laboratory animals. A distinction is made between the methodology used to assess the effects of substances whose effects can be related directly to bioconcentration (direct uptake via water) and those where also indirect uptake via the food may contribute significantly to the bioaccumulation.

Highly bioaccumulative substances have both a very high bioconcentration potential (log K_{ow} typically > 4.5 or BCF > 500) and are also resistant to biotransformation in animals. Biomagnification (increased food chain accumulation) of such chemicals is a major risk to the top predators of food webs, as the consumption of contaminated food is a major source of contaminants in predatory marine birds and mammals. In contrast the direct uptake of substances from the environment (that is from water and sediment) is only of minor relevance (Biddinger and Gloss, 1984; Opperhuizen, 1991). Factors that make these very hydrophobic substances of particular concern to the marine environment include longer food chains, migratory and reproductive aspects that may cause especially high exposure of progeny of marine species likely, long-life of many marine predators, and a higher fat content. However, whilst steady state levels in birds may be reached within weeks depending on the biological half-life of the chemical (Pearce et al., 1989), contamination levels in mammals may continually increase with age, with a plateau only being evident after several years (Thompson, 1990; Teigen et al., 1993).

No distinction can effectively be made between the spatial scales in the approach to the assessment since the predators will take food from sources spread across local and regional marine scenarios, as well as from the open sea. In the assessment it is therefore proposed to use a $PEC_{seawater}$ based on the mean of the local and regional concentrations for the assessment of the local situation, and for the regional situation to apply a spatially broader scale. Given that marine predators may have a wider range of foraging and that the regional sea concentrations will normally be lower, this is considered as a reasonable worst-case assumption.

Bioaccumulation of metallic species is not considered explicitly in this section.

3.9.3.2 Assessment of bioaccumulation and secondary poisoning

The assessment scheme

The principal endpoints for the secondary poisoning assessment are the predators and top predators that prey on organisms that are in direct contact with the marine aqueous phase and receive the substances from this source. A relatively simple food chain is modelled which consists of the seawater phase, marine food, marine fish and two separate levels of predators. This food chain is visualised in **Figure 16**. As can be seen from this scheme risks for three different trophic levels need to be assessed:

1. *risks to marine fish:* No specific calculation needs to be performed for estimating the risk to marine fish as this is covered by the risk assessment for aquatic organisms.

2. *risks to marine predators:* The risk to marine predators is calculated as the ratio between the concentration in their food (marine fish) and the no-effect concentration for oral intake ($PNEC_{oral,\ predator}$). The concentration in the marine fish (C_{fish}) is obtained from bioconcentration of the substance from the aqueous phase and (for very hydrophobic substances) as a result of bioaccumulation from the food the fish consumes (which consists of different types of aquatic organisms). Therefore, both a bioconcentration factor (BCF) and a biomagnification factor (BMF_1) are used to calculate C_{fish}. Note that for the BCF_{fish} also information for other organisms such as mussels may be considered.
3. *risks to marine top predators:* The risk to marine top-predators is calculated as the ratio between the concentration in their food (marine predators) and the no-effect concentration for oral intake ($PNEC_{oral,\ top\ predator}$). Since very hydrophobic substances may biomagnify in the tissue and organs of the predator, for the calculation of the internal concentration of the predator an additional biomagnification factor (BMF_2) must be applied. Note that no additional BMF factor for the top predator itself is required since the comparison between PEC_{oral} and $PNEC_{oral}$ is not based on internal concentrations but on intake rates.

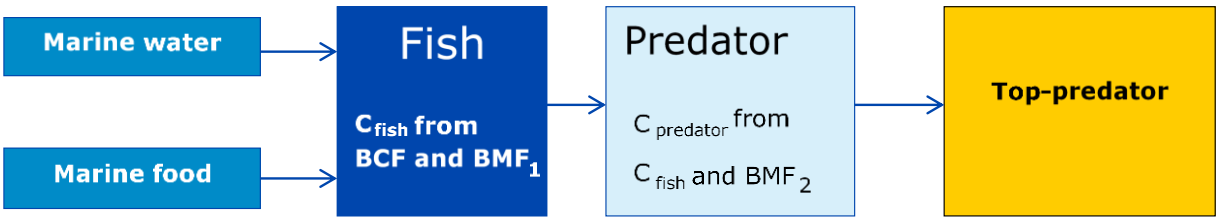

Figure 16: Secondary poisoning food chain.

It is realised that food chains of the marine environment can be very long and complex and may consist of 5 or more trophic levels. The possible extent of bioaccumulation in marine food chains with more than the above three to four trophic levels should be evaluated case by case if necessary input data for such an evaluation is available, using the principles for the shorter food chain. Also if further data are available it may be possible to refine the assessment of secondary poisoning via marine food chains by employing more advanced modelling that takes the differences in for instance uptake and metabolic rates into account for the different trophic levels.

In the relatively simple food chain given above the concentration in the fish (i.e. the food for the fish-eater) ideally should take account of all possible exposure routes, but in most instances this will not be possible because it is not clear what contribution each potential exposure route makes to the overall body burden of a contaminant in fish species. Therefore, for very hydrophobic substances a simple correction factor for potential biomagnification on top of the bioconcentration through the water phase is applied.

Calculation of PEC in food of predators

The actual calculation of the concentration of a chemical in the food of the predators and top predators will include the following steps:

$$PEC_{oral,toppredator} = PEC_{oral,predator} \cdot BMF_2 = PEC_{water} \cdot BCF_{fish} \cdot BMF_1 \cdot BMF_2$$ **Equation 106**

$$PEC_{oral,predator} = PEC_{seawater} \cdot BCF_{fish} \cdot BMF_1$$ **Equation 107**

Explanation of symbols

$PEC_{oral,\ predator}$	concentration in the food of the predator	[mg·kg^{-1}]	
$PEC_{oral,\ top\ predator}$	concentration in the food of the top predator	[mg·kg^{-1}]	
$PEC_{seawater}$	concentration in seawater	[mg·l^{-1}]	
BCF_{fish}	bioconcentration factor	[l·kg^{-1}]	**Equation 92**
BMF_1	biomagnification factor in fish	[-]	**Table 30**
BMF_2	biomagnification factor in the predator	[-]	**Table 30**

The BMF used should, ideally, be based on measured values. BMFs can be derived from trophic magnification studies. Additional guidance can be found in the Water Framework Directive Technical Guidance for deriving Environmental Quality Standards. However, the limited availability of such data means that in most instances the default values described below may have to be used. The use of a default value represents a screening approach designed to identify substances for which it may be necessary to obtain more detailed information on the biomagnification factor.

Although there may be relationships between the magnitude of the BMF and the log K_{ow} of the substance under defined conditions, the available data are not conclusive. Other more complex intrinsic properties of substances, than the lipophilicity (log K_{ow}), seems to be important as well as the species under consideration (e.g. its biology in relation to uptake, metabolism etc.). As a simple screening approach, however, it seems reasonable to assume that for organic substances with a log K_{ow} up to 4.5 biomagnification seems generally to be low and thus BMF = 1. For higher log K_{ow} the biomagnification increases up to around log K_{ow} 7 and then it decreases again to be low around log K_{ow} 9 (Fisk et al., 1998). Based on data published by Rasmussen et al. (1990), Clark and Mackay (1991), Evans et al. (1991) and Fisk et al. (1998), the default BMF values in **Table 30** are suggested. If a BCF for fish is available, it is possible to use that as a trigger instead of log K_{ow}. The BCF triggers recommended are less conservative than the log K_{ow} triggers because they more realistically take the potential for metabolism in biota (i.e. fish) into account. Due to this increased relevance, the use of BCF as a trigger would take precedence over a trigger based on log K_{ow}.

Table 30: Default BMF values for organic substances with different log Kow or BCF in fish

log Kow	BCF (fish)	BMF1	BMF2
< 4.5	< 2,000	1	1
4.5 - < 5	2,000-5,000	2	2
5 – 8	> 5,000	10	10
> 8 – 9	2,000-5,000	3	3
> 9	< 2,000	1	1

The derivation of appropriate default BMFs can only, at this stage, be considered as preliminary for use in screening of chemicals for the purposes of identifying those that need further scrutiny. In reviewing the appropriateness of the BMF applied in any particular assessment, it should be recognised that factors other than the log K_{ow} and BCF should also be taken into account. Such factors should include the available evidence that may indicate a potential for the substance to metabolise or other evidence indicating a low potential for biomagnification. Evidence of a potential for significant metabolism may include:

- data from in vitro metabolism studies;
- data from mammalian metabolism studies;

- evidence of metabolism from structurally similar compounds;
- a measured BCF significantly lower than predicted from the log K_{ow}, indicating possible metabolism.

Where evidence exists suggesting that such metabolism may occur, the BMF detailed above may be reduced. Where such reductions are proposed, a detailed justification must be provided.

Application of different spatial scales

Apart from the fact that for the assessment of the risks to the top predator an additional biomagnification factor is used the assessment also differs in terms of the input values that are used for the seawater concentrations that lead to the concentrations in the food of the different predators. For the first tier (or trophic level) of predators a worst-case assumption is that they obtain their prey equally from the local and regional area, respectively. This is in line with the assessment for freshwater and terrestrial organisms where a similar choice is made. For the calculation of the PEC_{oral} for the predators this implies the following:

$$PEC_{seawater} = 0.5 \cdot \left(PEClocal_{seawater,ann} + PECregional_{seawater}\right)$$ **Equation 108**

When $PEC_{seawater}$ is substituted in **Equation 89** this results in the following equation:

$$PEC_{oral,predator} = \left(PEClocal_{seawater,ann} + PECregional_{seawater}\right) \cdot 0.5 \cdot BCF_{fish} \cdot BMF_1$$ **Equation 109**

Explanation of symbols

$PEC_{oral,\ predator}$	concentration in the food of the predator	$[mg \cdot kg^{-1}]$	
$PEC_{seawater}$	concentration in seawater	$[mg \cdot l^{-1}]$	
BCF_{fish}	bioconcentration factor	$[l \cdot kg^{-1}]$	**Equation 90**
BMF_1	biomagnification factor in fish	[-]	**Table 30**
$PECregional_{,seawater}$	predicted environmental concentration in the region	$[mg \cdot l^{-1}]$	
$PEClocal_{,\ seawater,ann}$	annual average predicted environmental concentration	$[mg \cdot l^{-1}]$	

For the second tier of organisms, the top predators, it can be assumed that they obtain their prey mainly from the larger-scale regional marine environment which is to a lesser extent influenced by point source discharges. However, since it cannot be ruled out that certain top predators prey on organisms that receive their food from relatively small areas it is proposed to assume, as a realistic worst case, a 90/10 ratio between regional and local food intake. For the calculation of the oral intake rate for the top predator ($PEC_{oral,\ top\ predator}$) this implies:

$$PEC_{oral,top-predator} = \left(0.1 \cdot PEClocal_{seawater,ann} + 0.9 \cdot PECregional_{seawater}\right) \cdot BCF_{fish} \cdot BMF_1 \cdot BMF_2$$ **Equation 110**

When PEC_{water} is substituted in **Equation 90** this results in the following equation:

$$PEC_{water} = 0.1 \cdot PEClocal_{seawater,ann} + 0.9 \cdot PECregional_{seawater}$$ **Equation 111**

Derivation of the $PNEC_{oral}$ values

In the derivation of the $PNEC_{oral}$ values only toxicity studies reporting on dietary and oral exposure are relevant as the pathway for secondary poisoning refers exclusively to the uptake of chemicals through the food chain. However, reliable toxicity data for predatory marine birds (such as gulls and penguins) and mammals (such as seals, dolphins, whales and polar bears) are extremely limited (Nendza et al., 1997). Furthermore, testing of such species would be ethically unsound and contrary to animal welfare concerns. Therefore, it is necessary to extrapolate threshold levels for marine species from terrestrial species assuming there are interspecies correlations between laboratory bird species and marine predatory bird species, and between laboratory mammals (e.g. rats) and the considerably larger marine predatory mammals. This procedure is identical to that applicable for other media (see **section 3.8.3.5** of this guidance).

3.9.3.3 Testing strategy

If the PEC/PNEC ratio based on use of default BMF values indicates potential problems at any trophic level it should first be considered whether a refinement of the PEC-assessment is possible, i.e. the release and exposure assessment, including the fate related parameters such as determination of log K_{ow} or BCF. In special cases it may even be considered to start with bioaccumulation studies in fish to determine the assimilation coefficient and the biological half-life of the substance (i.e. to determine BMF_1) prior to estimating or determining the bioconcentration factor (BCF). Also a refinement of the $PNEC_{oral}$ could be considered, i.e. to require a long-term feeding study with laboratory mammals or birds to derive a more realistic $NOEC_{oral}$ value. In conducting such a study according to current test methods, it may in special cases be considered whether to extend such studies to include satellite groups for determination of the concentration of the substance in the animals during exposure (i.e. to measure BMF_2 values). Alternatively or supplementary to actual testing can be monitoring of biota for which it is clear that they have lived in the environment that is covered in the assessment. Of course no active sampling of (top) predators should be performed, but for instance animals that are found dead can be used to get an indication about possible biomagnification factors in wildlife. Useful information might also be obtained from eggs or from biopsies of skin or blubber of marine birds or mammals.

3.10 Effects assessment for rapidly degrading substances

3.10.1 Introduction

This chapter was provided as a proposal for harmonisation in the use of the time weighted average (TWA) and other available approaches to define effect data endpoints in aquatic and soil studies where the test concentrations cannot be maintained throughout the test.

Much of the available guidance on environmental testing, exposure and risk assessment strategies concentrates on the issue of persistence and does not sufficiently address the issue of rapidly degrading substances. This is of particular concern for risk assessors and experimenters when testing the effects of non-persistent or rapidly degrading substances in tests where method modifications such as flow-through or static-renewal are not practical i.e. algal, sediment and soil ecotoxicological tests. Furthermore, several biocidal uses result in a continuous or semi-continuous long-term emission of such non-persistent substances. Therefore, additional guidance on how and when to assess the no effect concentration is desirable for substances in aquatic and soil studies where the concentrations cannot be maintained throughout the exposure period of the test.

Special care should be taken in the evaluation of such rapidly degrading substances that this rapid degradation is sufficiently considered for a balanced risk characterisation (PEC/PNEC). If a substance shows a rapid degradation, this is normally already considered for the exposure estimation, leading to a correspondingly lower PEC. To use nominal or initial measured concentrations on the effects side instead of (mean) measured concentrations would lead to an underestimation of the risk for the environment. This

means, there is no disadvantage of degradable substances by using the approach outlined below but it ensures a balanced risk assessment. However, the reverse situation often occurs in the risk assessment for the terrestrial compartment. $PNEC_{soil}$ is often based on studies with initial soil concentrations, i.e. exposure in tests is not corrected for degradation. Therefore, for the soil compartment the PEC_{soil} should not be corrected for degradation, given that if the PEC_{soil} was corrected but the test soil concentrations were not, that would lead to an underestimated risk quotient ($PEC_{soil}/PNEC_{soil}$).

3.10.2 Proposal for a harmonised assessment

The following proposals provide a basis for a consistent approach to assess ecotoxicological endpoints for active substances that rapidly degrade in the test system. These proposals only apply to robust tests conducted following standard guidelines where the substances tested cannot be maintained throughout the test even using techniques such as semi-static or flow-through. These rules cannot be applied for endpoints to be derived from unacceptable or poor quality studies.

The proposals are based on the OECD Guidance Document No. 23 (2000) on aquatic toxicity testing of difficult substances and mixtures, with additional consideration of the potential exposure patterns for biocidal products. These approaches are to be used for the determination of the mean exposure concentration in acute or chronic tests where a substance can be shown to degrade significantly over the course of a test (< 80 % of nominal reported).

The following options are available:

a) If measured concentrations at test start and end are available for all concentration levels tested or for the concentration levels that are close to the derived effect value, the geometric mean of the concentrations measured at test start and test end for each treatment may be calculated as an approximation of the actual exposure.

b) When concentrations have been determined on more than two occasions during a test, the time weighted average concentration may be calculated according to Annex 2 of OECD Guidance Document 23 (OECD, 2000):

$$C_{\text{twa}} = \text{antilog}\left[\frac{1}{2\cdot(t_n - t_1)}\cdot\sum_{i=1}^{i=n}(\log(C_i)+\log(C_{i+1}))\cdot(t_{i+1}-t_i)\right]$$

Equation 112

Explanation of symbols

C_{twa}	time weighted average concentration
$t_n - t_1$	total time period over which the weighted concentration is calculated
C_1	initial concentration
C_i	concentration at time point *i*,
C_{i+1}	concentration at next time point after *i*
n	last time point at which a concentration measurement is available

It is noted that equal results are obtained when the natural logarithm of concentrations is used with base *e* instead of $\log_{10}$ values and base 10.

If only concentrations at test start and end are available, this equation is mathematically equal to the calculation of the geometric mean (see option a).

It is noted that OECD guideline 211 (OECD, 2012) gives an alternative equation for calculation of the weighted mean concentration for tests in which the concentrations of the test substance decline over the period between medium renewals. The outcome of the equations is similar to that of OECD GD 23 for DT50 values of ~ 2 days and higher (difference is a factor of 1.02 at DT50 2 days).

The difference in outcome of OECD GD 23 and OECD guideline 211 is explained as follows. Departing from the assumption of a concentration decrease following first order kinetics, OECD GD 23 uses logarithmised concentrations and the resulting degradation pattern is a straight line. OECD guideline 211 also departs from the assumption of first order kinetics, but uses a non-transformed, linear concentration axis. If a renewal test is performed according to OECD guideline 211, the calculation method of that guideline applies.

c) Where a measured concentration at the end of the exposure period is absent or where it indicates that the substance is not detected, the validity of the test should first be reconfirmed. If analytical data indicates that the substance could not be:

i. detected by the end of the study, the final concentration may be taken as the limit of detection (LOD) and the mean (geometric) measured concentrations can be calculated as in (a).

ii. quantified by the end of the study, the final concentration may be taken as half the limit of quantification (LOQ/2) for the method and the mean (geometric) measured concentrations can be calculated as in (a).

Since there may be various methods for determining the above parameters, the method selected to determine mean measured concentrations should be made explicit in the reporting of test results. This is because the concentration might not be measurable.

The above mentioned options that are taken directly from the OECD GD on Difficult Substances and apply mainly to aquatic studies including algae. Aquatic studies for rapidly degrading substances performed without any analytical monitoring have to be regarded as invalid as a deviation of more than 20 % from the nominal concentration is expected. This also applies to studies in which analytical monitoring was performed in a selection (not all) of the tested concentrations, and in which the analysed concentrations do not include the effect level (EC50, EC10 and NOEC). Only if it is clear that decline is not concentration dependent, degradation rates observed in the analysed test levels may be extrapolated to other levels.

Soil and sediment studies

The calculation of a time averaged concentration for static soil (or sediment) tests is only used for substances that do not degrade too fast in the test system as this would lead to unrealistically low effect values. The following cases are proposed:

1) Substances with an expected degradation half-life of < 2 d:

It is unlikely that a sensitive endpoint from a static soil or sediment study (test duration normally in the range of 14 – 21 d) can be derived, as the use of a time averaged concentration would result in unrealistically low effect values. For such substances, any toxicity observed in the tests might predominantly be caused by one or more degradation product(s). The use of the nominal or initial measured concentration is nevertheless justified if the PNEC derived from these tests is compared with the initial PEC without considering degradation, if the true exposure pattern due to the biocidal use is similar to that of the effect test method. In addition, a risk assessment for the relevant metabolites would need to be performed. If the environmental exposure is due to a semi-continuous pattern, it is

proposed to sum, in the exposure assessment, the PEC of the active substance and the PEC of the metabolite(s), then this PEC would be compared with the PNEC based on nominal or initial measured concentrations.

2) Substances with an expected degradation half-life of ≥ 2 d:

As indicated above, if the exposure pattern due to the biocidal use is similar to that of the terrestrial ecotoxicity test, it is justified to compare the PNEC based on nominal or initial measured concentrations with the initial PEC. However, when the predicted environmental concentration (PEC) is expressed as a time averaged concentration, the PNEC for soil/sediment studies is derived using the time averaged method. The risk assessment should also consider the relevant metabolite(s).

This approach may also be applicable to substances with a half-life < 2 d for which continuous release or repeated emissions result in continuous or increasing exposure in soil. As indicated in **section 2.3.5.7**, a case-by-case decision on the selection of initial or time averaged PEC and PNECsoil should be taken to ensure that the risk assessment is protective.

If analytical monitoring was also performed in soil studies the approaches given above under a) - c) may also apply to these studies. In most soil studies, however, analytical monitoring is absent and the mean exposure concentration may be calculated according to the TWA approach as detailed for Plant Protection Products (see e.g. EFSA 2009, Appendix H; FOCUS, 2014, section 11.4.1).

$$C_{\text{tavg}} = C_0 \times \left(\frac{1 - e^{-kt}}{kt}\right)$$ **Equation 113**

Explanation of symbols

C_0	Initial concentration (at test start) in terrestrial toxicity test
k	degradation rate constant from aerobic soil degradation study =ln2/DT_{50}
t	Test duration of terrestrial ecotoxicity test

The half-life to be used for the estimation of *k* should be selected from experimental soil degradation studies based on expert judgement. It should be corrected to the standard test temperature of the ecotoxicity test. However, the calculation of a time averaged concentration is only valid when the degradation pattern follows first order kinetics. It is assumed that application of half-lives derived for natural soil to ecotoxicological studies performed with artificial soil, represents a worst-case situation, as the degradation of the test substance in the artificial soil is likely lower than in natural soils due to the lower microbial activity. However, as normally no other information on degradation in the experimental soil is available, it is recommended to use these half-lives as a first approach. If a risk is identified based on the half-lives from soil degradation studies, a new effect test could be performed with chemical analysis of the test substance concentration in the test system at least at test start and test end; for long-term tests or if fast degradation is expected additional measurements between test start and end (in separate analytical vessels) are advisable.

The absence of biological observations at different time intervals during the test hamper a proper evaluation of the relationship between exposure and effects. Any information on the time to effects in the ecotoxicity test should be used to decide on the appropriate averaging time for deriving a TWA-concentration. If for a substance there is information on the mode of action from which it can be concluded that effects are only expected to be acute (e.g. oxidising substances), the initial concentrations can be used for the effects assessment and

compared with the initial PEC for the risk characterisation. Examples for such substances are hydrogenperoxide or hypochlorite. However, for most biocidal active substances this information is not available. It has to be considered that the information available on the mode of action from efficacy tests cannot automatically be used to conclude on the mode of action in ecotoxicity tests, as a substance can act by different mode of actions (e.g. herbicidal and insecticidal activity) or the available information does not allow a statement on acute versus chronic effects.

3.11 Assessment of exclusion criteria

Active substances cannot be approved if they fulfil the exclusion critera according to Article 5(1) of the BPR:

1. are carcinogens category 1A or 1B, mutagens category 1A or 1B, or toxic for reproduction category 1A or 1B,
2. have endocrine-disrupting properties, or
3. are persistent, bioaccumulative and toxic (PBT) or very persistent and very bioaccumulative (vPvB)

Derogations apply according to Article 5(2) of the BPR if the risk is negligible, the substance is essential to control a serious danger to human or animal health or to the environment, or the non-approval will have disproportionate negative impact for society.

Ad 2): For the assessment of endocrine disrupting properties, guidance is currently under preparation.

Ad 3): PBT substances are substances that are persistent, bioaccumulative and toxic, while vPvB substances are characterised by a particular high persistence in combination with a high tendency to bio-accumulate, but not necessarily proven toxicity. These properties are defined by the criteria laid down in section 1 of Annex XIII of REACH (*Criteria for the Identification of Persistent, Bioaccumulative and Toxic Substances, and very Persistent and very Bioaccumulative Substances*, henceforth "the PBT and vPvB criteria").

Experience with PBT/vPvB substances has shown that they can give rise to specific concerns that due to their potential to accumulate in parts of the environment and/or biota, and the effects of such accumulation are unpredictable in the long-term; such accumulation is practically difficult to reverse as cessation of emission will not necessarily result in a reduction in the substances concentration.

Furthermore, PBT or vPvB substances may have the potential to contaminate remote areas that should be protected from further contamination by hazardous substances resulting from human activity as the intrinsic value of pristine environments should be protected.

These specific concerns occur particularly with substances that can be shown both to persist for long periods and to bioaccumulate in biota and which can give rise to toxic effects after a longer time and over a greater spatial scale than chemicals without these properties. These effects may be difficult to detect at an early stage because of long-term exposures at normally low concentration levels and long life-cycles of species at the top of the food chain. In case of vPvB chemicals, there is concern that even if no toxicity is demonstrated in laboratory testing, long-term effects might be possible since high and unpredictable levels may be reached in human or the environment over extended time periods.

Guidance on how to conduct a PBT assessment as well as the screening criteria and information for the identification of PBT/vPvB properties on substances can be found in the *Guidance on information requirements and chemical safety assessment* Chapter R.11: PBT Assessment according to the criteria stated in Annex XIII of REACH. Nevertheless, the information requirement for the BPR may differ than that required for REACH.

Moreover, Article 2(3) of the BPR outlines the Directives and Regulations to which the BPR must also apply. The provisions for substance under these Directives and Regulations should also be considered for the assessment of exclusion criteria of biocidal active

substances.

3.12 Assessment of long-range environmental transportation

In accordance with the criteria set out in Article 19(1)(b) of the BPR, the biocidal product may be authorised provided that it has 'has no unacceptable effects itself, or as a result of its residues, on the environment, having particular regard to contamination of surface waters (including estuarial and seawater), groundwater and drinking water, air and soil, taking into account locations distant from its use following long-range environmental transportation.

Therefore it needs to be assessed whether the active substance is meeting the criteria for being a persistent organic pollutant (POP) under Regulation (EC) No 850/2004. This involves checking if the active substance or its degradation product is listed on Annex I of the Regulation (EC) No 850/2004 and assessing whether it exhibits the characteristics of persistent organic pollutants in accordance with the criteria set out in paragraph 1 of Annex D of the to the Stockholm Convention on Persistent Organic Pollutants. In this assessment, meeting of the following characteristics of persistent organic pollutants needs to be addressed:

- Assessment of long-range transport potential (LRTAP):
    - Vapour pressure <1000 Pa and
    - half-life in air > 2 days or
    - Monitoring data in remote area showing that the substance is found in remote regions or
    - Result of multi media modelling.
- The active substance or a degradation product is vP/vB or T.

4. Risk characterisation

According to BPR Annex VI, the risk characterisation for the environment considers the estimation of the incidence and severity of the adverse effects likely to occur in environmental compartments due to actual or predicted exposure to any active substance or substance of concern in a biocidal product.

For any given environmental compartment, the risk characterisation must, as far as possible, entail comparison of the PEC with the PNEC so that a PEC/PNEC ratio may be derived. If it has not been possible to derive a PEC/PNEC ratio, the risk characterisation must entail a qualitative evaluation of the likelihood that an effect is occurring under the current conditions of exposure or will occur under the expected conditions of exposure.

4.1 Introduction

Having conducted the exposure assessment and the dose (concentration) - response (effect) assessment for all environmental compartments, either a quantitative risk characterisation or a qualitative risk characterisation is carried out.

The quantitative risk characterisation is carried out by comparing the PEC with the PNEC. This is done separately for each of the environmental compartments identified in **section 1.1** and **Table 1** and
Table 2: Exposure levels used for indirect human exposure
Inland environmental compartments:

- aquatic ecosystem (including sediment);
- terrestrial ecosystem;
- atmosphere;

- top predators;
- microorganisms in sewage treatment plants;

Marine environmental compartments:

- aquatic ecosystem (inlcuding seawater sediment);
- top predators.

A list of the different PEC/PNEC ratios that should be considered for the inland and marine environments is given in **Tables 31** and **32**, respectively.

Table 31: Overview of PEC/PNEC ratios considered for fresh-/surface water risk assessment*

Local	Regional
$PEClocal_{, water}/PNEC_{water}$	$PECregional_{, water}/PNEC_{water}$
$PEClocal_{, sed}/PNEC_{sed}$	$PECregional_{, sed}/PNEC_{sed}$
$PEClocal_{, soil}/PNEC_{soil}$	$PECregional_{, agr.soil}/PNEC_{soil}$
$PEC_{stp}/PNEC_{stp}$	
$(0.5 \cdot PEClocal_{, oral, fish} + 0.5 \cdot PECregional_{, oral, fish})/PNEC_{oral}$	
$(0.5 \cdot PEClocal_{, oral, worm} + 0.5 \cdot PECregional_{, oral, worm})/PNEC_{oral}$	

* It has to be noted that these ratios have to be derived for all stages of the life-cycle of a compound.

Table 32: Overview of PEC/PNEC ratios considered for marine risk assessment *

Local	Regional
$PEClocal_{, seawater}/PNEC_{seawater}$	$PECregional_{, seawater}/PNEC_{seawater}$
$PEClocal_{, seased}/PNEC_{seased}$	$PECregional_{, seased}/PNEC_{seased}$
$[(PEClocal_{, seawater,ann} + PECregional_{, seawater}) \cdot 0.5 \cdot BCF_{fish} \cdot BMF_1]/PNEC_{oral, predator}$	
$[(0.1 \cdot PEClocal_{, seawater,ann} + 0.9 \cdot PECregional_{, seawater}) \cdot BCF_{fish} \cdot BMF_1 \cdot BMF_2]/PNEC_{oral, top predator}$	

* It has to be noted that these ratios have to be derived for all stages of the life-cycle of a compound.

When no quantitative risk characterisation can be carried out, for example for remote marine areas or when either PEC or PNEC cannot be properly derived, a qualitative risk characterisation should be conducted. This is described in **section 4.4** of this guidance.

4.2 General premises for risk characterisation

In general, the risk characterisation phase is carried out along the following steps:

- determine the PEC/PNEC ratios for the different environmental compartments considered. Care should be taken to ensure that PEC and PNEC values are expressed in a harmonized way. For example, for the sediment compartment both exposure and effect concentrations should be expressed on a dry weight basis, normalised to sediment with 2% organic carbon, if appropriate (see **Info-box 9** for further details).

Dependent on these PEC/PNEC ratios:

- determine whether further information/testing may lead to a revision of these ratios;
- ask for further information/testing when appropriate;

- refine the PEC/PNEC ratio.

This iterative process should be continued until a final conclusion regarding the environmental risks can be reached. The risk characterisation should describe the assumptions and uncertainties in a transparent manner.

For the risk characterisation for the aquatic and terrestrial ecosystems, including secondary poisoning, a direct comparison of the PEC and PNEC values is carried out, presuming that the relevant data are available. If the PEC/PNEC ratio is greater than one the substance is "of concern" and further action has to be taken.

For the air compartment usually only a qualitative assessment of abiotic effects is carried out. If there are indications that one or more of these effects occur for a given substance, expert knowledge should be consulted or the substance be handed over to the relevant international group, e.g. to the responsible body in the United Nations Environment Programme (UNEP) for ozone depleting substances. In some cases also an assessment of the biotic effects to plants can be carried out.

The risk characterisation for top predators is made by comparing the PEC_{oral} with the $PNEC_{oral}$ in accordance with the procedure described in **sections 3.8** and **3.9.3**. If the ratio PEC_{oral} / $PNEC_{oral}$ is greater than one and a refinement of the PEC_{oral} or the $PNEC_{oral}$ is not possible or reasonable, risk reduction measures should be considered.

The risk characterisation for microorganisms in sewage treatment systems is done by comparing the PEC_{stp} with the $PNEC_{stp}$. If the ratio of these two values is greater than one, this indicates that the substance may have a detrimental effect on the function of the STP and therefore is "of concern".

When PEC/PNEC ratios greater than one have been calculated, the competent authority should consult industry in order to see if additional data on exposure and/or ecotoxicity can be obtained in order to refine the assessment.

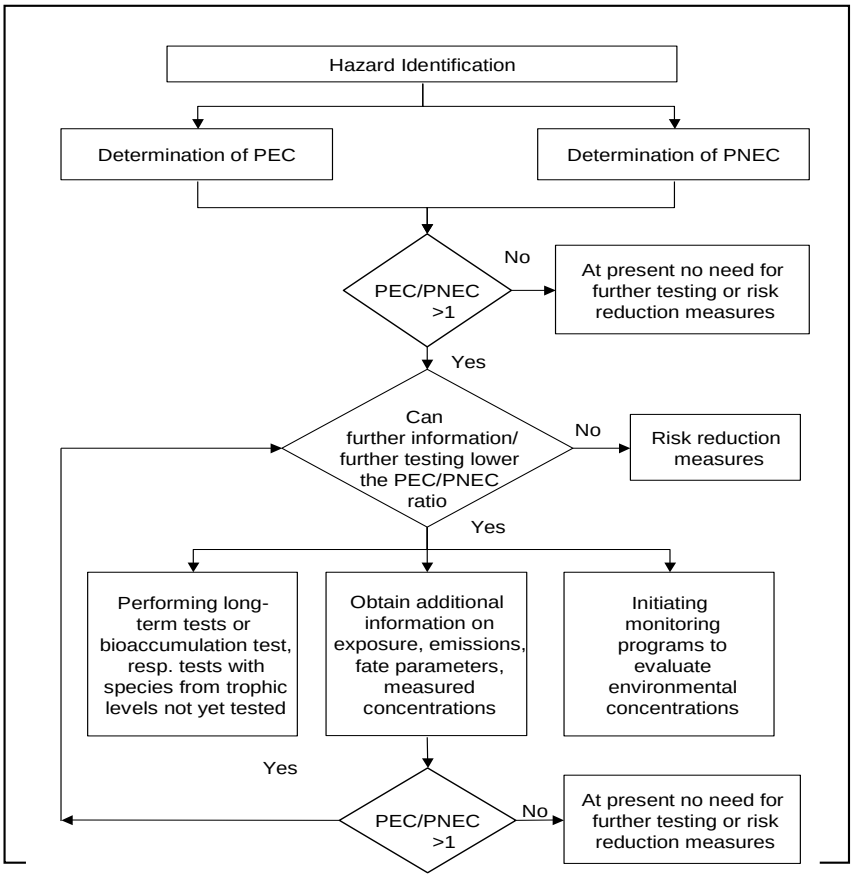

Figure 17: General procedure for environmentall risk assessment

Dependent on the value of the PEC/PNEC ratio, there may be cases where, assuming realistic PEC values which cannot be further refined (e.g. representative monitoring data) any further testing which lowers the assessment factor cannot decrease the PEC/PNEC ratio below one. In that case, no further testing should be required and risk reduction and mitigation measures are needed for the substance.

If a refinement of the risk characterisation is possible but the necessary data are not available, further information and/or testing needs to be requested. On a case-by-case basis, a decision must be taken as to whether both the PEC and PNEC will be revised or only one of them. Consideration should be given to which of the parameters that will be most sensitive to revision as a result of further testing. The decision by the competent authority to request additional data should be transparent and justified and should be based on the principles of lowest cost and effort, highest gain of information and the avoidance of unnecessary testing on animals. This iterative approach has precautionary aspects as data gaps are filled by worst-case assumptions or high assessment factors. Detailed guidance on how to use (Q)SARs in order to clarify whether further testing is necessary, and how these (Q)SARs can assist in deciding on the testing strategy, is given in Guidance on information requirements and chemical safety assessment. *Guidance on information requirements and chemical safety assessment Chapter R.6: QSARs and grouping of chemicals*.

Furthermore, the PEC for groundwater and surface water must be compared with the maximum permissible concentrations laid down by Directive 98/83/EC for groundwater and Directive 2000/60/EC and Directive 98/83/EC where the surface water in or from the area of envisaged use is intended for the abstraction of drinking water (see Annex VI, points 67-69 of the BPR).

4.3 Specific premises for the risk characterisation for biocides

The environmental risk characterisation for biocidal active substances in the context of BPR Annex VI involves i.a. the comparison of PEC and PNEC values for relevant environmental compartments as well as for non-target organisms. The possible results of the risk assessment are:

- there is a need for further information and/or testing;
- the substance has unacceptable effects on the environment and consequently, it cannot be included in the Union List of Authorised Active Substances of the Regulation (in the following referred to as Union List);
- the substance may be considered for inclusion in the Union List.

Info-box 17: Tiered approach

The risk to environmental compartment follows in general a tiered approach. The first tier is a general conservative evaluation of the behaviour and toxicity of the substance in the environment. It is in general based on model data regarding exposure, laboratory toxicology studies and for example, the equilibrium partitioning for certain PNEC derivations.

If the trigger values of the first tier of the evaluation are not met, the applicant is offered the opportunity to submit additional data for conducting a refined risk evaluation (higher tier). In general this includes additional chronic studies (aquatic and soil) and/or more realistic exposure data. Alternatively, the applicant can choose for risk reduction measures, but the applicant must prove that these measures are in practice realistic, effective and reduce the risk(s) to acceptable levels.

The decision on inclusion in the Union List of the BPR also depends on other criteria regarding, e.g., other unacceptable effects and efficacy (cf. Regulation 528/2012 and the Practical guide chapters in relation to Active Substances). The inclusion may, where appropriate, be subject to certain requirements and conditions for use.

Additional to these main conclusions, some substances included in the Union List may be candidates for substitution (Article 10 of the BPR Regulation). See also **section 4.7** of this guidance.

If the PEC/PNEC ratio is > 1 the competent authority must judge, on the basis of the size of that ratio and on other relevant factors, if further information and/or testing are required to clarify the concern, if risk reduction measures are necessary or if the substance cannot be included in the Union List at all.

Finally, if a quantitative risk characterisation cannot be conducted, a qualitative risk characterisation should be conducted, cf. below. For in-situ generated active substances, the risk assessment includes also the possible risks from the precursor(s).

Info-box 18: Risk assessment and data requirements for bees and beneficial arthropods

At the moment no method is available for biocides on how to perform the risk assessment for bees and non-target arthropods. The methods applied under the pesticides EU framework are not directly applicable. However, if tests on bees or non-target arthropods are performed, or are available, these could be use for a qualitative risk assessment if exposure pattern is comparable. Based on the outcome of these tests risk mitigation measures can be considered.

If tests on non-target arthropods have to be performed, tests on soil dwelling organisms like springtails are preferred.

With respect to the data requirement for bees and non-target arthropods (NTA) tests are required only in case of large scale-outdoor applications like fogging (e.g. products against mosquitoes for human health reasons).

Additionally, for neonicotinoid substances or other instecticide substances with high toxicity to bees, exposure to bees should also be quantified. When no data is available, a qualitative assessment should be performed.

4.4 Qualitative risk characterisation

Although the use of quantitative PEC/PNEC ratios is the preferred procedure for carrying out an environmental risk assessment, there may be cases where a quantitative risk characterisation cannot be carried out. Situations for which this might be the case include: the assessment of risks for remote marine areas, substances where either PEC or PNEC cannot be properly calculated, or when expert judgement suggests that the use of certain molecules will lead to negligible emissions (e.g., the use of ethanol, hydrogen peroxide or peracetic acid on surfaces). In these cases, the risk characterisation must entail a qualitative evaluation of the likelihood that an effect will occur under the expected conditions of exposure.

For some substances it may not be possible to undertake a full quantitative risk assessment, using a $PEC_{water}/PNEC_{water}$ ratio because of the inability to calculate a $PNEC_{water}$. This can occur when no effects are observed in short-term tests. However, an absence of short-term toxicity does not necessarily mean that a substance has no long-term toxicity, particularly when it has low water solubility and/or high hydrophobicity. For such substances, the concentration in water (at the solubility limit) may not be sufficient to cause short-term effects because the time to reach a steady-state between the organism and the water is longer than the test duration.

For these substances, therefore, it is recommended to conduct a qualitative risk assessment in order to decide if further long-term testing is required. Such an assessment should take full account of the level of exposure as well as of the probability that long-term effects may occur despite the absence of short-term effects. Thus, especially for non-polar organic substances with a potential to bioaccumulate (log K_{ow} > 3), the need for long-term testing is more compelling. For ionised substances or surfactants the determination of a trigger value on the basis of other physico-chemical properties, e.g. K_d should be sufficient to ask for long-term tests. Taking all this into account, long-term toxicity tests should be asked for immediately for substances with log K_{ow} > 3 (or BCF > 100) and a PEClocal or PECregional > $1/100^{th}$ of the water solubility.

The water solubility should, where possible, be based on the solubility in the aquatic toxicity test water rather than distilled water (presuming that this solubility is measured after filtration (0.45 μm) of the test solution or after centrifugation). When the log K_{ow} is not a good indicator of bioconcentration, or where there are other indications of a potential to bioconcentrate (see **section 3.8** of this guidance), a case-by-case assessment of the presumable long-term effects will be necessary.

4.5 Risk characterisations for specific substance groups

4.5.1 Risk characterisation for metals and metal compounds

4.5.1.1 Introduction

This section gives a general outline on how to perform risk assessments for metals using the methods that are available for risk assessment of active substances as a starting point. There are a number of fundamental differences between metals and organic chemicals that must be taken into account when assessing the risks to man and the environment, e.g.:

- unlike most organic chemicals, metals, and a limited number of organometallo compounds like methylmercury and methyltin, are a class of chemicals of natural origin. Consequently natural background concentrations and the exposure due to these background concentrations should be taken into account during risk assessment;
- the availability of metals for uptake by organisms under field conditions is limited, will vary from site to site and is highly dependent on the speciation of the metal. Hence, it is of utmost importance that both PEC and PNEC are based on similar levels of availability in both exposure and effect assessment, taking the speciation into account;
- the same toxic form can originate from a variety of different substances, e.g. Zn^{2+} from $ZnSO_4$, $ZnCl_2$. Therefore it is in general necessary to take into account all metal species that are emitted to the environment which in the end lead to concentrations of the toxic form.

Substantial levels of information are available regarding the fate and toxicity of metal ions and this information will be examined to improve the assessment process. However, it is recognised that many of the specific fate and toxicity extrapolations are either not appropriate or need modification. The interaction of metal ions with the media in both the aquatic and soil compartments may result in a high level of uncertainty regarding the true level of bioavailablity of the toxic species necessary for a practical assessment.

Organo-metallic compounds are not explicitly covered by this procedure unless they act, through their degradation products, as significant sources of the toxic metal ion. It is considered that these organo-metallic compounds can generally be assessed as individual substances in accordance with the procedures laid down in **section 3** of this guidance. When the emissions of these substances are major contributors to the toxic metal ion concentration in either a local or regional environment, they will be further assessed according to the procedures laid down in this document.

When describing the topics that need to be taken into consideration for the risk assessment of metals, there is often a misunderstanding with regard to definitions of some of the key terms.

The following definitions will be used for these key terms:

General:

- **total concentration of a metal**: for terrestrial systems, the concentration of a metal that is determined after complete destruction of the mineral matrix. For aqueous systems, the total amount of metal present, including the fraction sorbed to particles and to dissolved organic matter and the fraction in the mineral matrix;
- **available fraction**: the fraction of the metal that is extractable from the substrate with chemical (e.g. neutral salt, water extraction) or physical means (shaking, pore water collection), and that is generally considered to be a better estimate for the fraction that is potentially available for organisms than the total concentration;
- **bioavailable fraction**: the fraction that is available for uptake by a specific organism. A single substrate has only one 'availability' for each of the possible

physico-chemical extraction procedures. The bioavailability differs, however, per biological species. Thus, taking soil as an example, for instance for worms in a certain soil the bioavailability may be high (it is in this case the concentration in the pore water that determines uptake), while for arthropods in the same soil the bioavailability may be low (uptake by the food is for these organisms the dominant uptake route);

- **natural background concentration**: the concentration that is present due to natural causes only;
- **ambient background concentration**: the concentration that is present due to natural background plus the immission of metals from diffuse sources of human origin[28].

For soils or sediments:

- **water extractable fraction or concentration**: the fraction or the concentration of the metal that is extracted after shaking the substrate in aqueous solution (usually distilled water);
- **neutral-salt solution extractable fraction or concentration**: the fraction or the concentration of the metal that is extracted after shaking the substrate in neutral salt solution;
- **pore water concentration**: the concentration of the metal that is present in the pore water collected from the substrate;
- **pore water activity**: the concentration of a metal in the aqueous fraction that is potentially biologically active (usually considered to be the concentration of metal ions that can be taken up by organisms).

4.5.1.2 Exposure assessment

For the assessment of metals it is in general necessary to take into account all metal species that are emitted to the environment which in the end lead to concentrations of the bioavailable species that may cause effects. In practice, a limited number of major emissions or uses predominate and these must initially be identified. The assessment will normally concentrate on the impact of these emissions since they will be the major contributors to the regional burden, but due care must be paid to the impact of local emissions of specific substances. An inventory of all relevant emission sources must be prepared and specific industry and use categories identified for assessment of both local and regional impact.

Two types of emission can be identified: diffuse emissions and point source emissions. For some metal compounds, diffuse sources such as emissions from agriculture, transport, corrosion, etc. can make a significant contribution to the overall levels. For many substances, however, local emissions from point sources will need to be considered as well as the wider contribution to the regional burden.

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[28] In case of soil, for all metals so-called reference lines were derived by correlating measured ambient background concentrations (total concen-trations in the soil-matrix) at a series of remote rural sites in the Netherlands to the percentage lutum (% L) and the organic matter content (% H) of these soils (Ministry of VROM, 1994). The same approach has been followed in Flanders, Belgium (Ontwerp uitvoeringsbesluit, 1995). To this end the 90-percentiles of the ambient background concentrations measured were used. The metal-specific parameters of the regression equations represent the strength of binding of the different metals to soils of different clay and humus contents. The reference lines are not only used to calculate ambient background concentrations at given sites, but also to enable the extrapolation of laboratory toxicity data to standard-soil conditions. Some typical examples of reference lines derived in The Netherlands ([ ] = ambient background concentration in mg/kg soil, L = % lutum, H = % organic matter): $[Cu] = 15 + 0.6 \cdot (L + H)$; $[Zn] = 50 + 1.5 \cdot (2L + H)$ or $[Ni] = 10 + L$.

Local exposure assessment

As with organic compounds, the precise emissions will need to be identified and quantified for the whole life-cycle of the substance. Emission factors should initially be based on the substance being considered. It is important to know whether the substance is soluble in water, or can be transformed into a soluble form. Thus some knowledge of the chemistry of the particular substance and its interaction with the receiving media is important. Where the metal compound is soluble or can be transformed to a soluble form, the prediction of the environmental concentration, PEClocal, can be based on the relevant soluble metal ion. The behaviour of the substance in a wastewater treatment plant can be modelled using SimpleTreat, although measured K_p values will have to be used (**section 2.3.7** of this guidance). Since the actual bioavailability of the metal ion will be determined by the properties of the receiving media, such as the pH and water hardness, the precise physico-chemical characteristics of this receiving media must be defined. In general, it will be defined in a way which optimises the bioavailability of the toxic species. Speciation models exist which may be used to determine the soluble fraction. The partitioning behaviour of the substance to sludge/sediment/soil can be based on the appropriate K_p values for the soluble ion.

In some cases, the metal compound will be only poorly soluble and sufficiently stable to not rapidly transform to a water soluble form. In these circumstances, the substance itself should be assessed taking into account its specific partitioning characteristics. For the aquatic environment, it can be assumed as a first estimate that the substance will dissolve up to its water solubility limit, and that this fraction will be the bioavailable form. Refinement of the assessment may take into account kinetics of the dissolution.

Regional exposure assessment

As for organic substances, all emissions from both point and diffuse sources are assumed to contribute to the regional concentration, PECregional. Because of the wide range of transformation processes and longer timescales involved, it is assumed that all the individual metal compounds are changed to the ionic species. Where possible, information on kinetics of transformation processes should be taken into account.

As bioavailability is influenced by various physico-chemical characteristics of the environment it is important to define a 'standard environment', especially for a regional assessment. It is proposed that a regional assessment is carried out under conditions that optimise the bioavailability with respect to ranges for pH, water hardness etc that are found in the natural environment. This environment will probably differ for each metal assessed. Multimedia fate models can be used to assess exposure of man and ecosystems to metals on a regional scale. In applying multimedia fate models all emissions, including point sources, are assumed to be diffuse.

Transport of metals between the aqueous phase and soil/sediment/suspended matter should be described on the basis of measured soil/water, sediment/water and suspended matter/water equilibrium partition coefficients (K_p), instead of using common mathematical relationships based on, for example, octanol-water partition coefficients, as is usually done for organic chemicals (see **section 2.3.4** of this guidance). The same applies to the bioconcentration factors required: only experimentally determined values should be used. For soils, the K_p values to be used should, as far as possible, be derived for the soil type of interest. The soil usage should also be taken into account (for instance cultivated versus non-cultivated soils) since this may be of importance for the most appropriate K_p values. Often volatilisation is to be ignored. In such cases, most of the metal present in the atmosphere is predominantly bound to aerosols which means that rates of dry and wet deposition (in combination with the scavenging ratio) of atmospheric aerosols will suffice to quantify transport from the atmosphere. If biotransformation occurs this must be taken into account.

More specific guidance on the use of regional fate models is given in **Figure 18**.

In general, the mathematical descriptions of fate processes used in multimedia fate models are also applicable to local models.

Background concentrations

When assessing the exposure of man and ecosystems to metals previous releases into the environment need to be considered. In view of differences in bioavailability it is important to distinguish between ambient background concentrations and natural background concentrations. One should be aware that natural background concentrations within an environmental compartment may vary from site to site by several orders of magnitude. Also, due to natural dynamic processes like weathering, natural background concentrations may change over time. This means that it is impossible to attribute single values to natural background concentrations of specific metals within a certain compartment. It should be noted that under natural conditions in certain regions, clearly elevated natural background concentrations can be encountered. When assessing the natural background concentration within a certain area, these "outliers" should not be used or included in the calculation of the standard background concentrations as they would give a non-representative picture thereof.

Several methods are available for determining background concentrations. Apart from the obvious method of measuring metal levels at selected sites considered to be undisturbed by human activities, additional methods include:

Geochemical modelling: estimation methods on the basis of the contribution of weathering processes (erosion). This method is shown to be well applicable for assessing natural background concentration in aqueous systems (rivers).

Assessment of metal concentrations in the deeper sediment layers, taking into account anthropogenic contributions and leaching to these layers.

For surface water having ground water as its origin: assessment of the metal concentrations in the deeper ground water.

For soils, ambient background concentrations can be calculated as described above (reference lines). Through this procedure the natural binding capacity of soils, making the metal more or less inert in the solid phase, is approximated. Application of this procedure to both laboratory toxicity data and to field soils is possible.

For surface water, extensive national monitoring programs exist for the follow-up of metals in the aquatic environment since most metals are considered in the Council Directive 2006/11/EEC of the European Parliament and of the Council of 15 February 2006 on pollution caused by certain dangerous substances discharged into the aquatic environment of the Community as list I ("black list") or list II ("grey list") substances. Extraction of representative natural background concentrations may be possible from these data. However, these monitoring programs often measure total instead of dissolved metal concentrations.

Equilibrium partitioning/bioavailability

One should be aware that K_p values are both environment (site) and compound specific, and depend on the speciation of the metal in both the solid and the liquid (pore water) phase. The speciation of metals is strongly influenced by environmental factors like for instance temperature, redox conditions, pH, and composition of both the liquid and solid phase.

Multimedia fate models can be used to estimate exposure to metals. However, there are several differences compared to the use of these models for organic compounds. Below, differences are described for applying regional models.

1. Physico-chemical properties (**section 2.3.2**)

   In general water solubility, boiling point and vapour pressure cannot be used. The octanol-water partition coefficient is not appropriate and measured partition coefficients Kp should be used instead.

2. Partition coefficients (**section 2.3.5**)

   Adsorption to aerosol particles

Most of the metal present in the atmosphere will be bound to aerosols. Therefore, an extremely low value for the vapour pressure should be used in formula 5, e.g. 10-20 Pa. This leads to a value for Fass, aer almost equal to one. If a valid measured value is available, this value can be used.

Volatilisation

Volatilisation can be ignored for metals, except for mercury-compounds and several organometallo compounds. Therefore the Henry-coefficient should be set to a very low value (formula 6).

Adsorption/desorption

Formula 8 and 9 cannot be used. As stated above, measured Kp values must be used for water-soil, water-sediment and water-suspended matter.

3. Biotic and abiotic degradation rates (**2.3.6**)
   Not important for regional models.
4. Elimation processes prior to the release in the environment (**section 2.3.7**)

   For applying models like SimpleTreat a partition coefficient is used for water-sludge. For metals a measured Kp value must be used. However, it should be noted that Kp values are different for the different metal species.
5. Calculation of PECregional (**section 2.3.7.7**)

   The values applied for model parameters for the regional model (**Table 11**), intermedia mass transfer coefficients (**Table 12**) and model parameters for the continental concentration (**Table 13**) can be used.

In a natural soil or sediment system, metals can be distributed over the following fractions:

- dissolved in the pore water;
- reversibly or irreversibly bound to soil or sediment particles;
- reversibly or irreversibly bound to organic ligands;
- encapsuled in secondary clay minerals and metal(hydr)oxides;
- encapsuled in the primary minerals.

It is recognised that for various organisms, only the metal species present in the aqueous phase (pore water) are potentially available for direct uptake by biota and thus mainly responsible for effects on biota. Other uptake routes may also be important, especially for metals with high K_p values, but at the moment little is known on how to treat these processes quantitatively in the risk assessment. Processes determining the availability of metals for direct uptake by biota from the aqueous phase include precipitation, dissolution, adsorption, desorption and complexation. All processes mentioned are not only pH-dependent (adsorption of metal cations for instance increases with pH), but are also strongly influenced by competition for adsorption sites and to all complexation reactions likely to increase the solubility of the metal.

At the moment most K_p values are expressed in terms of total concentrations present in both the aqueous and the solid phase. As can be derived from the possible distribution sites for metals mentioned above, availability of metals for uptake by biota can differ from site to site and, due to amongst others weathering and (de)sorption processes, may change over time. At this stage it is of importance to realise that in general the bioavailability of metals in test systems (expressed as the fraction of the total amount of metal present in the system) may be higher than the bioavailability under field conditions.

When performing risk assessment it is of utmost importance that both PEC and PNEC are based on similar levels of availability. What is required is that for both exposure and effect

assessment, K_p values are expressed in terms of concentrations available for uptake by biota in both the aqueous and the solid phase:

$$K_p = \frac{total\ available\ concentration\ in\ solid\ phase}{concentration\ in\ aqueous\ phase}$$ **Equation 114**

It is of importance to be aware that **Equation 111** differs from the commonly used expressions for K_p in the sense that instead of total concentrations in both the solid and liquid phase, available concentrations are to be used. Reason for this is that part of the metal present in the solid phase may be incorporated in the mineral fraction and is therefore not available. Several experimental extraction techniques have been developed to determine available concentrations of metals, thus enabling the calculation of K_p values according to **Equation 111**. However, up till now the underlying concepts for a standardised approach towards partition coefficients representing availability have not yet been sufficiently worked out.

Finally, with regard to availability of metals it should be noted that apart from the general processes denoted above, under certain environmental conditions additional complexation and precipitation processes may take place that may strongly diminish aqueous metal concentrations. An example of such a process is the formation of insoluble metalsulphides under anaerobic conditions (the so-called Acid Volatile Sulphide, or AVS-concept).

Monitoring data

Metals are a group of compounds for which relatively many reliable monitoring data in all environmental compartments are present. Given the fact that the group of metals is limited to a small number of compounds, for which usually sufficient monitoring data are available, risk assessment may well be based on monitoring data. In general monitoring data are preferred over model calculations. When interpreting the data, natural background concentrations, ambient background concentrations and availability for uptake by biota need to be taken into account.

One should be aware that for the aquatic environment metal concentrations may sometimes be reported as dissolved concentrations and sometimes as total concentrations. Dissolved concentrations can be derived from total concentrations by means of the concentrations of dissolved organic matter and suspended particulate matter and partition coefficients between water and either organic or particulate matter. Since, as indicated before, risk assessment is to be performed on the basis of availability, dissolved concentrations should preferably be used since these indicate the bioavailable metal fraction in the aquatic environment.

For soils and sediments sufficient information is only rarely available from monitoring data to directly determine the bioavailable metal fraction. By applying the appropriate K_p values, estimates of the available metal concentrations can be obtained. PECs from calculations and PECs from monitoring data can be compared. In cases where calculated PECs are below PECs based on measured concentrations, natural background and ambient background concentrations should be taken into consideration.

4.5.1.3 Effects assessment

Availability of data

Toxicity data are available for most metals in sufficient quantity, since there are few compounds, and various toxicity data exist at least for the soluble metal salts. Most data are available for the toxic effects of metals on aquatic organisms, to a lesser extent data are present for terrestrial and sediment-dwelling organisms. Usually most data are based on total concentrations of the metals under investigation. For essential metals deficiency data must be taken into account.

The data are available both on short and long-term tests, and are present for species from various trophic levels. These data can be used for the effect assessment in all

compartments following the procedures for assessing the adequacy of data as presented in **section 3.2** of this guidance. However, some metal-specific criteria must be taken into account:

- physico-chemical test conditions that define the metal speciation and bioavailability should be relevant for field conditions: water hardness, pH, alkalinity, presence of complexing agents (humic acids and EDTA);
- content of metal already present in the test medium, especially for soils taken from the field and natural waters. As metals are natural constituents of the biosphere these background concentrations can influence the test results. However, it should be noted that the bioavailability of the background concentration for soils is probably less than that of the "added" metal;
- for essential metals organisms of a given habitat are conditioned to the natural concentration range for essential elements. Within this range they can regulate their metal uptake in such a way that their internal concentration is kept relatively stable (homeostasis). This implies that organisms tested should originate and be cultivated within this optimal concentration range.

Derivation of the PNEC

PNECs can be derived through the application of assessment factors on the basis of the available data assessed according to the criteria given above. Standard methods applied elsewhere (e.g. for organic compounds) can be used for this (see **section 3.3** and **section 3.7**). However, because of the specific mode of action that metals may have for some species, care should be taken in extrapolating short-term toxicity data to the PNEC using the standard assessment factors in **section 3.3** of this guidance. For many metals sufficient long-term toxicity data for aquatic organisms may be present to enable statistical extrapolation, results of which can support the results of PNECs calculated using assessment factors.

Calculated PNECs derived for essential metals may not be lower than natural background concentrations.

A prerequisite for the derivation of the PNEC is that it is done on the basis of the same level of availability as in exposure assessment.

Results from aquatic toxicity tests are usually expressed as total concentrations. As a first approach total concentrations have to be recalculated to dissolved concentrations using partition coefficients. If this is not possible, the total concentration can be set equal to the dissolved concentration. Differences in test systems, e.g. (semi-)static versus continuous flow systems and natural versus standard water have to be considered.

For the terrestrial compartment many data exist, but most are only expressed as total concentration that has been added to the test media. This added amount will be partitioned among the aqueous and the solid phase. Application of partition coefficients to calculate the available concentration in soil can be applied. Soil type correction, using reference lines should be applied to correct for differences among soil types (see also **section 3.6.2** of this guidance).

In future risk assessment for the terrestrial compartment one should be aware of the different routes of exposure that exist among terrestrial species: for species that are not exposed through the aqueous phase, the (physico-chemically) available fraction needs not be correlated to the bioavailability.

Some of the metals are essential metals, having a function in biological processes at low concentrations. Shortage of micronutrients may cause malfunction. This implies that in setting the PNEC information on deficiency levels should be taken into account. It should, however, be noted that often no information on deficiency levels of various metals for various species is available.

Though some exceptions exist, in general ionic metal species are considered to be the dominant metal species taken up, and are thus considered to be the metal species

responsible for the toxic effect. Data on the concentration of ionic species in aquatic and terrestrial systems are not readily available, and cannot, as yet, be applied on a regular basis in risk assessment.

Bioaccumulation of essential metals

Metals are taken up by organisms. For essential metals, biota regulates their uptake by means of the general physiological mechanism of homeostasis. By this mechanism, organisms will keep within a certain range of varying external concentrations, their intracellular levels relatively constant, in order to satisfy their requirements for that essential element. Homeostasis implies that organisms can deliberately concentrate essential elements if concentrations in the environment are very low. This may lead to high BCF values. On the other hand, the homeostatic regulation capacity will be exceeded at a given higher external concentration beyond which the element will accumulate and become toxic. From the above it is clear that it is not appropriate to apply classical concepts (e.g. use of BCF,BMF) to metals as they are applied to organic substances. At the same time, log K_{ow} values for metals and other inorganic compounds are not applicable for predicting their bioaccumulation potential and scientific judgement and/or studies are necessary.

4.5.1.4 Risk characterisation

The risk characterisation of metals basically follows the principles set out in **section 4.2** of this guidance. However, it should be stated again that is very important that both PEC and PNEC are based on similar levels of availability. In addition, when PEC/PNEC ratios greater than one are found, it is very important to have information on the natural and/or ambient background levels in order to decide upon further actions to be taken to reduce the risks.

Since for most metals sufficient monitoring data are obtainable, risk assessment will often be based on measured instead of calculated environmental concentrations, especially for a regional assessment. Usually most monitoring data deal with total concentrations. Especially in case of aqueous systems it is often possible to convert measured total concentrations to dissolved concentrations. For terrestrial systems this is possible by applying the appropriate K_p values.

4.5.2 Risk characterisation for petroleum substances

4.5.2.1 Introduction

In this section the Hydrocarbon Block Method (HBM) is described, which is under development and may be used for environmental risk assessment of petroleum substances. The method was originally devised by CONCAWE (The Oil Companies' European Organisation for Environmental and Health Protection) and was discussed in a workshop in Ispra in December 1994 (CONCAWE, 1995; EU, 1995). The approach has only recently been devised and hence experience with its application is limited. Although there has been work to validate the general approach, it should be recognised that there are still uncertainties regarding some technical details which should be borne in mind, when considering the outcome of the risk characterisation.

4.5.2.2 Outline of the method

There are many petroleum substances (e.g. refinery streams and solvents) which although described by a single EINECS number are hydrocarbon mixtures of varying degrees of complexity. The compositional complexity of many petroleum hydrocarbon substances is compounded by the fact that their composition will vary depending on the source of crude oil and the details of the process used in their production. This compositional complexity poses particular problems when environmental risk assessment is required.

Difficulties in carrying out a risk assessment for petroleum substances arise because individual components of them have specific and different physico-chemical and ecotoxicological properties, and potentials to be degraded in the environment. Each will be subjected to different distribution and fate processes on release. This means that on release

to the environment, each component will behave independently and reach its own concentration in each environmental compartment. It follows from this that a PEC for the whole petroleum substance does not exist. It would, in theory, be possible to identify each individual component of a petroleum substance and then to determine a PEC for each of them. In practice this approach demands a degree of analytical resolution that is not achievable for most petroleum substances and even where possible, handling such large quantities of data would be impractical. However, since hydrocarbons of similar structure will have similar physico-chemical properties and potentials to be degraded in the environment they will have similar distributions and fates within a given environment. It is therefore possible to group or block such hydrocarbons, so that components having similar properties may be considered together (it should be recognised that a block may consist of a single component or a large number of components with similar fate and distribution properties). Once the blocks for a substance have been established, PEC values can be calculated for each block for each environmental compartment. Given that PECs can only be obtained for single components, or groups of similar components, it follows that PNECs must also be estimated for the same individual components or groups of components.

Therefore, ecotoxicity data obtained on the whole substance, whether obtained using water accommodated fractions (WAFs) or dispersions, cannot be used to estimate PNECs. PNECs must be based on the toxicity of the individual blocks, which can be either single or multiple component blocks. These blocks should show similar modes of action.

From the above it is clear that the PEC/PNEC ratio of the whole substance cannot be derived directly, as neither the PEC, nor the PNEC for the whole substance will be available. The PEC/PNEC ratio is therefore derived from the PEC/PNEC ratios of the blocks of components, based on the proportional contribution of each of the blocks to additive:

$$\frac{PEC}{PNEC}_{whole\ substance} = \frac{PEC_A}{PNEC_A} + \frac{PEC_B}{PNEC_B} + \frac{PEC_C}{PNEC_C}\ etc. \qquad \textbf{Equation 115}$$

where: A,B,C etc. are the blocks.

This is referred to as the Hydrocarbon Block Method (HBM). Please see Part II Biocidal Products, which contains more recent research and updated reflections on general mixture toxicity aspects.

In relation to the above it should be noted that where the petroleum substance is of such limited complexity that it can be considered to constitute a single blocks (e.g. some narrow-cut hydrocarbon solvents) then the risk assessment is identical to that for a simple single component substance i.e. the substance is a single block and therefore, the PEC for the petroleum substance and the blocks are the same, the ecotoxicity data used to obtain the PNEC can be based on the toxicity of the whole substance, and the PEC/PNEC ratio can be obtained directly.

Given the complexity of many of the petroleum substances and hence the number of blocks that will be created, allied with the need for flexibility in the assessment procedures, it is considered that the use of this method of risk assessment for petroleum substances will, in practice, only be possible using computer based assessment procedures.

In view of the fact that particular blocks of hydrocarbons may be present in more then one petroleum substance, there may be a need to consider the contribution to the overall environmental risk from more than one petroleum substance. In principle the HBM allows to calculate the combined environmental risks of different petroleum substances in specific situations or for the comparison of combined PEC values with monitoring data. For this, the PEC/PNECs of the different discharged petroleum substances (or the values for their specific blocks) can be combined in the same way as the blocks for a specific petroleum substance are combined, assuming that the effects will be concentration additive.

Outline of the application of the HBM

The following outlines the principal steps in the application of the HBM:

- obtain compositional data for the substance that are sufficient to assign components to blocks;
- define blocks by grouping components on the basis of similar structural and/or physico-chemical properties, degradation parameters and ecotoxicological properties. If desired, blockscan be defined as single components;
- obtain production and use data;
- establish release estimates for each blocks. A single release estimate for a petroleum substance may not always be adequate: blocks with markedly different physico-chemical properties may require different release estimates;
- assign representative values for physico-chemical properties, degradation rate constants and LC/EC_{50}s and NOECs for each blocks;
- determine the PEC value for each compartment for each blocks (local as well as regional);
- determine the PNEC value for each blocks;
- calculate PEC/PNEC ratio for each blocksand sum proportionally.

Summarising, once the blocks with their physico-chemical and ecotoxicological properties are defined, there is no difference between the approach presented in the above sections and the HBM. This means that a PEClocal and PECregional can be calculated as described in **section 2** of this guidance and a PNEC can be derived as described in **section 3** of this guidance.

Points for special consideration when using the HBM for risk assessment

The more detailed description of certain aspects of the application of the HBM, which follows, is largely based on the application of the HBM to risk assessment for the aquatic environment. This is because it is considered that given the present state of the development of environmental risk assessment, and of the use of the HBM in particular, the use of this compartment best exemplifies the principles, the applicability and the issues associated with the use and further development of the HBM.

Composition of petroleum substances

The composition of many petroleum substances is complex, with a single substance often containing a large number of component chemicals, varying in chemical type, molecular weight and isomeric structure.

For some petroleum substances the differences in the physico-chemical properties of the different blocks will be such that a single release estimate for the substance may not be sufficient and separate release estimates for some blocks or groups of blocks may be required.

The complexity of some petroleum substances is further compounded by the fact that their composition may vary depending on the source of the crude oil from which they are produced and the method of their production. It is therefore necessary, that adequate information should be available not only on composition but also, where relevant, on variations in composition. This information can be used to allow several calculations of the PEC/PNEC for a substance to take account of likely variations in composition. For petroleum substances, adequate information on composition may allow risk assessment of groups of substances to be undertaken at the same time, for example whole groups of naphthas or kerosines.

It is clear that for many petroleum substances a complete identification of the composition is neither achievable nor necessary to be able to carry out a risk assessment. But it is

essential that compositional data, including information on variability, is sufficient to allow blocks to be properly defined for the purpose of risk assessment.

It should be borne in mind that some petroleum substances will contain a relatively narrow range of components and be much more consistent in composition e.g. some narrow-cut hydrocarbon solvents. In some cases it may be appropriate to regard such substances as a single block.

Many of the components of petroleum substances will be present in many of the substances. In general, it is desirable to ensure that when similar components are present in different petroleum substances the same approach to "blocking" is taken. This will allow the development of PEC/PNEC ratios for blocks applicable to a range of petroleum substances (data on physico-chemical and degradation properties and toxicity values for these common blocks will only need to be generated once).

Definition of blocks

Blocks will primarily be defined on the basis of those physico-chemical and degradation properties that are key in determining the distribution and fate of their components. Care should be taken to ensure that blocks are not so wide as to encompass components that will not have broadly similar fates and distributions on release. Similarly, blocks should, whenever possible, contain substances with a similar mode of action and a narrow range of toxicity. Both the fate and toxicity criteria for blocks definition need to be satisfied simultaneously.

Verburgh et al. (1995) carried out "trial calculations" using the HBM based on data for 500 hydrocarbons with a non-specific mode of action, using non-polar narcotic toxicity QSARs and with the Mackay level III model of the EU standard environment defined for calculating the PECregional. It appeared that for definition of the blocks the log K_{ow} is the main parameter. This implies that blocks can be defined on equally spaced log K_{ow} values: e.g. <3.0; 3-3.5; 3.5-4.0 etc.

It is proposed to start with such a "block definition" for application of the HBM. Based on the results of the risk assessment the blocks may be further refined.

Blocks based on, or containing, non-hydrocarbons

Certain petroleum substances contain non-hydrocarbon components. Special care should be taken when assessing these substances to ensure that "blocking" is appropriate and in 25particular that the range of toxicities of components in the block is small and that where necessary, due account is taken of differences in mode of action.

Additivity of toxicity

It is generally accepted that for chemicals with the same mode of action, acute toxicities can be considered as additive (EIFAC, 1987). There is increasing evidence that this is also true for chronic toxicity (Hermens, 1989). Please see Part II Biocidal products, which contains more recent research and updated reflections on general mixture toxicity aspects.

Whether a chemical, or a group of related chemicals, act by non polar narcosis can be based on a comparison of test results with QSAR estimates for base line toxicity. Schemes exist that allow the classification of large numbers of organic chemicals according to their mode of action (Verhaar et al., 1992).

Petroleum hydrocarbons are mainly composed of hydrocarbons. These act via a similar mode of toxic action, non-polar narcosis. In the light of the above it can be assumed that for the hydrocarbon components of petroleum substances, effects will be simple concentration additive.

The situation is less clear with regard to chemicals with different modes of action. Components of petroleum hydrocarbons with specific modes of action are likely to be blocked together, provided they have the same specific mode of action. In the first instance the PEC/PNEC ratio of this block must be added to the total PEC/PNEC ratio. From this it will be clear if the PEC/PNEC ratio for that block influences any potential for environmental risk

for the specific petroleum substance. If it does, further investigation whether or not there is additivity of the modes of action, would be required.

Chemicals which may have a specific mode of action present in petroleum substances can be metallic constituents (e.g. vanadium and nickel in crude oil, fuel oils and asphalt) and heterocyclic compounds (e.g. carbazole compounds in cracked fuels) and mutagens/ carcinogens (e.g. PAHs such as benzo(a)pyrene, 7,12-dimethylbenzo(a)anthracene). However, they are present in low concentrations compared to the non-specific acting components. Nevertheless, these specific acting constituents should on a case-by-case basis be taken into account in the environmental risk assessment, at least in a qualitative way.

QSARs

The identification of the blocks when applying the HBM may be dependent on the use of QSARs for the estimation of physico-chemical properties (e.g. log K_{ow}, water solubility, melting point and vapour pressure) and degradation rates (e.g. photodegradation and hydrolysis rates), when measured values are not available. There are reasonably well accepted methods for the generation of these data using readily available data bases, or QSARs. There are no widely accepted QSARs for biodegradation, but it is considered adequate, at least for screening, if experimentally determined rate constants for the blocks of interest are not available, to use QSAR estimates for block identification, according the principles laid down in *Guidance on information requirements and chemical safety assessment,* Chapter R.6: QSARs and grouping of chemicals.

The use of QSARs is well established for predicting the acute toxicity of simple hydrocarbons, and can be used to supplement the available ecotoxicity data. Whilst the accuracy of QSARs for more complex hydrocarbons and for chronic toxicity may need further consideration, they provide an adequate default where experimental data are not available (in particular where the values are found not to be key to the outcome of the risk assessment).

The minimum data-set available for each priority petroleum substances, is usually not sufficient for risk assessment using the HBM, because it will usually comprise tests conducted with the whole petroleum substance. Since in the HBM process individual hydrocarbons are blocked together on the basis of their environmental fate and ecotoxicological properties, additional data on these hydrocarbons are also required. These may be measured data, but it is foreseen that values derived from QSARs will be helpful for filling datagaps in the establishment of blocks. When the overall risk assessment for the petroleum substance is undertaken (with the PEC/PNEC ratios for the blocks calculated and summed), those blocks contributing most to the overall PEC/PNEC ratio can be identified. It should be noted that any decision on the final outcome of the risk assessment when the overall PEC/PNEC ratio is close to or greater than one, will need to be based on measured (rather than QSAR) data. Hence, for each block (unless the contribution of the particular block is found to be irrelevant to the outcome of the risk assessment) representative measured core data should be available. These data could be on any component of the block, since by definition, blocks are comprised of hydrocarbons with similar fate and ecotoxicological properties. Data on some individual hydrocarbons suitable for this purpose are already available as the IUCLID database shows.

For block identification, QSARs for short (algae, daphnids and fish) and long-term (daphnids and fish) toxicity are given in Chapter 4 of the TGD (2003) on the use of QSARs. These QSARs can be used for chemicals with a non-specific mode of action, i.e. for most petroleum substance components. Considering the assessment factors presented (see Section 3.3.1 of this guidance) a factor of 10 on the QSAR derived long-term NOEC is proposed.

Blocks which do not exhibit acute toxicity

There will be a number of blocks for which no acute toxicity is indicated at the limit of water solubility. Adema (1986, 1991) found no short-term toxicity for n-decane or higher homologues and for alkylbenzenes with a carbon number higher than 14. This does not necessarily mean that these blocks will not contribute to chronic toxic effects. There may be

several approaches to estimate the chronic toxicity for such chemicals if there are no measured long-term toxicity data available:

- use the QSAR for long-term toxicity as presented in *Guidance on information requirements and chemical safety assessment, Chapter R.6: QSARs and grouping of chemicals* (http://echa.europa.eu/guidance-documents/guidance-on-information-requirements-and-chemical-safety-assessment). However, these QSARs can only be applied in a range of log K_{ow} from approximately 2-6. For chemicals with higher log K_{ow} the resulting NOEC is often higher than the water solubility;
- for blocks which do not demonstrate acute toxicity at or below their water solubility, QSARs (irrespective of the fact that the result may exceed the water solubility) may be used as a basis for the PNEC by application of a suitable assessment factor. This calculated value is taken to represent the PNEC of the block unless it is itself greater than the water solubility. In this case the water solubility should be substituted as the PNEC. It should be noted that for very high log K_{ow} values, this may lead to unrealistic PNEC values;
- as an indication above log K_{ow} 6, a parabolic equation to derive a BCF for fish can be used (see **section 3.8.3.2** of this guidance) in combination with the critical body burden (CBB) concept (McCarty & Mackay, 1982) to calculate the chronic toxicity. This critical body burden concept indicates that the long-term critical body burden is equal to the NOEC multiplied by the BCF (CBB = BCF·NOEC) (Sijm et al., 1992; ECETOC, 1995). To be able to perform a risk assessment, there may be a need to develop measured chronic data to support this QSAR prediction.

Undissolved material

Petroleum substances (or components of them) can enter the aquatic environment either in solution or as undissolved material in slicks or dispersions. Hydrocarbons in undissolved form might have direct local effects. It is considered that undissolved hydrocarbons will not be present at the regional level, but in any event this will have to be confirmed by calculating the PECregional.

Monitoring data

For substances consisting of only a single component sound and relevant monitoring data may be available for several compartments. For petroleum substances there are a number of difficulties related to the use of monitoring data that need specific consideration. Frequently there will be measurements of total hydrocarbons or of particular hydrocarbon components that may have come from a range of different petroleum substances.

Such release or monitoring data may be used to provide a worst-case estimate of the concentration of a block for screening purposes, assuming that the whole of the release is attributable to the particular petroleum substance. However, it should be noted that the measured concentrations represent the sum of all sources of a block whereas the calculated concentrations for a specific block represents only the fraction of the total concentration of this block in the environment related to the specific petroleum substance under study. Therefore, monitoring data are most suitable for the assessment of a certain block, as they represent the actual concentration the organisms are exposed to in the environment, related to all relevant sources.

Compartments other than the aquatic

The description of the use of the HBM for the environmental risk assessment of petroleum substances given above has focused on the aquatic environment. This is because at the present time it is only for this environmental compartment that sufficient data and experience are available to allow anything approaching a full risk assessment. However, the principles of the HBM are applicable to all environmental compartments and it is anticipated that as familiarity with the approach extends, knowledge will increase and it will prove possible to apply it to the soil and air compartments. Particular shortcomings in relation to its wider application at the present time are the lack of data on the toxicity of chemicals,

including hydrocarbons, to terrestrial organisms and hence the absence of adequate (Q)SARs.

Contribution of computer based risk assessment to the use of the HBM

The use of computer based risk assessment provides the capability to carry out many iterations of the risk characterisation which in turn facilitates:

- investigation of effects of compositional changes;
- investigation of alternative "blocking" schemes;
- identification of blocks which are the principal contributors to the PEC/PNEC ratio for the whole substance and therefore, where most refinement of the data, through for example the generation of experimental values as opposed to (Q)SAR estimates would be most valuable;
- maintenance of a data base of information on blocks which are common to more than one petroleum substance.

Testing strategies

Based on the identification of the blocks, the estimation of the block properties and the compositional information in combination with exposure scenarios a PEC/PNEC is calculated. Further refinement of the PEC or PNEC may be necessary in order to improve the data estimates for the properties of the blocks.

A form of sensitivity analysis may be useful in confirming the selection of blocks to represent a particular petroleum substance; this approach may also be used to identify those particular parameters which are important in defining the fate and effects of the block. This approach may be useful to identify the most relevant additional data that would influence the outcome of the risk assessment.

Further refinement of the data estimates for the block properties should be made when:

1. specific blocks have PEC/PNEC values > 1 or;
2. the total sum of the blocks results in a PEC/PNEC ratio > 1.

For the blocks with a PEC/PNEC ratio > 1, one or some representative components should be selected. For these component(s) the testing principles from the TGD (2003) can be followed and the results can be used as representative for the specific block. If the combination of blocks with individual PEC/PNECs < 1 gives a PEC/PNEC > 1 it is suggested to focus on the major contributing blocks. For the relevant blocks again representative components can be selected and the general testing principles applied.

Application of the method to other UVCBs

It is apparent that this method may be applicable to other UVCB substances, but this will need to be explored on a case-by-case basis. Its broader applicability will be determined by the ability to define acceptable blocks and to provide the necessary data to support the derivation of PECs and PNECs for the blocks and for their additivity, which is needed to be able to derive an overall PEC/PNEC ratio.

4.5.3 Risk characterisation for ionising substances

4.5.3.1 Introduction

The degree of ionisation of an organic acid or base greatly affects both the fate and the toxicity of the compound. The water solubility, the adsorption and bioconcentration, as well as the toxicity of the ionised form of a substance may be markedly different from the corresponding neutral molecule.

When the dissociation constant (pKa/pKb) of a substance is known, the percentage of the dissociated and the neutral form of the compound can be determined. For example, for an acid with a pKa of 5.5, the pH dependency of the behaviour of the substance can be

described as follows:

- 1% dissociated at pH 3.5;
- 10% dissociated at pH 4.5;
- 50% dissociated at pH 5.5;
- 90% dissociated at pH 6.5;
- 99% dissociated at pH 7.5.

Thus, even slight changes in the pH of the environment considerably affect the form in which the substance is present in the environment. This is the case especially for substances with pKa/pKb values around the pH values of the environment (i.e. pH 4-9 for surface water). In the assessment of ionised substances, due attention has to be paid as to how much fate and effects of the substance are affected by the pH of the environment.

4.5.3.2 Exposure assessment

The water solubility of organic acids and bases are very much dependent on the pH. The water solubility of the dissociated compound can be orders of magnitude higher than the neutral species. Therefore, the pH dependence of the water solubility should be known. At least the pH of the test water needs to be identified. This also applies to log K_{ow}.

The basic parameters used in the exposure assessment (log K_{ow}, Henry's law constant, adsorption/desorption coefficients) are only applicable to the non-ionised form of the substance. Therefore, every time when partitioning of a substance between water and air or solids is concerned, a correction needs to be made in order to take only the undissociated fraction of the compound into account at a given pH. In practice, this implies that Henry's law constant and K_p in soil, sediment, and suspended solids need to be corrected. This can be done by using a correction factor (see **Equation 1**).

The correction can only be used for partition coefficients which refer to the unionised form of the substance. This means that for estimated partition coefficients, water solubility and K_{ow} need to be determined for the neutral form. The choice of relevant pH values to be used in the calculation should be based on the pKa/pKb of the compound in concern and any relevant knowledge of the actual toxic form of the substance. For experimentally determined partition coefficients the need for correction should be assessed on a case by case basis, depending on the pH in the test.

These principles apply also to the fate of the substance in sewage treatment plant. However, since the STP is a well buffered environment, a default pH of 7 can be used in the calculations. The role of pH in the experimental determination of the bioconcentration should also be acknowledged.

4.5.3.3 Effects assessment

Ionisation can markedly alter the toxicity of the substance. Normally, this is caused by the different bioavailability of the dissociated and neutral species. Consequently, when testing toxicity, the tests should preferably be carried out at both sides of the pKa, to fully characterise the possible differences in toxicity. Since this may not be possible in every case, the role of pH should at least be discussed qualitatively in the assessment.

4.5.3.4 Risk characterisation

Care should be taken that the PEC and the PNEC in the risk characterisation represent similar conditions. PEC/PNEC comparisons should preferably be made at both sides of the pKa values, within environmentally relevant pH-range. The higher PEC/PNEC ratio should be used in the risk characterisation, following the realistic worst-case approach. If it is not possible to carry out a quantitative analysis, the assessor should take the pH effect into account qualitatively.

4.6 Risk assessment of sources not covered by the life-cycle of the substances

4.6.1 Introduction

Exposure may occur from other sources than the life-cycle of the active substance under assessment. Such sources have been referred to as "unintentional sources". Examples are substances of natural origin and indirect emissions of the substance, e.g. as by-product, contaminant or degradation product of another substance. In these cases information is necessary on emissions which are not covered by the life-cycle of the substance being assessed.

Knowledge of the extent of the sources not covered by the life-cycle of the substance under review is necessary for a full evaluation of the risks posed by the active substance. The information is needed for example for a correct interpretation of measured environmental concentrations. The information is also required for an evaluation of the relative contribution of the emissions of the substance under review to the overall risks posed by the substance through all possible sources. Such information might be relevant in the eventual development of a risk reduction strategy. In the following sections, some recommendations are given on how to deal with these kinds of sources.

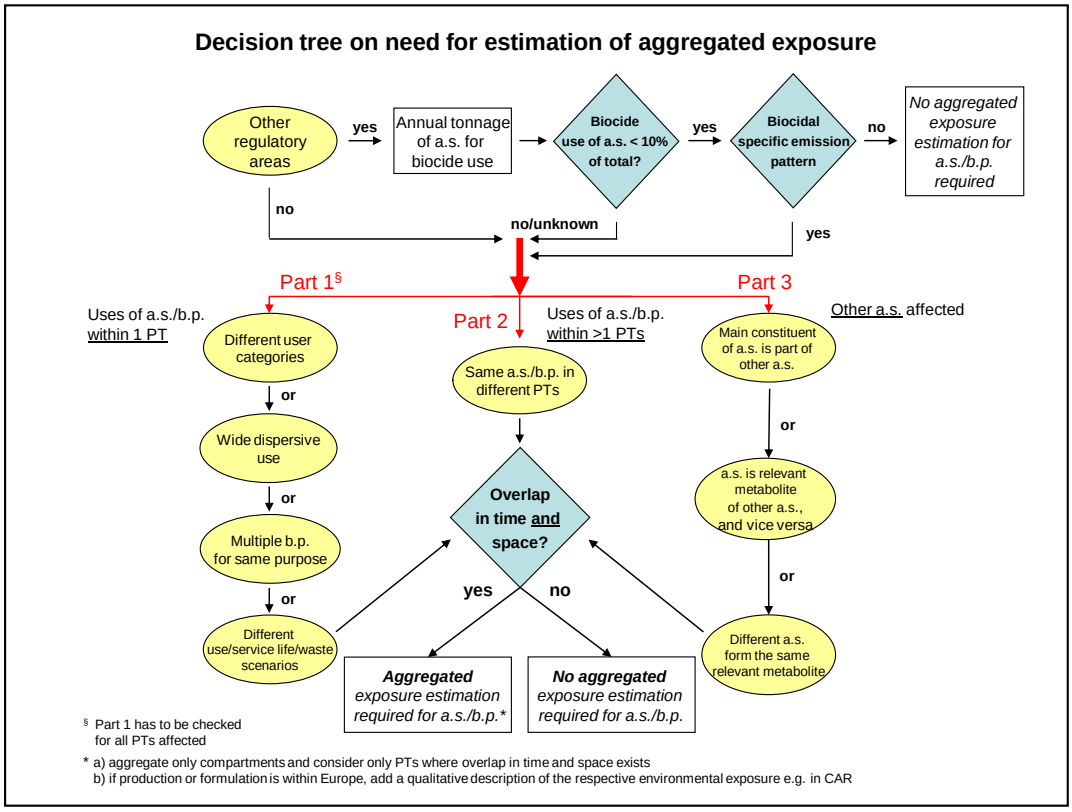
4.6.2 Legal backround

The BPR states that cumulative effects from the biocidal products containing the same active substances must be taken into account, where relevant, in the assessment of a biocidal active substance.

For biocides, sources which include substances of natural origin or releases from other biocidal uses should be taken into account in the risk assessment. When it comes to cumulative effects of a substance used also outside the scope of the BPR (e.g. in plant protection products) and maybe regulated with another Regulation there is, at the time of the preparation of this guidance, still a need for a common EU decision on how to handle such cases. Exclusion of other than only biocidal uses from the assessment causes difficulties, for example, when using monitoring data or comparing measured residue data with Maximum Residue Limits.

4.7 Assessment of aggregated exposure

Guidance currently under development: to be added at a future update. The following decision scheme has been discussed:


Decision tree on need for estimation of aggregated exposure
Other regulatory areas
yes
Annual tonnage of a.s. for biocide use
Biocide use of a.s. < 10% of total?
yes
Biocidal specific emission pattern
no
No aggregated exposure estimation for a.s./b.p. required
no
no/unknown
yes
Part 1§
Part 2
Part 3
Uses of a.s./b.p. within 1 PT
Different user categories
or
Wide dispersive use
or
Multiple b.p. for same purpose
or
Different use/service life/waste scenarios
Uses of a.s./b.p. within >1 PTs
Same a.s./b.p. in different PTs
Overlap in time and space?
yes
no
Aggregated exposure estimation required for a.s./b.p.*
No aggregated exposure estimation required for a.s./b.p.
Other a.s. affected
Main constituent of a.s. is part of other a.s.
or
a.s. is relevant metabolite of other a.s., and vice versa
or
Different a.s. form the same relevant metabolite
§ Part 1 has to be checked for all PTs affected
* a) aggregate only compartments and consider only PTs where overlap in time and space exists
b) if production or formulation is within Europe, add a qualitative description of the respective environmental exposure e.g. in CAR

Appendix 1. Assignment of organisms to trophic levels

Primary producers

Primary producers photo-/chemo-autotrophically synthesise organic compounds using inorganic precursors. They include:

- chlorophyll-containing species of vascular plants;
- algae (e.g. green algae: *Selenastrum, Scenedesmus, Chlorella*; blue-green algae: *Microcystis*);
- purple sulphur bacteria, chlorobacteria;
- chemoautotrophic bacteria (nitrifying bacteria, sulphur bacteria).

Primary consumers

They live mainly on living or dead autotrophic organisms or on microorganisms. Representatives of this trophic level are especially plant-eating animals (i.e. species that are not carnivorous of the following taxonomic groups):

- Protozoa (e.g. *Uronema, Entosiphon, Tetrahymena*);
- Annelida (e.g. *Tubifex, Enchytraeus*);
- Crustacea (e.g. *Artemia, Daphnia Spp.*, *Copepoda, Gammarus, Asellus*);
- Molluscs (e.g. *Dreissena, Mytilus, Ostrea*; several gastropods: *Patella, Viviparus*);
- Insects (some insect larvae that are not carnivorous);
- Nematoda (those species which are living in water).

Secondary consumers

They live mainly on primary consumers. Among them are:

- predatory insects and larvae of insects (e.g. *Chaoborus*);
- carnivorous protozoa;
- Rotifera;
- Ctenophora
- Cnidaria (e.g. *Hydra*);
- predatory copepods;fish (Teleostei: e.g. *Cyprinus carpio*, *Brachydanio rerio*, *Poecilia reticulata*, *Oryzias latipes*, *Pimephales promelas*, *Lepomis macrochirus*, *Oncorhynchus mykiss* (previously: *Salmo gairdneri*, *Leuciscus idus melanotus*, *Cyprinodon, Carassius*);
- Amphibians (e.g. *Rana, Xenopus*)

Decomposers

Organisms of this trophic level break down dead organic material to inorganic constituents.

Standard organisms are underlined

Organisms used in ecotoxicological tests can be assigned to different trophic levels, taxonomic groups, life forms (e.g. sessil, planktonic or swimming), and feeding strategies

(e.g. autotrophic, carnivorous, herbivorous, detritivorous, scavengers, omnivorous, deposit or filter feeders). These assignments are related to differences in morphology, behaviour, and physiology, including their ability to take up, metabolise and excrete chemicals. Furthermore, these assignments may also to some extent determine the likelihood, extent and way the organisms may be exposed. Taken together the mentioned differences may explain the observed variability among organisms regarding their sensitivity to the toxicity of chemicals, even though it may be difficult or impossible to attribute which differences between two organisms are the actual reasons for their sensitivity to a certain toxic chemical.

The standard organisms which are usually used in standard tests (plankton micro-algae, Daphnia and fish) represent three trophic levels (primary producers, primary consumers and secondary consumers), three taxonomic groups (green algae, crustaceans and bone fish), two life forms (plankton or nekton) and three feeding strategies (photosynthetic, herbivorous filter feeder and carnivorous).

Accordingly, non-standard organisms can be assigned to equivalent trophic levels, taxonomic groups, etc.

The assignment of an organism to a trophic level is based on the energy balance of the ecosystem concerned and is not primarily dependent on the species. Therefore, a given population may represent more than one trophic level depending on the spectrum and amount of nutrition for the species. In addition, earlier life stages may live on completely different nutrition compared to adults of the same species.

Appendix 2. Toxicity data for fish-eating birds and mammals

The endpoints of the tests should be expressed as a concentration in food (mg test substance/kg food). Often test results for birds and mammals are expressed in mg/kg body weight/day. These data should be converted to a concentration in food (mg/kg). For the conversion, data on body weight and daily food intake during the tests need to be known. This conversion is only advisable when no other toxicity data for birds and mammals are available. If this information cannot be obtained from the test report, the values on body weight, daily food intake and daily water intake that are given in the table can be used for the transformation. For transformation of toxicity data expressed on the basis of body weight or water intake to food intake, the toxicity data should be multiplied by the conversion factor (BW/DFI or DWI/DFI).

Table 33: Conversion factors for toxicity data (Sax, 1989; Romijn et al., 1993)

	BW	DFI	DWI	BW/DFI	DWI/DFI
Canis domesticus	10,000	250		40	
Macaca spec.	5,000	250		20	
Microtus spec.	25	3		8.3	
Mus musculus	25	3		8.3	
Oryctolagus cuniculus	2,000	60		33.3	
Rattus norvegicus (> 6 weeks old)	200	10		20	
Rattus norvegicus (< 6 weeks old)				10	
Gallus domesticus		64.3	128.5		2

BW	: body weight (g)
DFI	: daily food intake (g/day)
DWI	: daily water intake (mg/l/day)
BW/DFI	: conversion factor from mg/kg body weight/day to mg/kg food
DWI/DFI	: conversion factor from mg/l/day to mg/kg food

Concentrations causing no effect after long-term exposure (NOEC) are preferred. If, in a study, a single dose or the lowest dose of a range causes < 20 % mortality, a NOEC may be calculated from LOEC/2. If the effect is more than 20 %, the data cannot be used.

Laboratory food for mammals and birds is usually grain. The energy content of grain is higher than fish. This means that in order to obtain the same amount of energy more wet weight of fish must be consumed compared to grain. Therefore a correction factor of 3 may be applied for the difference in caloric content of the diet of laboratory animals and the diet of fish-eating birds or mammals (Everts et al., 1993).

Appendix 3. Transformation pathways

In the table below biodegradation and transformation pathways of some organic compounds are summarised. The mechanisms and pathways presented here are not comprehensive and other mechanisms and pathways may therefore occur. It should also be noted that the assessment of transformation pathways may be complicated due to the interaction between different functional groups within a molecule. The following references give further detail:

Neilson AH (1994). Organic Chemicals in the Aquatic Environment: Distribution, Persistence, and Toxicity. Lewis Publishers, Boca Raton, FL, USA, 448 pp.

Larson RA and Weber EJ (1994). Reaction Mechanisms in Environmental Organic Chemistry. Lewis Publishers, Boca Raton, FL, USA.

Table 34: Summary of biodegradation and transformation pathways of certain organic compounds.

GROUP	METABOLIC PATHWAY	TRANSFORMATION PRODUCT(S)
Aldehydes	Oxidation	Carboxylic acids
Alkanes, branched acids	Oxidation/carboxylation	Alcohols/carboxylic
Alkanes, unbranched	beta-Oxidation	Alcohols, carboxylic
Alkanols	Oxidation	Aldehydes, ketones
Alkenes	Epoxidation	Epoxides, diols
Alkynes	Addition of water	Ketones
Amides and related compounds	Hydrolysis	Amines, carboxylic acids
Amines, primary/secondary/tertiary	Oxidative deaminiation/reductive dealkylation/reductive dealkylation	Carboxylicacids/primary amines/secondary amines
Anilines	Ring oxygenation	Catechols
Aromatic hydrocarbons	Oxygenation	Catechols
Azo compounds, aromatic	Reduction	Anilines
Carbamates	Hydrolysis	Amines, alcohols
Carboxylic acids	beta-Oxidation	Acetic acid
Catechols	Oxidation with ring cleavage	Carboxylic acids
Esters (carboxylic/sulfuric/ phosphoric)	Hydrolysis	Alcohols and carboxylic/ phosphoric/sulfuric acids
Ethers, aliphatics	Reductive or oxidative dealkylation	Alcohols
Halogenated aliphatics	Hydrolysis/elimination/reductive dehalogenation	Alkanols/alkenes/alkanes
Halogenated aromatics	Oxygenation	Halogenated catechols
Heteroaromatics	Oxygenation	Similar to aromatics
Ketones	Monooxygenation	Esters
Nitriles	Hydrolysis	Amides, carboxylic acids
Nitro compounds	Reduction	Amines
Nitro aromatics	Dioxygenation (elim. of NO_2^-)/ reduction	Catechols/anilines
Organomercurials (C-Hg bond)	Reductive cleavage	Alkanes,inorg.mercury
Organophosphonate (C-P bond)	Reductive cleavage	Hydroxybenzoates/catechols
Phenols	Carboxylation (anaerobic)/ Oxygenation (aerobic)	Hydroxybenzoates/catechols
Sulfoxides	Reduction	Thioethers, thiols
Sulphonates, aromatic	Elimin. of sulfite by dioxygenation	Catechols
Sulphates, alkyl	Hydrolysis	Alcohols, inorg. sulphate
Ureas	Hydrolysis	Amines

Appendix 4. Connection to Sewage Tratment Plans in Europe

There is overall a development towards a higher proportion of the population being connected to urban wastewater treatment plants[29]. For example in Malta , where coverage reached 100 % in 2011 — up from 20.7 % in 2010 — due to the construction of new wastewater treatment plants. Apart from the rapid increase in connection rates in Malta, the next highest rates of change were recorded in Belgium, Hungary, Poland, Bulgaria and Slovenia. In 2013, the highest connection rates in the EU-28 were recorded in Malta (100 %), the United Kingdom (99.5 %; 2010 data), the Netherlands (99.4 %; 2012 data), Luxembourg (98.2 %), Spain (97.8 %; 2012 data) and Germany (96.4 %; 2010 data).

Table 35 presents information on the proportion of the population connected to at least secondary wastewater treatment plants. This share has also been generally increasing and was above 80 % in 14 of the EU Member States for which data are available (mixed reference years). The share of the population connected to at least secondary wastewater treatment plant rose to above 90 % in the United Kingdom (2010 data), the Netherlands (2012 data), Luxembourg, Germany (2010 data), Spain, Austria, Malta and Greece (2012 data for all four), as well as Denmark. At the other end of the range, less than one in two households were connected to at least secondary urban wastewater treatment plants in Romania and Croatia (2011 data), while the same was also true in Turkey (2012 data), Albania, Serbia, Bosnia and Herzegovina, and Kosovo.

Table 35: Share of the population connected to at least secondary urban wastewater treatment, 2003–13 (%).

	2003	2004	2005	2006	2007	2008	2009	2010	2011	2012	2013
Belgium	51.4	53.2	*54.4*	*57.4*	68.7	71.0	72.8	75.0	77.0	82.0	84.0
Bulgaria	37.9	38.0	38.3	38.8	39.7	41.4	42.7	45.1	53.6	53.9	54.5
Czech Republic	70.6	70.8	72.8	71.9	73.0	75.4	75.7	76.9	78.0	78.0	79.8
Denmark	:	:	:	:	:	:	89.4	88.0	88.4	88.4	90.1
Germany	:	93.8	97.3	:	91.9	:	:	95.3	:	:	:
Estonia	70.0	71.0	73.0	73.0	73.5	79.5	79.5	78.3	81.1	81.2	82.1
Ireland	:	:	:	:	:	:	:	:	:	:	:
Greece	:	:	:	:	85.0	:	87.3	87.3	88.1	92.0	:
Spain	:	:	:	88.0	:	88.0	:	93.0	:	94.8	:
France	:	79.5	:	:	:	:	:	:	56.1	*56.1*	*55.4*
Croatia	:	:	:	:	:	:	:	:	27.0	:	:
Italy	:	:	93.6	:	:	:	83.0	:	:	:	:
Cyprus	22.9	28.4	29.8	:	:	:	:	:	:	:	:
Latvia	68.3	64.3	63.8	62.9	60.9	54.3	60.9	58.1	63.9	66.0	67.2
Lithuania	27.6	:	:	:	:	:	:	:	:	63.1	:
Luxembourg	88.1	:	:	:	:	:	:	91.3	90.9	96.1	96.3
Hungary	38.9	40.2	*41.7*	*45.3*	*49.8*	*50.0*	*52.1*	*69.5*	*71.1*	*72.8*	*72.6*
Malta	16.1	13.3	*13.2*	*9.3*	*8.4*	*14.8*	*15.2*	6.6	*93.2*	*93.1*	*92.9*
Netherlands	98.6	98.9	99.0	99.1	:	99.3	:	99.4	:	99.4	:
Austria	:	88.9	:	:	:	*92.6*	:	*93.9*	:	94.5	:
Poland	55.5	56.8	58.1	60.7	61.8	62.9	64.1	64.5	65.5	68.5	70.2
Portugal	32.0	:	42.6	37.0	51.0	52.0	55.8	:	:	:	:
Romania	:	*16.9*	16.9	:	:	:	:	22.0	31.0	32.7	35.5
Slovenia	19.9	29.3	32.1	47.6	48.8	51.1	52.9	52.5	54.0	54.2	54.9
Slovakia	:	:	:	:	:	:	:	:	:	:	:
Finland	:	:	:	:	:	:	:	83.0	*83.0*	*83.0*	*83.0*
Sweden	86.0	86.0	86.0	86.0	86.0	86.0	86.0	86.0	86.0	87.0	87.0
United Kingdom	:	:	:	:	:	96.9	97.0	99.5	:	:	:
Iceland	1.0	1.0	2.0	:	:	2.0	:	:	:	:	:
Norway	55.4	56.2	58.0	58.6	58.5	58.8	59.3	59.2	61.4	62.6	62.6
Switzerland	:	:	:	:	:	:	:	:	:	:	*98.0*
Albania	:	:	:	:	:	:	:	4.7	4.7	7.4	*22.0*
Serbia	5.4	5.8	6.4	6.9	6.9	7.5	8.9	8.6	8.9	9.0	9.4
Turkey	21.1	24.8	:	:	31.1	31.4	35.2	37.6	:	42.0	:
Bosnia and Herzegovina	1.5	1.5	1.5	1.6	1.6	1.7	1.7	1.7	1.8	1.8	1.8
Kosovo	:	:	:	:	:	:	:	:	0.6	0.6	0.6

Source: Eurostat (online data code: env_ww_con)

Based on these data, a figure of 90% connection to wastewater treatment is therefore

[29] http://ec.europa.eu/eurostat/statistics-explained/index.php/Water_statistics#Wastewater

proposed for the generic region. A figure of 90 - 95% was also proposed in the TGD (2003) for use following full implementation of the UWWTD. This coincides with the likely ultimate degree of connection and treatment capacity for urban regions of the EU.

Urban Waste Water Treatment

In terms of treatment levels tertiary wastewater treatment was most common (again mixed reference periods) in the Netherlands, Germany, Austria, Sweden and Greece, where at least four in every five persons were connected to this type of wastewater treatment. By contrast, no more than 1 % of the population was connected to tertiary wastewater treatment in Bulgaria.

The residual of wastewater treatment is sewage sludge. While the amount of sludge generated per inhabitant depends on many factors and hence is quite variable across countries, the nature of this sludge – rich in nutrients, but also often loaded with high concentrations of pollutants such as heavy metals – has led countries to seek different pathways for its disposal. Typically, four different types of disposal make up a considerable share of the total volume of sewage sludge treated: more than two thirds of the total was used as fertiliser in agriculture in Spain and Ireland, while another eight Member States (Lithuania, Hungary, Bulgaria, Cyprus, Luxembourg, France, the Czech Republic and Latvia), as well as Norway, reported between one and two thirds of their total mass of sewage sludge being disposed of through agricultural uses. By contrast, more than two thirds of sewage sludge was composted in Estonia and Slovakia. Otherwise, alternative forms of disposal may be used to reduce or eliminate the spread of pollutants on agricultural or gardening land; these include incineration and landfill. While the Netherlands, Slovenia, Belgium, Germany and Austria (as well as Switzerland) reported incineration as their primary pathway for disposal, its discharge into controlled landfills was practised as the primary pathway in Greece, and was used exclusively in Malta (Eurostat, 2012).

Appendix 5. PNECoral derivation for the primary and secondary poisoning assessment of anti-coagulant rodenticides

Derivation of $PNEC_{oral}$ for primary and secondary poisoning has been discussed at the Biocides Technical Meeting I in 2006 when discussing the substances difethialone and coumatetralyl. Norway provided a discussion document which resulted in the following guidance.

There was a general agreement that the principles laid down in the TGD do not reflect the special situation with regard to rodenticides very well. In addition to the secondary poisoning assessment from the TGD (PEC_{oral}, fish and PEC_{oral}, worm compared to a PNEC for fish- or worm-eating mammals or birds) another food chain rodenticide (bait) or rodent or rodent-eating mammal or rodent-eating bird has to be assessed here. A predicted environmental concentration, which corresponds to the PEC_{oral}, predator in the TGD needs to be defined. According to the emission scenario developed for product-type 14 in the EUBEES project "…it will then be compared with the predicted no-effect concentration $PNEC_{oral}$ according to the TGD". However, the guidance for PNEC derivation given in the TGD refers to an exposure situation which is completely different from the exposure situation for rodenticides. Also in the ESD PT14 it is questioned "…if the $PNEC_{oral}$ calculated according to the TGD is really very suitable for rodenticides".

One issue not yet discussed at TM regarding $PNEC_{oral}$ derivation for the primary and secondary poisoning assessment of rodenticides is whether it is considered necessary to derive separate $PNEC_{oral}$ for an acute and a chronic exposure situation to rodenticides as done by most MS.

In ESD PT14 it is stated that "…it could be argued that both an acute and a chronic risk assessment should be done for anticoagulants, because although the mode of action is generally chronic, some anticoagulants have substantial acute toxicity." ESD PT14 states also that "…the time periods implied by the exposure and effects assessments should be comparable. If possible these two should be made consistent". The ESD PT14 gives no clear guidance on whether two separate $PNEC_{oral}$ values have to be derived and on how to do this.

The $PNEC_{oral}$ derivation described in the TGD for the secondary poisoning assessment considers the oral intake of a chemical via fish or worms and a more or less continuous exposure situation and no guidance is given at all regarding primary poisoning. The TGD does not state to derive a separate short-term $PNEC_{oral}$ in addition to the long-term $PNEC_{oral}$. Therefore no guidance is available on how to derive a short-term $PNEC_{oral}$.

At TM I '06 it was not possible to find another way of deriving $PNEC_{oral}$ than the approach described in the TGD and it was agreed to follow the TGD. However, for the short-term exposure and for primary poisoning no guidance is given in the TGD.

This Appendix provides a proposal for harmonising the primary and secondary poisoning assessment of anticoagulant rodenticides so that a future comparative assessment of anticoagulant rodenticides would be possible. .

Item 1: Do we need both a short-term and a long-term $PNEC_{oral}$?

As described in general in the TGD only one PNEC is derived for any effects assessment, which, if not exceeded, should ensure an overall protection of the environment. This PNEC can be considered as a long-term value.

The situation with respect to anticoagulant rodenticides is different. Most anticoagulant rodenticides are acutely toxic to mammals and birds and there is the possibility of an acute poisoning situation in addition to a long-term exposure of non-target mammals and birds. This situation is not reflected in the TGD, however, it is considered especially relevant for primary poisoning, whereas for secondary poisoning the long-term exposure seems to be more relevant than the acute exposure situation.

Comparing an acute poisoning incident, which represents a single uptake of the

anticoagulant rodenticide by a non-target mammal or a bird, with a $PNEC_{oral}$ which has been derived in accordance with the TGD, considerably overestimates the risk due to the choice of long-term studies as a basis for deriving the $PNEC_{oral}$.

On the other hand no guidance is available on how to derive $PNEC_{oral}$ values for an acute poisoning situation. Every MS which derived short-term $PNEC_{oral}$ values for their evaluations chose its own approach. Different studies, different endpoints and different assessment factors have been used as no harmonised guidance is available at the moment. When discussing this issue it became clear that the situation is that complex that it will not be possible to reflect the real life situation in the primary and secondary poisoning assessments of the evaluation reports. It remains unclear which studies should be chosen for a derivation of an acute $PNEC_{oral}$ and also which assessment factors should be applied to them. Due to these problems it is considered more than difficult to reach a compromise regarding the derivation of a $PNEC_{oral}$ for acute poisoning situations. Having in mind the importance of harmonising the primary and secondary poisoning assessment of anticoagulant rodenticides for a future comparative assessment the following pragmatic approach is suggested for the time being. When revising the ESD PT14, guidance should be included on how to derive a $PNEC_{oral}$ for acute exposure situations.

Qualitative risk assessment for acute situation

At the moment it is suggested not to conduct a quantitative risk assessment for the acute primary as well as the acute secondary poisoning situation. Instead a qualitative description of the toxicity of the substance compared to the possible single uptake should be given.

Example primary poisoning Tier 2, single uptake without excretion:

> Concentration of a.s. in bait 25 mg/kg
>
> Tree sparrow: daily food uptake 7.6 g/day
>
> Body weight: 22 g
>
> Expected content of the a.s. in the sparrow for a single uptake incident if the sparrow consumes 100% of its daily food uptake on rodenticide bait: 8.64 mg/kg bw
>
> LD_{50} of the a.s. (bird) = 0.264 mg/kg bw

From this calculation it becomes clear that the sparrow dies if consuming 100% of its daily food uptake on rodenticide bait, even without applying an assessment factor to a single dose LD_{50}. The same comparison can be made for an acute situation at Tier 1 secondary poisoning with Frodent = 1.

It is important to stress that this qualitative assessment is not intended to be used for the risk assessment of primary and secondary poisoning of rodenticides. This comparison only gives a first indication of the acute toxicity of the substance. If an anticoagulant rodenticide with a lower acute toxicity e.g. has a LD_{50} (bird) which is above the expected content in the sparrow the conclusion of this comparison should not be that the substance is not acutely toxic or "unproblematic" with regard to the acute primary poisoning situation because a comparison is made with a single dose LD_{50} without applying an assessment factor. This comparison is not intended to be used for risk characterisation: no PNEC must be derived and hence no PEC/PNEC ratio can be established, and must not be used for a comparative assessment.

The object of a qualitative risk assessment should be:

- Primary poisoning:
  - Tier 2 for 1 days exposure with and without excretion, where the PEC_{oral} is the expected concentration of the a.s. in the non-target animal after 1 day exposure (single meal) [mg/kg bw]. A default excretion factor of 0.3 (for birds and mammals) should be used in case no data is available. For a first step worst case it is assumed that:

- Avoidance factor (AV)[30]: the contaminated diet is not avoided. AV = 1;
- Fraction of diet obtained in treated area (PT): animals satisfy their entire food demand in the treated area. PT = 1;
- Fraction of food type in diet (PD): animals feed exclusively on contaminated diet. PD = 1.

For a more realistic worst case AV = 0.9, PT = 0.8 and PD = 1.

- Secondary poisoning
  - Tier 1, where the PEC_{oral} is the concentration in the rodent immediately after a last meal on day 5 [mg/kg food]. For a short-term exposure PD is 1 (rodents have fed entirely on rodenticide) and F_{rodent} = 1 (non-target animals consume 100 % of their daily intake on poisoned rodents). For comparison calculations with PD = 0.5 and PD = 0.2 could also be included.

Quantitative risk assessment for long-term situation

For the long-term exposure, as described in the ESD PT14, a quantitative risk assessment for primary and secondary poisoning should be carried out. For that the $PNEC_{oral}$ should be derived in accordance with the TGD.

The object of a quantitative risk assessment should be:

- Primary poisoning:
  - Tier 1 where the PEC_{oral} is the concentration of the actives substance in the food (bait) [mg/kg food]
  - Tier 2 for 5 days exposure, considering excretion, where the PEC_{oral} is the expected concentration of the active substance in the non-target animal after 5 days exposure [mg/kg bw]. A default excretion factor of 0.3 (for birds and mammals) should be used in case no data are available. As a worst case, the parameter AV, PT and PD are all 1.
- Secondary poisoning
  - Tier 1 for a long-term exposure. The PEC_{oral} is the concentration in the rodent immediately after a last meal on day 5 [mg/kg food]; PD = 1 and F_{rodent} = 0.5 (non-target animals consume 50 % of their daily intake on poisoned rodents). For comparison calculations with PD = 0.5 and PD = 0.2 could also be included.
  - Tier 2 for a long-term exposure. The PEC_{oral} is the concentration in non-target animals after a single day of exposure [mg/kg bw]; PD = 1 and F_{rodent} = 0.5.

For a comparative assessment the long-term PEC/PNEC values of the respective substances should be compared. As a worst case, PEC/PNEC ratios of the smallest bird and the smallest mammal should be compared for primary as well as secondary poisoning.

Item 2: Choice of studies for the long-term risk assessment for primary and secondary poisoning

It is suggested using the NOEC from an avian reproduction study or, if not available, the LC_{50} from a 5 days feeding study with birds for $PNEC_{oral,\ bird}$ derivation.

For mammals the NOAEL from a 28 or a 90 days repeated dose toxicity study or from a chronic study should be used.

For converting the $PNEC_{oral}$ values from a concentration in food [mg/kg food] to a dose related $PNEC_{oral}$ [mg/kg body weight], and vice versa, the following equation should be used:

[30] AV has to be set to 0.5 for birds if the product is a paste in an envelope

Daily dose [mg/kg bw day] = conc. in food [mg/kg] · daily food consumption [g/bird day]/body weight [g]

Data from animals used in the test should be used for conversion (i.e. body weight and daily food intake of the test species) and not default values given in EUBEES.

Item 3: Assessment factors

The AF laid down in **section 3** of this guidance should be used for $PNEC_{oral}$ derivation for the long-term risk assessment.

Appendix 6. Tonnage-based approach – Emission factors for different use categories (A&B tables of TGD, 2003)

This Appendix represents the former Appendix I to Chapter 3 of the TGD (2003). The TGD was prepared for chemicals and biocides. The descriptions below therefore include also the description of uses of chemicals with regard to life cycle, use classes (UC) and industrial categories (IC). However, the emission factors also apply to biocides when the exposure assessment is performed using the tonnage based approach.

1. Introduction to the release tables

For all ICs estimates have been generated for:

- the emission factors for the following stages of the life-cycle, i.e. (1) production, (2) formulation, (3) industrial use, (4) private use, service life and (5) waste treatment; these estimates have been collected in the "**A-tables**". When possible defaults occurring in emission scenario documents have been implemented
- the fraction of the main source and the number of emission days (point sources); these estimates have been collected in the "**B-tables**". When possible data on the model source of emission scenario documents have been implemented.

Many tables are applied for more than one category, but are given only once (at the first occurrence). For other categories, reference is made to the number of those tables.

Within one IC many different processes may take place involving many substances with very variable functions. Thus, the emission factors also may be very variable depending on process and process conditions. Function and physico-chemical properties may have a considerable influence.

It should be noted that only for a limited number of ICs and specific applications (use categories (UC)) studies have been performed (resulting in so-called emission scenario documents or use category documents). These emission scenario documents are presented in Chapter 7 of the Technical Notes for Guidance (2003). They provide a solid basis for the estimates. Emission scenario documents give a good description of processes and the function of substances involved.

2. Types of substances and levels of production and use

New substances are usually produced at a rather low level. For existing substances high production volume chemicals (HPVC) have also to be considered. At present the IUCLID database contains over 2,500 existing substances that are produced or imported at amounts in excess of 1,000 tonnes/year. For the B-tables, default values for every industrial category have been introduced, above which a substance is considered to be an HPVC (unless the substance is considered as a HPVC by the notifier or when a tonnage is indicated for a HPVC in the relevant emission scenario document provided in Chapter 7 of the TGD (2003)). If the (production) volume of a substance is rather high (HPVC), it may be unrealistic to use the standard size for the STP. A correction may be made in a more refined stage of the assessment.

In the text the term "volume" will be used instead of "production volume", as the volume applied in the EU is considered. This means that the volume equals the production volume + the volume imported in the EU - the volume exported from the EU (the substance as such, not the quantities imported in products).

A substance can have applications in more than one IC and/or UC. As an assessment has to be made for all relevant applications of the substance, the input of fractions for different industrial and use category combinations must be realised according to 3: Use and stages of the life-cycle.

3. Aspects of production

If specific data on emissions at production are known, these can be used instead of the

tables. Also for the fraction of the main source specific data may be entered, either as the capacity (tonnes/day) or as the period (days/year) in which the substance is produced.

4. Aspects of formulation

For this stage of the life-cycle specific data may be entered on the fraction of the main source and the emissions/emission factors. For the emissions, a refinement may be achieved by discriminating between cleaning with/without water and soap. This has not been done yet.

In case a substance is applied in a formulation (i.e. biocidal product)[31]/treated article at a rather low level, unrealistic values for the fraction of the main source and the number of days will be derived from the tables using the tonnage as such.

In such cases the number of release days can be obtained from the table below where the default number of release days corresponds to the generic assumption that a process with a small capacity may only be run for a limited number of days per year. The table further provides default daily tonnage for formulation/treatead article at industrial sites, as a function of the size of the site in terms of annual capacity.

Tonnage of formulation/treated article in which the substance is included for the use (or group of uses) per year[32]	**No. of release days (days/year)**	**Substance daily use amount (tonnes/day)**
Tonnage < 100	10	Tonnage/10
100 < Tonnage < 2 000	100	Tonnage /100
Tonnage > 2 000	300	Tonnage /300

The tonnage of formulation/treated article needs to be used to estimate the fraction of the main source using the A- and B-tables. It is possible to calculate an average in the case where a range of contents has been specified.

5. Aspects of industrial use

Industrial/professional use is referred to as "processing" in the A- and B-tables. Specific data on the fraction of the main source and the emissions may be used as input. This will be repeated for every specified IC-UC combination. In case a specific scenario for an IC-UC combination exists, specific data will be asked.

6. Aspects of service life

The life cycle stage service life is only considered for articles produced in textile industry.

7. Aspects of private use

Specific data on the fraction of the main source and the emissions may be used. This will be possible for every specified IC-UC combination for which the stage of private use is relevant.

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[31] The tonnage of the biocidal product will be used as basis to derive relevant default values, since it represent the worst case (as compared to the using the tonnage of the end-product).

[32] The tonnage of mixture formulated or used in industrial uses indicates a capacity, from which the default number of release days is derived (central column). The site tonnage to be calculated refers to the substance (right column). If the applicant has no information on the tonnage of the formulation, he can use the tonnage of the substance in the first column, which results in a more conservative daily use at the site and, as consequence, in a more conservative release estimation. Alternatively, if the applicant knows the fraction of the substance in the formulation, he can estimate the formulated tonnage (first column) via the equation: tonnage of formulation = tonnage of the substance /percentage of substance in the formulation. In that case this may lead to a change of tonnage band.

8. Aspects of waste treatment

Specific data on the fraction of the main source and the emissions may be used. This will be possible for every specified IC-UC combination for which the stage of waste treatment is relevant. For waste treatment only situations where a material – which contains the chemical of interest – is recovered and processes to make it suitable for re-use in its original application (recycling) or another application are taken into account.

9. Interpretation and use of the classification in "Main categories"

The main categories (MCs) were intended originally to provide a general impression of the relevance of the exposure during the whole life-cycle. The categorisation procedure outlined in Chapter 5 of TGD (2003) allows for one entry of the MC only, for all stages of the life-cycle.

In the context of environmental risk assessment MCs are often used to characterise release scenarios for the estimation of emissions to the environment at individual stages of the life-cycle, i.e. at production, formulation and use. They can therefore be allocated to release fractions, which are used as default values where specific information is lacking.

MC I "Use in closed systems"

This MC refers to the stage of production and industrial/professional use. At the stage of production a substance should be assigned only to this category if it remains within a reactor or is transferred from vessel to vessel through closed pipework. The HEDSET (EC/OECD Harmonised Electronic Data Set) distinguishes between three subcategories for intermediates.

For the stage of industrial/professional use this MC refers to substances that are used in closed systems, e.g. the application of a substance in a transformer or the circulation circuit of refrigerators.

MC II "Use resulting in inclusion into or onto a matrix"

Use consisting of inclusion into or onto matrices means all processes where chemicals are incorporated into products or articles from which they (normally) will not be released into the environment. This is applicable to the stage of formulation, e.g. when a substance is included in the emulsion layer of a photographic film. It also may refer to the stage of processing, e.g. when a paint additive ends up in the finished coating layer.

MC III "Non-dispersive use"

Non-dispersive use refers to chemicals which are used in such a way that only certain groups of workers, with knowledge of the process, come into contact with these chemicals. This means that the use of these chemicals is related to the number (and size) of the emission sources. So, this MC indicates industrial use at a limited number of sites (where emission reduction measures may be common practice).

MC IV "Wide dispersive use"

The term wide dispersive use should be used for a wide range of activities particularly when end users come into contact with the products. This means a large number of small point sources like households or line sources like traffic.

Although the HEDSET allows for one entry of the MC only for all stages of the life-cycle, the approach of MCs is used in EUSES in many cases for several stages of the life-cycle. As can be seen from **Table 37** interpretation is often different.

Table 35: Interpretation of main category (MC) for relevant stages of the life-cycle

MC	Life-cycle stage	Interpretation
Ia	Production	Non-isolated intermediates (Industrial category 3 or 9 & Use category 33)
Ib	Production	Isolated intermediates stored on-site, or substances other than intermediates produced in a continuous production process
Ib	Formulation	Dedicated equipment and (very) little cleaning operations
Ic	Production	Isolated intermediates stored off-site, or substances other than intermediates produced in dedicated equipment
Ic	Formulation	Dedicated equipment and frequent cleaning operations
II	Formulation	Inclusion into or onto a matrix
II	Processing [1)]	Non-dispersive use (industrial point sources), or processing of intermediates in multi-purpose equipment
III	Production	Multi-purpose equipment
III	Formulation	Multi-purpose equipment
III	Processing [1)]	Non-dispersive use (industrial point sources), or processing of intermediates in multi-purpose equipment
IV	Processing [1)]	Wide dispersive use (many small point sources or diffuse releases; normally no emission reduction measures)

Note to Table 37: [1)] Processing refers to industrial / professional use

10. Remarks on the industrial categories

This paragraph defines the scope of the ICs and presents some short remarks on the ICs in relation to the A- and B-tables. The definition is based on the examples specified in the HEDSET for substances classified in the appropriate ICs. One of the main problems using the A- and B-tables is the fact that it is often difficult to determine the correct tables to be used, i.e. to determine the correct IC/UC combination. The cause can be divided into two:

1. Correct categorisation is impossible because no suitable use category can be determined on account of the notification. Furthermore, problems may arise when the application of a substance takes place in a process that occurs in more than one industrial category, or
2. The specification of the industrial category and/or use category by the notifier is wrong, and determination of the proper combination fails due to the fact that the

detailed information of the notification may be cryptic.

A table is presented for every IC in which for every possible stage of the life-cycle the MCs are marked (with 'X'), which can be chosen or which are used automatically by the program on account of the choice made for the UC. If an MC can not be chosen or if no MC is needed a dot (.) has been placed in the table. Processing refers to industrial / professional use.

IC 1. Agricultural industry

Agricultural industry deals with the activities of growing crops (vegetables, grains, etc.) and raising cattle (for dairy products, meat and wool). It also comprises all allied activities such as pest control (application of pesticides, veterinary medicines), manuring. There are no emission scenarios and use category documents for this IC. Emissions due to the application (stage of processing) of pesticides are beyond the scope of the TGD. Several UCs are distinguished in the release scenario of the A-tables, e.g. UC = 19 Fertilisers and UC = 41 Pharmaceuticals.

Table 36: Table for IC 1 of the MCs for the possible stages of the life-cycle which may be chosen on account of the UC chosen (for interpretation of the MC see Table 37)

Stage	Main category					
	Ia	Ib	Ic	II	III	IV
Production	.	X	X	.	X	.
Formulation	.	X	X	.	X	.
Processing	.	.	.	.	.	.

IC 2. Chemical industry: basic chemicals

The HEDSET considers two different ICs for chemical industry, the industry where substances are produced through chemical reactions. The raw materials for chemical industry come from petrochemical industry (IC 9 "Mineral oil and fuel industry"), from plant or animal materials, or coal. IC 2 is dedicated to *basic chemicals*, where the definition for use of the release estimation tables is based on the examples given in the HEDSET: basic chemicals are substances used generally throughout all branches of chemical industry and usually in considerable amounts. Important basic chemicals are solvents (UC 48) and pH-regulating agents (UC 40) (acids, alkalis).

There are no emission scenario and use category documents for this IC. In case a basic chemical is formulated A- and B-tables have been provided. Recovery is not considered as a feasible emission stage; emissions of chemicals such as catalysts are included in the emissions at the stage of processing. No distinction between UCs has been made in the emission tables so far; however, apart from UC = 48 "Solvents" most chemicals will have to be classified as UC = 40 "pH-regulating agents", UC = 55/0 "Others", and probably as UC = 43 "Process regulators".

Table 37: Table for IC 2 of the MCs for the possible stages of the life-cycle which may be chosen on account of the UC chosen (for interpretation of the MC see Table 37)

Stage	Main category					
	Ia	Ib	Ic	II	III	IV
Production	.	X	X	.	X	.
Formulation	.	X	X	.	X	.
Processing	.	.	.	.	.	.

IC 3. Chemical industry: chemicals used in synthesis

The definition for chemicals used in synthesis based on the examples given in the HEDSET is: chemicals used in synthesis are substances either regulating the chemical reaction process (e.g. catalysts) or being used as an intermediate (i.e. chemicals that are formed and can be isolated at an intermediate step between starting material and the final product in a sequence of chemical processes). The HEDSET includes monomers in intermediates, which is only valid in the release estimation tables for the stage of production. For the processing stage the tables of IC 11 "Polymers industry" are used (see also subparagraph 4.2.5).

Apart from UC = 33 "Intermediates" most chemicals in this IC will have to be classified as UC = 43 "Process regulators" or UC = 55/0 "Others". Formulation may be applicable for some chemicals, whilst recovery is unlikely.

Table 38: Table for IC 3 of the MCs for the possible stages of the life-cycle which may be chosen on account of the UC chosen (for interpretation of the MC see Table 37)

Stage	Main category					
	Ia	Ib	Ic	II	III	IV
Production (UC ≠ 33)	.	X	X	.	X	.
Production (UC = 33)	X	X	X	.	.	.
Formulation (UC ≠ 33)	.	X	X	.	X	.
Processing	.	X	X	.	X	.

IC 4. Electrical/electronic industry

In electrical/electronic industry a wide range of products is manufactured. It comprises both the manufacture of components like resistors, transistors, capacitors, diodes, lamps, etc. and the production of televisions, radios, computers (PC's as well as mainframes), radar installations, complete telephone exchanges, etc. In the manufacturing processes constituent processes may take place. The main constituent processes are electroplating, polymer processing, and paint application. The emissions of substances used in these separate processes are not covered in IC 4, but in the following ICs:

- IC 8. "Metal extraction, refining and processing industry": electroplating and other metal

processing (e.g. use of metalworking fluids);

- IC 11. "Polymers industry": polymer processing (shaping of thermoplastics and curing of prepolymers e.g. for the embedding of electronic components);
- IC 14. "Paints, lacquers and varnishes industry": application of coating products by all means of methods like spraying, curtain coating, etc.

There are no emission scenario and use category documents for IC 4. There are many different applications, however, in this IC, which may be characteristic and specific for it, e.g. the production of printed circuit boards, semiconductors and the application of dielectric fluids in transformers and capacitors.

Table 39: Table for IC 4 of the MCs for the possible stages of the life-cycle which may be chosen on account of the UC chosen (for interpretation of the MC see Table 37)

Stage	Main category					
	Ia	Ib	Ic	II	III	IV
Production	.	X	X	.	X	.
Formulation	.	X	X	.	X	.
Processing	.	.	.	X	X	.

IC 5. Personal/domestic

In this IC the use and application of substances in household for maintenance and care of houses, furniture, kitchenware, gardens, etc., and personal care (hygiene, make-up, etc.) is covered. In many cases chemicals used in this IC could be present in formulations, e.g. in cleaners (soaps, detergents, washing powders, etc.), cosmetics, and products for the care of leather, textile and cars. Emissions will be very diffuse and only for wastewater the emissions to an STP are regarded as a point source. The release scenario in the A-tables considers 18 specific UCs. It is assumed that emissions take place during the whole year.

The application of substances for some specific purposes is covered in the following ICs at the stage of private use:

- IC 9. "Mineral oil and fuel industry": fuels and fuel additives;
- IC 10. "Photographic industry": photochemicals;
- IC 14. "Paints, lacquers and varnishes industry": paint products.

Table 40: Table for IC 5 of the MCs for the possible stages of the life-cycle which may be chosen on account of the UC chosen (for interpretation of the MC see Table 37)

Stage	Main category					
	Ia	Ib	Ic	II	III	IV
Production	.	X	X	.	X	.
Formulation	.	X	X	.	X	.
Private use	.	.	.	.	.	.

IC 6. Public domain

This IC covers application and use of substances in a variety of places by skilled workers, such as offices, public buildings, waiting rooms, various workshops such as garages, professional cleaning and maintenance of buildings, streets, parks, etc.

Most chemicals in this IC could be present in formulations, e.g. in "cleaners" (UC = 9 "Cleaning and washing agents and disinfectants"), non-agricultural biocides (UC = 39 "Biocides, non-agricultural"), and products for the maintenance of roads, buildings, etc. Different numbers of emission days are used for the identified UCs. The emissions in this IC could still be diffuse, but the number of days over which emissions occur are expected to be different for the UCs (many products will be used only during working days or even during a short time period). UCs 9 and 39 have been distinguished besides UC = 55/0 "Others" in the release scenarios in the A- and B-tables.

Table 41: Table for IC 6 of the MCs for the possible stages of the life-cycle which may be chosen on account of the chosen UC (for interpretation of the MC see Table 37)

Stage	Main category					
	Ia	Ib	Ic	II	III	IV
Production	.	X	X	.	X	.
Formulation	.	X	X	.	X	.
Processing	.	.	.	.	.	.

IC 7. Leather processing industry

The leather processing industry is considered to be the industry where leather is made out of raw hides, leather is dyed and where products are made out of leather (e.g. shoe manufacture).

For this IC an emission scenario document exists (focusing on leather dyeing, UC=10 "Colouring agents"). A general scenario is presented in the A- and B-tables with default values for common functions of chemicals like tanning (UC = 51 "Tanning agents". The release scenarios of the A- and B-tables make no distinction between UCs, only between MC = 2 and 3. Leather care such as for shoes belongs to IC = 5 "Personal/domestic".

Table 42: Table for IC 7 of the MCs for the possible stages of the life-cycle which may be chosen on account of the UC chosen (for interpretation of the MC see Table 37)

Stage	Main category					
	Ia	Ib	Ic	II	III	IV
Production (UC ≠ 10)	.	X	X	.	X	.
Production (UC = 10)	.	.	.	.	.	.
Formulation	.	X	X	.	X	.
Processing	.	.	.	X	X	.

IC 8. Metal extraction, refining and processing industry

This IC covers the extraction of metals from ores, the manufacture of primary/secondary steel and non-ferro metals (as well "pure" metals as alloys), and the manifold of metal working processes ("shaping") like cutting, drilling, rolling, etc.

There are emission scenario and use category documents for one aspect of the processes in this IC, namely the application of metalworking fluids. The first is only for water based fluids and the local situation. On the basis of the use category document the release scenarios in the A- and B-tables distinguish the main function of (substances used in) metalworking fluids as being cooling and lubrication: UC = 29 "Heat transferring agents" and UC = 35 "Lubricants and additives".

Table 43: Table for IC 8 of the MCs for the possible stages of the life-cycle which may be chosen on account of the UC chosen (for interpretation of the MC see Table 37)

Stage	Main category					
	Ia	Ib	Ic	II	III	IV
Production	.	X	X	.	X	.
Formulation (UC ≠ 29 & 35)	.	X	X	.	X	.
Formulation (UC = 29 / 35)	.	.	.	.	.	.
Processing	.	.	.	X	X	.

IC 9. Mineral oil and fuel industry

Mineral oil and fuel industry involves the petrochemical industry, which processes crude mineral oil. By means of physical and chemical processes (e.g. separation by means of distillation, cracking and platforming) a wide range of hydrocarbons serving as raw materials for the chemical industry and (often after adding a series of additives) fuels for heating and combustion engines, are produced.

There are no emission or use category documents for this IC. General release scenario tables are used in the A- and B-tables and do not make a distinction between UC = 27 "Fuels", UC = 28 "Fuel additives" and UC = 35 "Lubricants and additives" or any other UCs.

Table 44: Table for IC 9 of the MCs for the possible stages of the life-cycle which may be chosen on account of the UC chosen (for interpretation of the MC see Table 37)

Stage	Main category					
	Ia	Ib	Ic	II	III	IV
Production	.	X	X	.	X	.
Formulation	.	X	X	.	X	.
Processing	.	.	.	.	.	.
Private use	.	.	.	.	.	.

IC 10. Photographic industry

The photographic industry is the industry where photographic materials are manufactured ("solid" materials like films and photographic "papers", but also preparations - either in a solid or a liquid form - for film and paper processing baths. The processing of films and photographic paper is also assigned to the photographic industry, including professional processing in so-called printshops. The treatment of films and photographic paper by the public at large is considered at the stage of private use.

There are both emission scenario and use category documents for this IC. As the first scenario only covers wastewater and the local situation specific release scenarios are found in the release scenarios of the A- and B-tables. The only specific UC in the scenarios is UC = 42 "Photo-chemicals".

Table 45: Table for IC 10 of the MCs for the possible stages of the life-cycle which may be chosen on account of the UC chosen (for interpretation of the MC see Table 37)

Stage	Main category					
	Ia	Ib	Ic	II	III	IV
Production	.	X	X	.	X	.
Formulation ("aqueous solutions")	.	X	X	.	X	.
Formulation ("solid materials")	.	.	.	.	.	.
Processing	.	.	.	X	X	.
Private use	.	.	.	.	.	.

IC 11. Polymers industry

In this report and in EUSES the polymers industry comprises the branch of chemical industry where 'plastics' (thermoplastics) are chemically produced, and industries where processing of thermoplastics and prepolymers takes place by means of a wide range of techniques (see below). These processes are all dealt with in IC 11 and not in branches of industry where polymers are produced (chemical industry) or processed (IC 4, 16 and 0).

On the basis of the available use category document and expert judgement general release scenarios have been provided in the A- and B-tables. First, there are tables for polymerisation processes, i.e. the processing stage of substances, which are converted into polymers by polymerisation reactions, polyadditions, polycondensations, etc. This has been done in order to be able to treat them specifically apart from substances produced in 'chemical industry' (in principle they may be regarded as process intermediates). Several types of functions, UCs and two polymerisation processes are distinguished.

Second, there are tables for the processing of polymers, i.e. shaping by all kinds of processes such as injection moulding, blowing, and extrusion. Although processing of polymers may occur in several ICs, e.g. IC 4 Electrical/electronic industry and IC 16 'Engineering industries: civil and mechanical', only one release scenario was introduced at the present IC. Several types of functions, UCs and thermoplastics and thermosetting resins are distinguished in the scenario.

Table 46: Table for IC 11 of the MCs for the possible stages of the life-cycle which may be chosen on account of the UC chosen (for interpretation of the MC see Table 37)

Stage	Main category					
	Ia	Ib	Ic	II	III	IV
Production	.	X	X	.	X	.
Formulation	.	X	X	.	X	.
Processing ("polymerisation")	.	.	.	.	.	.
Processing	.	.	.	.	.	.
Recovery	Not yet considered					

IC 12. Pulp, paper and board industry

Strictly speaking only the production of pulp, paper and cardboard out of wood or waste paper belongs to this IC. As the HEDSET categorisation does not specifically distinguish the reprographic industry this important activity has been separated from the general category 0 "Others".

For this IC both emission scenario and use category documents are available. The emission scenario document deals with wastewater and the local situation. The release scenarios in the A- and B-tables are applicable to the stage of processing printing and allied processes, and the production of pulp, paper and board (including paper dyeing). The stage of recovery (paper recycling) is also considered in the tables.

Two UCs are specifically considered, i.e. UC=10 "Colouring agents" used as pigments in inks and as dyes for paper mass colouring, UC 20 and 31 ("Fillers" and "Impregnation agents") both used in paper production and UC 45 "Reprographic agents" which is a "collection" of all kinds of uses and functions of substances in printing and allied processes.

Table 47: Table for IC 12 of the MCs for the possible stages of the life-cycle which may be chosen on account of the UC chosen (for interpretation of the MC see Table 37)

Stage	Main category					
	Ia	Ib	Ic	II	III	IV
Production (UC ≠ 10)	.	X	X	.	X	.
Production (UC = 10)	.	.	.	.	.	.
Formulation	.	X	X	.	X	.
Recovery	.	.	.	.	.	.

IC 13. Textile processing industry

This IC covers treatment of fibres ("cleaning", spinning, dyeing, etc.), weaving, and finishing (e.g. impregnation, coating, etc.).

For this IC both emission scenario and use category documents are available. The release

scenarios in the A- and B-tables are specific for IC 10 "Colouring agents" and general for other relevant UCs.

Table 48: Table for IC 13 of the MCs for the possible stages of the life-cycle which may be chosen on account of the UC chosen (for interpretation of the MC see Table 37)

Stage	Main category					
	Ia	Ib	Ic	II	III	IV
Production (UC ≠ 10)	.	X	X	.	X	.
Production (UC = 10)	.	.	.	.	.	.
Formulation	.	X	X	.	X	.
Processing	.	.	.	.	.	.
Private use (only UC = 10)	.	.	.	.	.	.

IC 14. Paints, lacquers and varnishes industry

Apart from the manufacture of coating products (stage of formulation) such as paints this report and EUSES also consider application of these products as belonging to this IC. This has been done because otherwise many release scenarios would have to be introduced in many other ICs. These could include for example IC 5 "Personal/domestic" for private use, IC 6 "Public domain" for professional application by house painters and in (small) workshops, and many industrial applications. The latter could include IC 16 "Engineering industries: civil and mechanical" in the manufacturing of motor cars, constructions, etc. and IC 8 "Metal extraction, refining and processing industry".

There is an emission scenario on paint manufacture and application (stages of formulation and processing respectively) and a use category document for paint manufacture. The A- and B-tables have release scenarios for both water-based and solvent-based coatings systems and distinguish 8 specific UCs; both industrial use (stage of processing) and private use. The stage of formulation concerns the manufacture of the coating products.

Table 49: Table for IC 14 of the MCs for the possible stages of the life-cycle which may be chosen on account of the UC chosen (for interpretation of the MC see Table 37)

Stage	Main category					
	Ia	Ib	Ic	II	III	IV
Production	.	X	X	.	X	.
Formulation	.	X	X	.	X	.
Processing	.	.	.	.	.	.
Private use	.	.	.	.	.	.

IC 15. Engineering industries: civil and mechanical

Industrial activities belonging to this IC include wood processing industries (e.g. wooden

furniture), motor car manufacture, building industry, etc. There are no emission or use category documents for this IC. Processes such as coating application take place in many of these activities; these processes are dealt with in the IC where the specific process belongs (coating application: IC 14 "Paints, lacquers and varnishes industry"). For the present IC the same general release scenarios as for IC 15 "Others" are used in the A- and B-tables.

Table 50: Table for IC 15 of the MCs for the possible stages of the life-cycle which may be chosen on account of the UC chosen (for interpretation of the MC see Table 37)

Stage	Main category					
	Ia	Ib	Ic	II	III	IV
Production	.	X	X	.	X	.
Formulation	.	X	X	.	X	.
Processing	.	.	.	X	X	X

IC 16. Others

All processes and activities, which can not be placed in one of the previous ICs, belong to this IC. An example is the food processing industry. General release scenarios are used in the A- and B-tables.

Table 51: Table for IC 16 of the MCs for the possible stages of the life-cycle which may be chosen on account of the UC chosen (for interpretation of the MC see Table 37)

Stage	Main category					
	Ia	Ib	Ic	II	III	IV
Production	.	X	X	.	X	.
Formulation	.	X	X	.	X	.
Processing	.	.	.	X	X	X

11. Relationship between industrial categories

In practice all chemicals originate from IC 2 & 3 "Chemical industry" and go from there to one of the other ICs (or remain in chemical industry). Substances such as monomers, cross-linking agents, and curing agents take a special position. These substances are basic chemicals (raw materials) for IC 11 "Polymers industry" for the production of polymers by polymerisation reactions and other reactions like polyaddition and polycondensation. Despite the fact that this may be seen as the stage of production in IC 3 (UC 33 "Intermediates") they have been introduced in the emission tables of IC 11 "Polymers industry" as UC 43 "Process regulators". Besides the production of polymers this IC also deals with the processing of the polymers (thermoplastics) and prepolymers (prepolymers are macromolecular substances such as polyester and epoxy resins which are transformed in thermosetting resins with the aid of curing agents, such as initiators - mainly organic peroxides - and cross-linking agents - mainly the monomer styrene - for polyesters, and curing agents like amines for epoxy resins). The processing stage of (pre) polymers involves the manufacture of all kind of articles and parts of objects from the basic materials.

The releases in both IC 5 "Personal/domestic" and IC 6 "Public domain" have a diffuse character. In IC 5 the use of chemicals in households is covered and in IC 6 the use in offices, public buildings, parks, railway stations, in the street, etc. The main differences will be found in the amounts (e.g. because of the size of the building) and the number of days that emissions occur.

12. History of the A- and B-tables

In the development of the quantitative risk assessment system for new substances DRANC (Dutch Risk Assessment System for New Chemicals) (Toet et al., 1991; Vermeire et al., 1992) emission tables were developed for a limited number of applications. The applications considered were textile dyes, photo-chemicals, metalworking fluids, hydraulic fluids, paper-chemicals, and intermediates. For these applications so-called use category documents were available. Nearly at the same time PRISEC (PRIority Setting system for Existing Chemicals) was developed (Van de Meent and Toet, 1992). For this system emission tables were developed for the 15 industrial categories distinguished at that time in the HEDSET (EC/OECD Harmonised Electronic Data Set). The emission factors were established by means of expert judgement and tended to the worst-case situation. For the local release estimation tables were supplied containing expert judgement for the order of magnitude of the daily amount of the substances for every relevant stage of the life-cycle on the basis of the tonnage. The ranges of the tonnages were typical for substances produced in limited amounts. When the TGD and EUSES were developed these tables were transformed into what are now referred to as the A- and B-tables (A-tables with emission factors and B-tables with size of the operation information) and extended in the following way:

1. extension of the tables with emission factors for several industrial categories. This may be for example for the introduction of main categories or specific use categories. This was also achieved by expert judgement trying to obtain realistic worst-case estimates;
2. insertion of the emission factors of the use category documents mentioned before in the appropriate industrial categories;
3. introduction of B-tables in order to cover higher tonnages for HPVCs. This was also done by expert judgement;
4. new A- and B-tables were developed for the new industrial category 16 'Engineering industries'.

The final tables were discussed and endorsed in a special EU Expert Meeting on Release estimation (Sept. 1995) that was held in the context of the development of the TGD. Subsequently, the tables were introduced in the TGD and EUSES.

13. Calculating releases per stage of the life-cycle

Using the fractions released from the A-tables, the total amount released (per stage of the life-cycle and for each environmental compartment) can be calculated with the following equations. For each stage (except for production) the losses in the previous stage are taken into account.

The fractions released in each stage of the life-cycle and to every compartment are denoted by $F_{i,j}$ where *i* is the stage in the life-cycle and *j* is the compartment:

i	stage of the life-cycle	*j*	compartment
1	production	a	air
2	formulation	w	water
3	processing	s	soil
4	private use		

5	recovery

Industrial/professional use is indicated as "processing" in the A- and B-tables. Service life is not included as a separate stage of the life-cycle. With respect to waste disposal, only recovery is addressed in the A- and B-tables.

The release per stage of the life-cycle (in tonnes per year) can be calculated by:

1. Production

Production	$RELEASE_{1,j}$	air	$F_{1,a} \cdot PRODVOL$
		water	$F_{1,w} \cdot PRODVOL$
		soil	$F_{1,s} \cdot PRODVOL$
		total	$\Sigma F_{1,j} \cdot PRODVOL$
	amount used:		TONNAGE

2. Formulation

Formulation	$RELEASE_{2,j}$	air	$F_{2,a} \cdot TONNAGE$
		water	$F_{2,w} \cdot TONNAGE$
		soil	$F_{2,s} \cdot TONNAGE$
		total	$\Sigma F_{2,j} \cdot TONNAGE$
	rest:		$(1-\Sigma F_{2,j}) \cdot TONNAGE$

3. Processing

Processing	$RELEASE_{3,j}$:	air	$F_{3,a} \cdot (1-\Sigma F_{2,j}) \cdot TONNAGE$
		water	$F_{3,w} \cdot (1-\Sigma F_{2,j}) \cdot TONNAGE$
		soil	$F_{3,s} \cdot (1-\Sigma F_{2,j}) \cdot TONNAGE$
		total	$\Sigma F_{3,j} \cdot (1-\Sigma F_{2,j}) \cdot TONNAGE$

4. Private use

Private use	$RELEASE_{4,j}$	air	$F_{4,a} \cdot (1-\Sigma F_{2,j}) \cdot TONNAGE$
		water	$F_{4,w} \cdot (1-\Sigma F_{2,j}) \cdot TONNAGE$
		soil	$F_{4,s} \cdot (1-\Sigma F_{2,j}) \cdot TONNAGE$
		total	$\Sigma F_{4,j} \cdot (1-\Sigma F_{2,j}) \cdot TONNAGE$
		rest:	$(1-\Sigma F_{3,j} - \Sigma F_{4,j}) \cdot (1-\Sigma F_{2,j}) \cdot TONNAGE$

5. Recovery

Recovery	$RELEASE_{5,j}$:	air	$F_{5,a} \cdot (1-\Sigma F_{3,j} - \Sigma F_{4,j}) \cdot (1-\Sigma F_{2,j}) \cdot$ TONNAGE
		water	$F_{5,w} \cdot (1-\Sigma F_{3,j} - \Sigma F_{4,j}) \cdot (1-\Sigma F_{2,j}) \cdot$ TONNAGE
		soil	$F_{5,s} \cdot (1-\Sigma F_{3,j} - \Sigma F_{4,j}) \cdot (1-\Sigma F_{2,j}) \cdot$ TONNAGE
		total	$\Sigma F_{5,j} \cdot (1-\Sigma F_{3,j} - \Sigma F_{4,j}) \cdot (1-\Sigma F_{2,j}) \cdot$ TONNAGE

Explanation of symbols

$F_{i,j}$	Fraction of tonnage released during stage *i* to compartment *j*	[-]	**Appendix 6**
PRODVOL	Production volume of the substance	[tonnes.yr^{-1}]	data set
TONNAGE	Tonnage of the substance	[tonnes.yr^{-1}]	eq.(4) (Ch.2)
$RELEASE_{i,j}$	Release during life-cycle stage *i* to compartment *j*	[tonnes.yr^{-1}]	

Abbreviations used in the tables

f	Fraction
HPVC	High Production Volume Chemicals
MC	Main category
IC	Industrial category
S	Solubility (in water) [mg/l]
T	Tonnage [tonnes/year]
UC	Use category
VP	Vapour pressure [Pa]

A-TABLES: ESTIMATES FOR THE EMISSION FACTORS (FRACTIONS RELEASED)

IC = 1: AGRICULTURAL INDUSTRY

IC = 2: CHEMICAL INDUSTRY: BASIC CHEMICALS

IC = 3: CHEMICAL INDUSTRY: CHEMICALS USED IN SYNTHESIS

IC = 4: ELECTRICAL/ELECTRONIC INDUSTRY

IC = 5: PERSONAL /DOMESTIC

IC = 6: PUBLIC DOMAIN

IC = 7: LEATHER PROCESSING INDUSTRY

IC = 8: METAL EXTRACTION, REFINING AND PROCESSING INDUSTRY

IC = 9: MINERAL OIL AND FUEL INDUSTRY

IC = 10: PHOTOGRAPHIC INDUSTRY

IC = 11: POLYMERS INDUSTRY

IC = 12: PULP, PAPER AND BOARD INDUSTRY

IC = 13: TEXTILE PROCESSING INDUSTRY

IC = 14: PAINTS, LACQUERS AND VARNISHES INDUSTRY

IC = 16: ENGINEERING INDUSTRY: CIVIL AND MECHANICAL

IC = 0: OTHERS

IC = 1: AGRICULTURAL INDUSTRY

PRODUCTION: **Table A1.1**

Compartment	Conditions		Emission factors			
	S (mg/l)	VP (Pa)	All MC's	MC=1b	MC=1c	MC=3 [1)]
Air		<1		0	0	0.00001
		1-10		0	0.00001	0.0001
		10-100		0.00001	0.0001	0.001
		100-1000		0.0001	0.001	0.0
		1000-10,0000		0.001	0.005	0.05
		≥10,000		0.005	0.01	0.05
	t (tonnes/year)					
Wastewater	<1000		0.02			
	≥1,000		0.003			
Soil			0.0001			

[1)] Default

FORMULATION: **Table A2.1**

Compartment	Conditions		Emission factors			
	S (mg/l)	VP (Pa)	All MC's	MC=1b	MC=1c	MC=3 [1)]
Air		<10		0.0005	0.001	0.0025
		10-100		0.001	0.0025	0.005
		100-1,000		0.0025	0.005	0.01
		≥1,000		0.005	0.01	0.025
	t (tonnes/year)					
Wastewater	<1,000		0.02			
	≥1,000		0.003			
Soil			0.0001			

[1)] Default

INDUSTRIAL USE: **Table A3.1***

UC's	Description	Emission factors to:		
		Air	Surface water	Soil
Default		0.1	0.1	0.8
3	areosol propellants	1	0	0
9, 10, 36	cleaning/washing agents and additives + colorants + odour agents	0	0.1	0.4
19	fertilisers	0	0.05	0.95
26	food/feedstuff additives	0	0	0.05
38, 50	pesticides + surfactants	0.05	0.1	0.85
41	pharmaceuticals (external application)	0	0	0.1
41	pharmaceuticals (internal application)	0	0	0
48	solvents	1	0	0

* Fertilisers and pesticides + surfactants go to agricultural soil on the regional and continental scale; the others go to industrial soil.

PRIVATE USE: Not applicable

WASTE TREATMENT: Not applicable

IC=2: CHEMICAL INDUSTRY: BASIC CHEMICALS

PRODUCTION: **Table A1.1**

FORMULATION: **Table A2.1**

INDUSTRIAL USE: **Table A3.2**

Conditions		Emission factors		
S (mg/l)	VP (Pa)	Air	Wastewater	Soil
<100	<100	0.65	0.25	0.0005
	100-1,000	0.8	0.1	0.0025
	≥1,000	0.95	0.05	0.001
100-1,000	<100	0.4	0.5	0.005
	100-1,000	0.55	0.35	0.002
	≥1,000	0.65	0.25	0.001
1,000-10,000	<100	0.25	0.65	0.005
	100-1,000	0.35	0.55	0.002
	≥1,000	0.5	0.4	0.001
≥10,000	<100	0.05	0.85	0.005
	100-1,000	0.1	0.8	0.002
	≥1,000	0.25	0.65	0.001

PRIVATE USE: Not applicable

WASTE TREATMENT: Not applicable

Remark: Emissions at recovery of chemicals such as catalysts are included in the emissions at industrial use.

IC = 3: CHEMICAL INDUSTRY: CHEMICALS USED IN SYNTHESIS

PRODUCTION: **Table A1.1** for UC ≠ 33 (intermediates)

Table A1.2 for UC = 33 (intermediates)

Compartment	Conditions		Emission factors			
	S (mg/l)	VP (Pa)	All MC's	MC=1a	MC=1b	MC=1c
Air		<1		0	0	0
		1-10		0	0	0.00001
		10-100		0	0.00001	0.0001
		100-1,000		0.00001	0.0001	0.001
		1,000-10,000		0.0001	0.001	0.01
		≥10,000		0.001	0.01	0.025
	Process	t (tonnes/year)				
Wastewater	Wet	<1,000	0.02			
		≥1,000	0.003			
	Dry		0			
Soil				0	0.00001	0.0001

FORMULATION: **Table A2.1**

INDUSTRIAL USE: **Table A3.3**

Compartment	Conditions		Emission factors			
	S (mg/l)	VP (Pa)	All MC's	MC = 1b	MC = 1c	MC = 3[1)]
Air		<1		0	0	0.00001
		1-10		0	0	0.0001
		10-100		0	0.00001	0.001
		100-1,000		0.00001	0.0001	0.01
		1,000-10,000		0.0001	0.001	0.025
		≥10,000		0.001	0.005	0.05

Compartment	Conditions		Emission factors			
	S (mg/l)	VP (Pa)	All MC's	MC = 1b	MC = 1c	MC = 3[1)]
	Process	t(tonnes/year)				
Wastewater	Wet	<1,000	0.02			
		≥1,000	0.007	0.0005		
	Dry		0			
Soil			0.0001			

[1)] Default

Remark: The releases at industrial use for use category 33 (intermediates) should be added to the releases at production unless the notifier states that the substance is processed elsewhere.

PRIVATE USE: Not applicable

WASTE TREATMENT: Not applicable

IC = 4: ELECTRICAL/ELECTRONIC INDUSTRY

PRODUCTION: **Table A1.1**

FORMULATION: **Table A2.1**

INDUSTRIAL USE: **Table A3.4**

Compartment	Conditions	Emission factors	
	VP (Pa)	MC = 2	MC = 3[1)]
Air	<100	0.0005	0.0005
	≥100	0.0005	0.001
Wastewater		0.0001	0.005
Soil		0.0001	0.01

[1)] Default

PRIVATE USE: Not applicable

WASTE TREATMENT: Not applicable

IC = 5: PERSONAL / DOMESTIC

PRODUCTION: **Table A1.1** for UC ≠ 9 (cleaning/washing agents) and 15 (cosmetics)

A1# for UC = 9 and 15 (if production volume < 1,000 tonnes/year then Table A1.1 applies)

Compartment	Conditions		Emission factors	
	S (mg/l)	VP (Pa)	Batch process [1)]	Continuous process [2)]
Air			0.000 001	0.000 001
Wastewater			[3)]	[4)]
Solid waste			0	0

Notes to the above table:

1) e.g., ethoxilation to nonionic surfactants and production of amphoteric and cationic surfactants

2) e.g., sulphonation and sulphation to anionic surfactants

3) According to the emission scenario document < 0.3 % (worst case = 0.003)

4) According to the emission scenario document < 0.1 % (worst case = 0.001)

FORMULATION: **Table A2.1** for UC ≠ 9 (cleaning/washing agents) and 15 (cosmetics)

Table A2# for UC = 9 (cleaning/washing agents) and UC15 (cosmetics)

Compartment	Conditions		Emission factors			
	S (mg/l)	VP (Pa)	Regular powder	Compact powder	Liquid	Unknown
Air			0.000 2	0.000 2	0.000 02	0.000 2
Wastewater			0.000 1	0.000 01	0.000 9	0.000 9
Solid waste			0.007 3	0.008 1	0.003 2	0.008 1

INDUSTRIAL USE: Not applicable

PRIVATE USE: **Table A4.1**

Compartment	Conditions			Emission factors
	Use category	S (mg/l)	VP (Pa)	
Air	2, 7, 8, 9, 10, 11, 15,			
	41, 47, 50			0
	3			1
	5			0.0005
	26		<5,000	0
			≥5,000	0.01
	35		<5,000	0
			≥5,000	0.05
	36		<100	0.05
			100-2,500	0.2
			2,500-10,000	0.5
			≥10,000	0.9
	38 (herbicides)			0.01
	(pesticides, garden)			0.05
	(pesticides, pets)		<100	0.05
			100-5,000	0.1
			≥5,000	0.8
	48, 55	<10	<10	0.005
			10-100	0.015
			100-1,000	0.15
			1,000-10,000	0.4
			≥10,000	0.6
	48, 55	10-100	<10	0.0015
			10-100	0.075
			100-1,000	0.125
			1,000-10,000	0.25

Compartment	Conditions			Emission factors
	Use category	S (mg/l)	VP (Pa)	
Air (continued)			≥10,000	0.4
	48, 55	100-1,000	<10	0.0015
			10-100	0.025
			100-1,000	0.1
			1,000-10,000	0.15
			≥10,000	0.225
	48, 55	≥1,000	<10	0.00075
			10-100	0.03
			100-1,000	0.075
			1,000-10,000	0.125
			≥10,000	0.175
Surface water	5, 35 (car products)			0.0005
Wastewater	2	25		0
		≥25		0.005
	3, 5, 19, 35			0
	7			0.01
	8 (household products)			0.95
	(cosmetics)			0.8
	9, 15			1
	50			0.99
	10 (cleaning products)			1
	(cosmetics)			0.8
	(else)			0.5
	11			0.8
	26			0.025
	36 (cosmetics)		<2,500	0.8

Compartment	Conditions			Emission factors
	Use category	S (mg/l)	VP (Pa)	
Wastewater (continued)			2,500-10,000	0.5
			≥10,000	0.1
	(cleaning products,…)		<100	0.9
			100-2,500	0.8
			2,500-10,000	0.5
			≥10,000	0.1
	(else)		<100	0.5
			100-2,500	0.3
			2,500-10,000	0.2
			≥10,000	0.05
	38 (herbicides)			0
	(pesticides, garden)			0
	(pesticides, pets)			0.1
	41 (external)			0.25
	(oral)			0.05
	47			0.9
	48, 55		<10	0.1
			10-100	0.2
			100-1,000	0.4
			≥1,000	0.6
Soil	2			0.0001
	3, 36, 41			0
	5			0.0005
	7			0.001
	8 (household products)			0.01
	(cosmetics)			0.001

Compartment	Conditions			Emission factors
	Use category	S (mg/l)	VP (Pa)	
Soil (continued)	9, 15			0
	47,50			0.01
	10 (cleaning products)			0.002
	(cosmetics)			0.0001
	(else)			0.01
	11			0.0001
	19			1
	26, 35			0.002
	38 (garden: herbicides, pesticides)			0.9
	(pesticides, pets)		<100	0.05
			100-5,000	0.01
			≥5,000	0.002
	48, 55		<10	0.2
			10-100	0.1
			100-1,000	0.05
			1,000-10,000	0.005
			≥10,000	0.002

WASTE TREATMENT: Not applicable

IC = 6: PUBLIC DOMAIN

PRODUCTION: **Table A1.1** for UC ≠ 9 (cleaning/washing agents) and 15 (cosmetics)

Table A1# for UC = 9 and 15 (if production volume < 1000 tonnes/year Table A1.1 applies)

FORMULATION: **Table A2.1** for UC ≠ 9 (cleaning/washing agents)

Table A2# for UC = 9 (cleaning/washing agents)

INDUSTRIAL USE: **Table A3.5**

Conditions		Emission factors		
Use categories		**Air**	**Wastewater**	**Soil**
9	(cleaning/washing agents)			
	≤ 1,000 tonnes/year	0.0025	0.9	0.05
	> 1,000 tonnes/year	0	1	0
39	(non-agric. pesticides)	0.1	0.05	0.8
All	other	0.05	0.45	0.45

PRIVATE USE: Not applicable

WASTE TREATMENT: Not applicable

IC = 7: LEATHER PROCESSING INDUSTRY

PRODUCTION: **Table A1.1** for UC ≠10 (colorants)

Table A1.3 for UC = 10 (colorants)

UC = 10 (Colorants)		
Compartment	Conditions S (mg/l)	Emission factors
Air		0.0008
Wastewater	<2,000	0.015
	2,000-10,000	0.02
	10,000-100,000	0.03
	100,000-500,000	0.05
	≥500,000	0.06
Soil		0.0001

FORMULATION: **Table A2.1**

INDUSTRIAL USE: **Table A3.6**

Compartment	Conditions		Emission factors		
	S (mg/l)	VP (Pa)	All MC's	MC = 2	MC = 3 [1)]
Air	<100	<100	0.001		
	<100	≥100	0.01		
	≥100		0		
Wastewater	<100			0.05	0.9
	100-1,000			0.15	0.99
	≥1,000			0.25	0.99
Soil			0.01		

[1)] Default

PRIVATE USE: **Not applicable**

WASTE TREATMENT: **Not applicable**

IC = 8: METAL EXTRACTION, REFINING AND PROCESSING INDUSTRY

PRODUCTION: **Table A1.1**

FORMULATION: **Table A2.1 for UC ≠ 29 & 35**

Table A2.2 for UC = 29 & 35

Compartment	Conditions VP (Pa)	Emission factors
Air	<1	0.00005
	1-10	0.00001
	10-100	0.0005
	100-1,000	0.0025
	≥1,000	0.025
Wastewater		0.002
Soil		0.00001

INDUSTRIAL USE: **Table A3.7**

Compartment	Conditions UC≠29&35 S (mg/l)	Emission factors MC = 2	MC = 3 [1)]
Air		0	0.25
Wastewater	<100	0.05	0.5
	100-1,000	0.1	0.5
	≥1,000	0.25	0.5
Soil		0	0.05

Compartment	Conditions UC=29&35 log k_H	Emission factors
Air	<2	0.0002
	≥2	0.002

Compartment	Conditions UC=29&35 log k_H	Emission factors
Wastewater	Pure oils	0.185
	Water based + unknown	0.316
Soil		0.0001

1) Default

Remark: UC 29 = heat transferring agents, UC 35 = lubricants and additives; both are used in metalworking fluids

PRIVATE USE: **Not applicable**

WASTE TREATMENT: **Not applicable**

IC = 9: MINERAL OIL AND FUEL INDUSTRY

PRODUCTION: **Table A1.1**

FORMULATION: **Table A2.1**

INDUSTRIAL USE: **Table A3.8**

Compartment	Conditions VP (Pa)	Emission factors
Air	<1	0.0001
	1-10	0.0005
	10-100	0.001
	100-1,000	0.005
	≥1,000	0.01
Wastewater		0.0005
Soil		0.001

PRIVATE USE: **Table A4.2**

Compartment	Conditions VP (Pa)	Emission factors
Air	<10	0.005
	10-100	0.015
	100-1,000	0.15
	1,000-10,000	0.4
	≥10,000	0.6
Wastewater		0.0005
Surface water		0.0001
Soil		0.0001

WASTE TREATMENT: **Not applicable**

IC = 10: PHOTOGRAPHIC INDUSTRY

PRODUCTION: **Table A1.1**

FORMULATION: **Table A2.1** default for formulations to be used in photographic baths (aqueous solutions)

Table A2.3 for UC=42, and other UC's in the manufacture of solid materials

Compartment	Conditions VP (Pa)	Emission factors
Air	<1	0.0001
	1-10	0.001
	10-100	0.3
	100-1,000	0.7
	≥1,000	1
Wastewater	Control of crystal growth	0.99
	Other functions	0.002
Soil		0.00025

INDUSTRIAL USE: **Table A3.9**

Compartment	Conditions	Emission factors VP (Pa)	MC=2	MC=3 [1)]
Air	Solid materials (e.g. films)		0	
	Else	<1		0.000035
		1-10		0.00025
		10-100		0.0075
		100-1,000		0.025
		≥1,000		0.075
Wastewater	Solid materials (e.g. films)		0	
	Aqueous solutions:			
	- coupler of dye			0.15

Compartment	Conditions	VP (Pa)	Emission factors MC=2	MC=3 [1)]
	- else			0.8
Soil	Solid materials (e.g. films)		0	
	Else			0.00025

[1)] Default

PRIVATE USE: Table A4.3

Compartment	Conditions UC=42 (photochemicals) for aqueous solutions only	Emission factors
Air		0
Wastewater		0.4
Soil		0

WASTE TREATMENT: Table A5.1

Compartment	Conditions UC=42 (photochemicals) for aqueous solutions only VP (Pa)	Emission factors
Air		<10.000005
	1-10	0.000025
	10-100	0.00075
	100-1,000	0.0025
	≥1,000	0.01
Wastewater		0.2
Soil		0

IC = 11: POLYMERS INDUSTRY

PRODUCTION: **Table A1.1**

FORMULATION: **Table A2.1**

INDUSTRIAL USE: **Table A3.10 for polymerisation processes**

In the polymers industry polymers are produced by:

A) Polymerisation reactions:

A.1) "Wet" (e.g. emulsion polymerisation)

A.2) "Dry" (e.g. gas phase polymerisation)

B) Other (e.g. polyadditions, polycondensations)

The use category (HEDSET) for all types of chemicals is 43: Process regulators, which can be subdivided according to the table below:

Type	Type of function
I	Monomers (UC 43 Process regulators)
II	Catalysts (UC 43 Process regulators)
III	Initiators, Inhibitors, Retarders, Chain transfer agents (UC 43 Process regulators), Vulcanising agents (UC 53 Vulcanising agents), etc.

N.B.

1. In principle this might be considered as stage 1. Production.
2. As no good information is available Process types "A" and "B" have been considered to have the same emission factors.

Compartment	Conditions	Emission factors					
		Type I		Type II		Type III	
	VP (Pa)	"Wet"	"Dry"	"Wet"	"Dry"	"Wet"	"Dry"
Air	<1	0.00001	0.00001	0	0	0	0
	1-10	0.0001	0.0001	0	0	0	0
	10-100	0.001	0.001	0	0	0	0
	100-1,000	0.01	0.01	0.0005	0.0005	0	0
	1,000-10,000	0.05	0.05	0.001	0.001	0.0005	0.0005

Compartment	Conditions	Emission factors					
		Type I		Type II		Type III	
	VP (Pa)	"Wet"	"Dry"	"Wet"	"Dry"	"Wet"	"Dry"
	≥10,000	0.05	0.05	0.01	0.01	0.001	0.001
Wastewater	**S (mg/l)**						
	<10	0.00001	0	0.005	0	0.0005	0
	10-100	0.0001	0	0.01	0	0.001	0
	100-1,000	0.001	0	0.025	0	0.0025	0
	≥1,000	0.01	0	0.05	0	0.005	0
Soil	**VP (Pa)**						
	<5,000	0	0	0.0005	0.0005	0.00025	0.00025
	≥5,000	0	0	0	0	0	0

INDUSTRIAL USE: Table A3.11 for polymer processing

Processing of polymers ("shaping" by all kind of techniques) occurs in many Industrial categories

Two categories of polymer processing are distinguished:

A Processing of thermoplastics

B Processing of thermosetting resins (prepolymers)

For the emission factors the following types of chemicals used are considered:

Type of chemicals	Emission factor	Type of function	
I	(A, B)	Additives	UC 7 (Anti-static agents), 22 (Flame retardants), 49 (Stabilisers) & 55 Others (e.g. antioxidants)
		Pigments	UC 10 (Colorants)
		Fillers	UC 20
II	(A)	Plasticisers	UC 47 (softeners)
III	(A, B)	Solvents	UC 48
IV	(A, B)	Processing aids	UC 6 (Anti-set off and anti-adhesive agents) & 35 (lubricants and additives)

Type of chemicals	Emission factor	Type of function	
V	(B)	Curing agents	UC 43 (Process regulators, e.g. initiators)
		Cross-linking agents	UC 43 (Process regulators: monomers)

Compartment	Conditions		Emission factors		Type of chemicals
	VP (Pa)	BP (°C)	A	B	
Air	<1	<300/unknown	0.001	0	I
		≥300	0.0005	0	
	1-100	*<300/unknown*	*0.0025*	0	
		≥300	0.001	0	
	≥100	<300/unknown	0.01	0	
		≥300	0.005	0	
		<400/unknown	0.01		II
		≥400	0.005		
	<100		0.1	0.1	III
	100-1,000		0.25	0.25	
	1,000-10,000		0.5	0.5	
	≥10,000		0.75	0.75	
	<1	<300/unknown	0.01	0	IV
		≥300	0.005	0	
	1-100	<300/unknown	0.025	0	
		≥300	0.01	0	
	≥100	<300/unknown	0.1	0	
		≥300	0.05	0	
	<100			0.075	V
	100-1,000			0.15	
	1,000-10,000			0.25	

Compartment	Conditions		Emission factors		Type of chemicals
	VP (Pa)	BP (°C)	A	B	
	≥10,000			0.35	
Wastewater			0.0005	0.0005	I
			0.001	0	II
			0	0	III
			0.0005	0.0005	IV
				0.00005	V
Soil			0.0001	0.0001	I
			0.0005	0	II
			0.00001	0.00001	III
			0.001	0.001	IV
				0.00001	V

PRIVATE USE: **Not applicable**

WASTE TREATMENT: **Not considered yet**

IC = 12: PULP, PAPER AND BOARD INDUSTRY

PRODUCTION: **Table A1.1 for UC ≠ 10 (colorants)**

Table A1.3 for UC = 10 (colorants)

FORMULATION: **Table A2.1 for UC ≠ 45 (reprographic agents)**

Table A2.1 for UC = 45 (reprographic agents)

INDUSTRIAL USE: **Table A3.12 for printing and allied processes**

Compartment	Conditions		Emission factors	
	Use categories	VP (Pa)	MC = 2	MC = 3 1)
Air	Default	<100	0	0.01
		100-1,000	0.05	0.2
		1,000-10,000	0.25	0.5
		≥10,000	0.5	0.75
	10 & 45		0	
	48	<100		0.05
		100-1,000		0.3
		1,000-10,000		0.65
		≥10,000		0.85
Wastewater		**S (mg/l)**	**MC = 2**	**MC = 3 [1)]**
	Default	<100	0.0001	0.01
		100-1,000	0.005	0.05
		≥1,000	0.001	0.1
	9			0.9
	10 & 45		0.0005	
	48	<100		0.0005
		100-1,000		0.001
		≥1,000		0.005
		VP (Pa)	**MC = 2**	**MC = 3 [1)]**
Soil	All	<100	0.0015	0.0015

Compartment	Conditions		Emission factors	
	Use categories	VP (Pa)	MC = 2	MC = 3 1)
		100-1,000	0.0001	0.0001
		1,000-10,000	0.00001	0.00001
		≥10,000	0	0

1) Default

INDUSTRIAL USE: Table A3.12 for pulp, paper and board production

Compartment	Conditions			Emission factors	
	Use category	S (mg/l)	VP (Pa)	MC=2	MC=3[1)]
Air	All	<100	<100	0	0.0001
			100-1,000	0.00001	0.001
			≥1,000	0.0001	0.01
		100-1,000	<100	0	0.00001
			100-1,000	0	0.0001
			≥1,000	0.00001	0.001
		≥1,000	<100	0	0
			100-1,000	0	0.0001
			≥1,000	0	0.001
Wastewater	Default	<100	<100	0.85	0.85
			100-500	0.75	0.75
			≥500	0.5	0.5
		100-1,000	<100	0.875	0.875
			100-500	0.85	0.85
			≥500	0.75	0.75
		1,000-10,000	<100	0.9	0.9
			100-500	0.875	0.875
			≥500	0.85	0.85
		≥10,000	-	0.95	0.95
	10:				

Compartment	Conditions			Emission factors	
	Use category	S (mg/l)	VP (Pa)	MC=2	MC=3[1)]
	- Basic dye, anion			0.023	0.023
	- Direct dye			0.04	0.04
	- Direct dye, kation			0.055	0.055
	- Direct dye, anion/kation			0.028	0.028
	- Acid dye, kation/unknown			0.079	0.079
	- Brightener			0.064	0.064
	20 & 31			0.05	0.05
Soil	All	<100		0.0015	0.0015
		100-1,000		0.0001	0.0001
		1,000-10,000		0.00001	0.00001
		≥10,000		0	0

[1)] Default

PRIVATE USE: **Not applicable**

WASTE TREATMENT: **Table A5.2**

Compartment	Conditions	Emission factors
Air		0
Wastewater	Use category = 10 (Colorants)	0.1
	Use category 45, for paper type:	
	- graphic	0.2
	- cardboard	0.01
	- newspaper	0.15
	- sanitary	0.01
	- packing	0.1
	- archives	0.05
	- other, or >1 application	0.2
Soil		0

IC = 13: TEXTILE PROCESSING INDUSTRY

PRODUCTION: **Table A1.1 for UC ≠ 10 (colorants)**

Table A1.3 for UC = 10 (colorants)

FORMULATION: **Table A2.1**

INDUSTRIAL USE: **Table A3.14**

Compartment	Conditions		Emission factors	
	S (mg/l)	VP (Pa)	UC<>10	UC = 10
Air	<100	<100	0.05	
		100-1,000	0.15	
		≥1,000	0.4	
	100-1,000	<100	0.025	
		100-1,000	0.05	
		≥1,000	0.15	
	1,000-10,000	<100	0.01	
		100-1,000	0.025	
		≥1,000	0.05	
	≥10,000	<100	0.005	
		100-1,000	0.01	
		≥1,000	0.025	
	Batch dyeing			0.0007
	Continuous dyeing			
	- thermosol/unknown			0.05
	- other			0.0025
	- printing			0.0025
Wastewater	<100	<100	0.85	
		100-1,000	0.75	
		≥1,000	0.5	
	100-1,000	<100	0.875	
		100-1,000	0.85	

Compartment	Conditions		Emission factors	
	S (mg/l)	VP (Pa)	UC<>10	UC = 10
		≥1,000	0.75	
	1,000-10,000	<100	0.9	
		100-1,000	0.875	
		≥1,000	0.85	
	≥10,000	-	0.95	

Table A3.14 continues below the following box:

WASTEWATER for UC = 10 (colorants):

Emission factor (EF) = Emission factor dyeing process (E.1) + Emission factor "handling, washing out and cleaning" (E.2)

E.1 = A / (1 + K . B) B = 1 / liquor ratio

(liquor ratio: default = 10 kg fibres / 1 l solution)

A = constant

K = equilibrium constant

INDUSTRIAL USE: Table A3.14 Continued

Compartment	Conditions Type of dye	(UC = 10) Type of dyeing	K	A	B	E.2
Wastewater, continued	Disperse	Continuous	115	5	1	0.055
	"	Printing	115	2	0.5	0.12
	Direct	Batch	73	1	0.1 [1)]	0.01
	Reactive - wool	Batch	190	1	0.1 [1)]	0.01
	Reactive - cotton	Batch	23	1	0.1 [1)]	0.01
	Reactive - general	Batch	57	1	0.1 [1)]	0.01
	Vat	Continuous	190	5	1	0.055
		Printing	190	2	0.5	0.12
	Sulphur	Continuous	40	5	1	0.055
		Printing	40	2	0.5	0.12

	Acid - one SO3	Batch	90	1	0.1 [1)]	0.01
	Acid - > 1 SO3	Batch	190	1	0.1 [1)]	0.01
	Basic	Batch	990	1	0.1 [1)]	0.01
	Azoic (naphtole)	Continuous	30	5	1	0.055
		Printing	30	2	0.5	0.12
	Metal complex	Batch	150	1	0.1 [1)]	0.01
	Pigment	Continuous	5000	5	1	0.055
		Printing	5000	2	0.5	0.12
	Unknown, low solubility	Continuous	190	5	1	0.055
		Printing	190	2	0.5	0.12
	Unknown, acid groups	Batch	90	1	0.1 [1)]	0.01

[1)] Default

Compartment	Conditions		Emission factors	
	S (mg/l)	VP (Pa)	UC<>10	UC = 10
Soil				0.005
	<100	<100	0.05	
		100-500	0.15	
		≥500	0.4	
	≥100	<100	0.025	
		100-500	0.05	
		≥500	0.15	

PRIVATE USE: **Table A4.4**

Compartment	Conditions S (mg/l)	Emission factors UC<>10	UC=10 1)
Air			0
Wastewater	<250		0.1
	250-1,000		0.15
	1,000-5,000		0.2
	≥5,000		0.3
Soil			0

1) For UC = 10 (Colorants) only, i.e. types used normally by industry for batch dyeing

WASTE TREATMENT: **Not applicable**

IC = 14: PAINTS, LACQUERS AND VARNISHES INDUSTRY

PRODUCTION: **Table A1.1**

FORMULATION: **Table A2.1**

INDUSTRIAL USE: **Table A3.15**

Compartment	Conditions		Emission factors	
	Use category	VP (Pa)	Water based	Solvent based
Air	3			1
	10, 14, 20		0	0
	50		0	
	47, 52, 55	<10	0	0
		10-500	0	0.001
		500-5,000	0.01	0.05
		≥5,000	0.05	0.15
	48		0.8	0.9
		S (mg/l)		
Wastewater	3			0
	10, 14, 20		0.005	0.001
	50	<10	0.005	
		10-100	0.01	
		≥100	0.05	
	47, 52, 55	<10	0.005	0.001
		10-100	0.01	0.005
		≥100	0.05	0.01
	48		0.1	0.02
Soil	3			0
	10, 14, 20		0.005	0.005
	50		0.005	
	47, 52, 55		0.005	0.005

	48		0.001	0.001

PRIVATE USE: **Table A4.5**

Compartment	Conditions		Emission factors	
	Use category	VP (Pa)	Water based	Solvent based
Air	3			1
	10, 14, 20		0	0
	50		0	
	47, 52, 55	<10	0	0
		10-500	0	0.001
		500-5,000	0.01	0.05
		≥5,000	0.05	0.15
	48		0.8	0.95
S (mg/l)				
Wastewater	3			0
	10, 14, 20		0.005	0.001
	50	<10	0.005	
		10-100	0.01	
		≥100	0.05	
	47, 52, 55	<10	0.005	0.001
		10-100	0.01	0.005
		≥100	0.05	0.01
	48		0.15	0.04
Soil	3			0
	10, 14, 20		0.005	0.005
	50		0.005	
	47, 52, 55		0.005	0.005
	48		0.01	0.01

WASTE TREATMENT: **Not applicable**

IC = 16: ENGINEERING INDUSTRY: CIVIL AND MECHANICAL

PRODUCTION: **Table A1.1**

FORMULATION: **Table A2.1**

INDUSTRIAL USE: **Table A3.16**

Compartment	Conditions		Emission factors		
	S (mg/l)	VP (Pa)	MC=2	MC=3[1)]	MC=4
Air	<100	<10	0.0001	0.001	0.01
		10-100	0.001	0.01	0.1
		100-1,000	0.01	0.1	0.25
		1,000-10,000	0.1	0.5	0.7
		≥10,000	0.5	0.75	0.9
	100-1000	<10	0.00001	0.0001	0.001
		10-100	0.0001	0.001	0.05
		100-1,000	0.001	0.05	0.1
		1,000-10,000	0.05	0.1	0.5
		≥10,000	0.25	0.5	0.75
	≥1,000	<10	0	0.00001	0.0001
		10-100	0.00001	0.0001	0.001
		100-1,000	0.0001	0.001	0.01
		1,000-10,000	0.001	0.01	0.1
		≥10,000	0.01	0.1	0.5
Wastewater	<100	<10	0.01	0.1	0.5
		10-100	0.001	0.01	0.1
		100-1,000	0.0001	0.001	0.01
		1,000-10,000	0.00001	0.0001	0.001
		≥10,000	0	0.00001	0.0001
	100-1000	<10	0.25	0.5	0.75
		10-100	0.05	0.1	0.5
		100-1,000	0.001	0.01	0.1

		1,000-10,000	0.0001	0.001	0.05
		≥10,000	0.00001	0.0001	0.001
	≥1,000	<10	0.5	0.75	0.9
		10-100	0.1	0.5	0.7
		100-1,000	0.01	0.1	0.25
		1,000-10,000	0.001	0.01	0.1
		≥10,000	0.0001	0.001	0.01
Soil	<100	<10	0.005	0.01	0.05
		10-100	0.001	0.005	0.01
		100-1,000	0.0005	0.001	0.005
		1,000-10,000	0	0.0005	0.001
		≥10,000	0	0	0.0005
	100-1000	<10	0.001	0.005	0.01
		10-100	0.0005	0.001	0.005
		100-1,000	0	0.0005	0.001
		1,000-10,000	0	0	0.0005
		≥10,000	0	0	0.0001
	≥1,000	<10	0.0005	0.001	0.005
		10-100	0	0.0005	0.001
		100-1,000	0	0	0.0005
		1,000-10,000	0	0	0.0001
		≥10,000	0	0	0

[1)] Default

PRIVATE USE: **Table A3.16**

WASTE TREATMENT: **Not applicable**

IC = 0: OTHERS

PRODUCTION: **Table A1.1**

FORMULATION: **Table A2.1**

INDUSTRIAL USE: **Table A3.16**

B-TABLES: ESTIMATES FOR THE FRACTION OF THE MAIN SOURCE AND THE NUMBER OF DAYS FOR EMISSIONS

IC = 1: AGRICULTURAL INDUSTRY

IC = 2: CHEMICAL INDUSTRY: BASIC CHEMICALS

IC = 3: CHEMICAL INDUSTRY: CHEMICALS USED IN SYNTHESIS

IC = 4: ELECTRICAL/ELECTRONIC INDUSTRY

IC = 5: PERSONAL/DOMESTIC

IC = 6: PUBLIC DOMAIN

IC = 7: LEATHER PROCESSING INDUSTRY

IC = 8: METAL EXTRACTION, REFINING AND PROCESSING INDUSTRY

IC = 9: MINERAL OIL AND FUEL INDUSTRY

IC = 10: PHOTOGRAPHIC INDUSTRY

IC = 11: POLYMERS INDUSTRY

IC = 12: PULP, PAPER AND BOARD INDUSTRY

IC = 13: TEXTILE PROCESSING INDUSTRY

IC = 14: PAINTS, LACQUERS AND VARNISHES INDUSTRY

IC = 16: ENGINEERING INDUSTRY: CIVIL AND MECHANICAL

IC = 1: AGRICULTURAL INDUSTRY

PRODUCTION **Table B1.1 for new substances and existing substances other than HPVC for UC ≠ 38 & 41**

T (tonnes/year)	f (main source)	No. of days
<1,000	1	0.1f.T
1,000-2,000	0.9	0.1f.T
2,000-4.000	0.75	0.1f.T
≥4,000	0.7	300

PRODUCTION **Table B1.2 for new substances and existing substances other than HPVC for UC = 38 & 41**

T (tonnes/year)	f (main source)	No. of days
<10	1	f.T
10-50	0.9	f.T
50-100	0.8	0.6667f.T
100-1,000	0.75	0.4f.T
1,000-2,500	0.6	0.2f.T
≥2,500	0.6	300

PRODUCTION **Table B1.3 for HPVC (default ≥10,000) for UC ≠ 38 & 41**

T (tonnes/year)	f (main source)	No. of days
<25,000	1	300
25,000-100,000	0.75	300
>100,000	0.6	300

PRODUCTION **Table B1.4 for HPVC (default ≥3,500) for UC = 38 & 41**

T (tonnes/year)	f (main source)	No. of days
<5,000	1	300
5,000-25,000	0.8	300

25,000-100,000	0.6	300
≥100,000	0.4	300

FORMULATION **Table B2.1 for new substances and existing substances other than HPVC**

T (tonnes/year)	f (main source)	No. of days
<100	1	2f.T
100-500	0.6	f.T
500-1,000	0.6	0.5f.T
≥1,000	0.4	300

FORMULATION **Table B2.2 for HPVC for UC ≠ 38 & 41**

T (tonnes/year)	f (main source)	No. of days
<15,000	1	300
15,000-50,000	0.75	300
≥50,000	0.6	300

FORMULATION **Table B2.3 for HPVC for UC = 38 & 41**

T (tonnes/year)	f (main source)	No. of days
<3,500	1	300
3,500-10,000	0.8	300
10,000-25,000	0.7	300
25,000-50,000	0.6	300
≥50,000	0.4	300

INDUSTRIAL USE **Table B3.1**

T (tonnes/year)	f (main source)	No. of days for use categories:			
		3,19,39,48,50	41	9,10,36	26
<10	0.05	2	10	50	300

10-100	0.01	2	10	50	300
100-1,000	0.005	2	10	50	300
1,000-10,000	0.001	2	10	50	300
10,000-50,000	0.0005	2	10	50	300
≥50,000	0.00001	2	10	50	300

PRIVATE USE **Not applicable**

WASTE TREATMENT **Not applicable**

IC = 2: CHEMICAL INDUSTRY: BASIC CHEMICALS

PRODUCTION **Table B1.1 for non-HPVC**

Table B1.5 for HPVC (default ≥10,000)

T (tonnes/year)	f (main source)	No. of days
<25,000	1	300
25,000-100,000	0.75	300
100,000-500,000	0.6	300
≥500,000	0.5	300

FORMULATION **Table B2.4 for non-HPVC**

If applicable!

T (tonnes/year)	f (main source)	No. of days
<10	1	2f.T
10-50	0.9	f.T
50-500	0.8	0.4f.T
500-2,000	0.75	0.2f.T
≥2,000	0.65	300

FORMULATION **Table B2.5 for HPVC**

If applicable!

T (tonnes/year)	f main source	No. of days
<25,000	1	300
25,000-50,000	0.75	300
≥50,000	0.4	300

INDUSTRIAL USE **Table B3.2**

T (tonnes/year)	f main source	No. of days
<10	0.8	2f.T
10-50	0.65	f.T
50-500	0.5	0.4f.T
500-2,000	0.4	0.25f.T
2,000-5,000	0.3	0.2f.T
5,000-25,000	0.25	300
25,000-75,000	0.2	300
≥75,000	0.15	300

PRIVATE USE **Not applicable**

WASTE TREATMENT **Not applicable**

IC = 3: CHEMICAL INDUSTRY: CHEMICALS USED IN SYNTHESIS

PRODUCTION **Table B1.2 for non-HPVC**

Table B1.6 for HPVC (default ≥7,000)

T (tonnes/year)	f main source	No. of days
<10,000	1	300
10,000-50,000	0.75	300
50,000-250,000	0.6	300
≥250,000	0.5	300

FORMULATION **Table B2.4 for non-HPVC**

Table B2.3 for HPVC

If applicable!

INDUSTRIAL USE **Table B3.2**

PRIVATE USE **Not applicable**

WASTE TREATMENT **Not applicable**

IC = 4: ELECTRICAL/ELECTRONIC INDUSTRY

PRODUCTION **Table B1.7 for non-HPVC**

T (tonnes/year)	f main source	No. of days
<100	1	0.1f.T
100-1,000	0.9	0.1f.T
1,000-2,500	0.8	0.1f.T
≥2,500	0.75	300

PRODUCTION **Table B1.6 for HPVC (default ≥ 7,000)**

FORMULATION **Table B2.4 for non-HPVC**

Table B2.3 for HPVC

INDUSTRIAL USE **Table B3.2**

PRIVATE USE **Not applicable**

WASTE TREATMENT **Not applicable**

IC = 5: PERSONAL/DOMESTIC

PRODUCTION **Table B1.7 for non-HPVC**

Table B1.6 for HPVC (default ≥ 7,000)

FORMULATION **Table B2.1 for non-HPVC**

Table B2.3 for HPVC

INDUSTRIAL USE **Not applicable**

PRIVATE USE (cosmetics) **Table B4.1 for UC ≠ 9 (cleaning/washing agents) and 15**

Only for wastewater!

T (tonnes/year)	f (main source)	No. of days:
	0.002	365

PRIVATE USE **Table B4# for UC = 9 and 15 (if production volume < 1,000 tonnes/year Table B4.1 applies)**

A) Based on tonnage

T (tonnes/year)	No. inhabitants region	No. inhabitants feeding STP	No. of days:
	$2.0.10^7$	10,000	365

WASTE TREATMENT **Not applicable**

IC = 6: PUBLIC DOMAIN

PRODUCTION **Table B1.7 for non-HPVC**

Table B1.6 for HPVC (default ≥ 7,000)

FORMULATION **Table B2.1 for non-HPVC**

Table B2.3 for HPVC

INDUSTRIAL USE **Table B3.3**

Only for wastewater!

T (tonnes/year)	f (main source)	No. of days for use categories:		
		9	39	Else
	0.002	200	15	50

PRIVATE USE **Not applicable**

WASTE TREATMENT **Not applicable**

IC = 7: LEATHER PROCESSING INDUSTRY

PRODUCTION **Table B1.8 for non-HPVC for UC ≠ 6, 9 10 & 31**

T (tonnes/year)	f (main source)	No. of days
<1,000	1	0.1f.T
1,000-4,000	0.9	0.1f.T
≥4,000	0.75	300

PRODUCTION **Table B1.9 for non-HPVC for UC = 6, 9 10 & 31**

T (tonnes/year)	f (main source)	No. of days
<10	1	f.T
10-50	0.9	f.T
50-500	0.5	f.T
500-1,500	0.2	f.T
≥1,500	0.2	300

PRODUCTION **Table B1.4 for HPVC (default ≥ 5,000) for UC ≠ 6, 9 10 & 31**

Table B1.4 for HPVC (default ≥ 2,500) for UC = 6, 9 10 & 31

FORMULATION **Table B2.4 for non-HPVC**

Table B2.3 for HPVC for UC ≠ 6, 9, 10 & 31

Table B2.6 for HPVC for UC = 6, 9, 10 & 31

T (tonnes/year)	f (main source)	No. of days
<100,000	1	300
100,000-250,000	0.7	300
≥250,000	0.4	300

INDUSTRIAL USE **Table B3.4**

T (tonnes/year)	f (main source)	No. of days
<10	0.8	2f.T
10-50	0.75	2f.T
50-500	0.6	f.T
500-1,500	0.5	0.4f.T
1,500-5,000	0.35	300
5,000-25,000	0.2	300
≥25,000	0.1	300

PRIVATE USE **Not applicable**

WASTE TREATMENT **Not applicable**

IC = 8: METAL EXTRACTION, REFINING AND PROCESSING INDUSTRY

PRODUCTION **Table B1.2 for non-HPVC for UC ≠ 29 & 35**

Table B1.10 for non-HPVC for UC = 29 & 35

T (tonnes/year)	f (main source)	No. of days
<10	1	f.T
10-50	0.9	f.T
50-500	0.8	0.6667f.T
500-1,500	0.5	0.4f.T
≥1,500	0.5	300

PRODUCTION **Table B1.6 for HPVC (default ≥ 7,000) for UC ≠ 29 & 35**

Table B1.4 for HPVC (default ≥ 2,500) for UC = 29 & 35

FORMULATION **Table B2.4 for non-HPVC**

Table B2.3 for HPVC

INDUSTRIAL USE **Table B3.5 for UC = 29 & 35**

T (tonnes/year)	No. of days	f (main source):	Field of application	
			Primary steelworks	Else
<1,000	300		1	0.8
1,000-5,000	300		0.9	0.5
5,000-50,000	300		0.75	0.3
≥ 50,000	300		0.6	0.2

INDUSTRIAL USE **Table B3.6 for UC ≠ 29 & 35**

T (tonnes/year)	f main source	No. of days
<10	1	2f.T
10-50	1	0.5f.T
50-500	0.9	0.4f.T

T (tonnes/year)	f main source	No. of days
500-2,000	0.8	0.1875f.T
2,000-10,000	0.7	300
10,000-50,000	0.6	300
≥ 50,000	0.5	300

PRIVATE USE **Not applicable**

WASTE TREATMENT **Not applicable**

IC = 9: MINERAL OIL AND FUEL INDUSTRY

PRODUCTION **Table B1.1 for non-HPVC for UC = 27**

Table B1.2 for non-HPVC for UC = 28+others

Table B1.4 for HPVC (default ≥3,000) for UC = 28+others

Table B1.11 for HPVC (default ≥25,000) for UC = 27

T (tonnes/year)	f main source	No. of days
<100,000	1	300
100,000-500,000	0.75	300
≥500,000	0.5	300

FORMULATION **Table B2.7 for non-HPVC for UC = 27**

T (tonnes/year)	f main source	No. of days
<1,000	1	100
1,000-2,000	0.8	200
≥2,000	0.6	300

FORMULATION **Table B2.8 for non-HPVC for UC = 28+others**

T (tonnes/year)	f main source	No. of days
<5	1	20
5-50	1	60
50-100	1	2f.T
100-500	0.8	f.T
500-1,000	0.6	0.5f.T
≥1,000	0.4	300

FORMULATION **Table B2.6 for HPVC for UC = 27**

Table B2.6 for HPVC for UC = 28+others

INDUSTRIAL USE **Table B3.7**

T (tonnes/year)	f main source	No. of days
<50	0.5	350
50-500	0.4	350
500-5,000	0.3	350
5,000-25,000	0.2	350
25000-100,000	0.05	350
≥100,000	0.02	350

PRIVATE USE **Table 4.1**

Only for wastewater!

WASTE TREATMENT **Not applicable**

IC = 10: PHOTOGRAPHIC INDUSTRY

PRODUCTION **Table B1.4 for HPVC (default ≥ 4,000)**

Table B1.12 for non-HPVC

T (tonnes/year)	f main source	No. of days
<5	1	f.T
5-50	1	0.5f.T
50-250	0.75	0.4f.T
250-3,000	0.5	0.2f.T
≥3,000	0.5	300

FORMULATION **Table B2.8 for non-HPVC**

Table B2.3 for HPVC

INDUSTRIAL USE **Table B3.8**

Company size	f main source	No. of days	
One company	1	300	(No private use)
Large companies	0.333	300	(No private use)
Small companies	0.05	300	

PRIVATE USE **Table B4.2**

Only for wastewater!

Only if company size at industrial use is small companies (otherwise f main source is zero)

F main source = 0.002.f private use

T (tonnes/year)	f private use	F main source	No. of days:
<10	0	0	200
10-50	0.00002	4.10^{-8}	200
50-500	0.0001	2.10^{-7}	200

T (tonnes/year)	f private use	F main source	No. of days:
500-5,000	0.0005	1.10^{-6}	200
≥5,000	0.0025	5.10^{-6}	200

WASTE TREATMENT Table B5.1

T (tonnes/year)	f main source	No. of days	One company
<10	1	150	(No private use)
≥10	1	300	

T (tonnes/year)	f main source	No. of days	Large companies
<30	0.333	150	
≥30	0.333	300	

T (tonnes/year)	f main source	No. of days	Small companies
<200	0.2	150	
≥200	0.2	300	

IC = 11: POLYMERS INDUSTRY

PRODUCTION **Table B1.9 for non-HPVC for UC ≠ 20, 47 & 43 (monomers, cross-linking agents & curing agents)**

Table B1.13 for non-HPVC for UC = 20, 47 & 43 (monomers, cross-linking agents & curing agents; not: initiators, retarders & inhibitors)

T (tonnes/year)	f main source	No. of days
<50	0.9	0.4f.T
50-500	0.75	0.2F.T
500-5,000	0.6	0.1f.T
5,000-25,000	0.75	200
≥25,000	0.5	300

PRODUCTION **Table B1.4 for HPVC (default ≥3,000) for UC ≠ 20, 47 & 43 (monomers, cross-linking agents & curing agents)**

PRODUCTION **Table B1.14 (default ≥60,000) for HPVC for UC = 20, 47 & 43 (monomers, cross-linking agents & curing agents; not: initiators, retarders & inhibitors)**

T (tonnes/year)	f main source	No. of days
<100,000	1	300
100,000-250,000	0.65	300
≥250,000	0.4	300

FORMULATION **Table B2.8 for non-HPVC**

Table B2.3 for HPVC for UC ≠ 20, 47 & 43 (monomers, cross-linking agents & curing agents)

Table B2.9 for HPVC for UC = 20, 47 & 43 (monomers, cross-linking agents & curing agents; not: initiators, retarders & inhibitors)

T (tonnes/year)	f main source	No. of days
<25,000	1	300
25,000-50,000	0.75	300
≥50,000	0.4	300

INDUSTRIAL USE **Table B3.9**

T (tonnes/year)	f main source	No. of days
<10	0.5	2f.T
10-50	0.35	f.T
50-500	0.25	0.4f.T
500-5,000	0.15	0.4f.T
5,000-25,000	0.1	300
≥25,000	0.05	300

PRIVATE USE **Not applicable**

WASTE TREATMENT **Not considered yet**

IC = 12: PULP, PAPER AND BOARD INDUSTRY

PRODUCTION **Table B1.8 for non-HPVC for UC ≠ 10 & 45**

Table B1.9 for non-HPVC for UC = 10 & 45

Table B1.4 for HPVC (default ≥ 4,500) for UC ≠ 10 & 45

Table B1.4 for HPVC (default ≥ 2,500) for UC = 10 & 45

FORMULATION **Table B2.1 for non-HPVC for UC ≠ 10 & 45**

Table B2.8 for non-HPVC for UC = 10 & 45

Table B2.3 for HPVC

INDUSTRIAL USE **Table B3.10**

T (tonnes/year)	f main source	No. of days
One company		
<10	1	2f.T
10-50	1	f.T
50-500	1	0.4f.T
≥500	1	300
Large companies		
<100	0.333	2f.T
100-250	0.333	f.T
250-600	0.333	0.5f.T
≥600	0.333	300
Small companies		
<200	0.05	2f.T
200-1,000	0.05	f.T
1,000-6,000	0.05	0.5f.T
6,000-25,000	0.05	300
≥25,000	0.02	300

PRIVATE USE **Not considered yet**

WASTE TREATMENT Table B5.2

T (tonnes/year)	f main source	No. of days
<100	0.5	150
100-1,000	0.4	200
1,000-10,000	0.3	250
10,000-100,000	0.2	300
≥100,000	0.1	300

IC =13: TEXTILE PROCESSING INDUSTRY

PRODUCTION **Table B1.2 for non-HPVC**

Table B1.6 for HPVC (default ≥7,000)

FORMULATION **Table B2.3 for HPVC**

Table B2.10 for non-HPVC

T (tonnes/year)	f main source	No. of days
<3,500	1	300
3,500-10,000	0.8	300
10,000-25,000	0.7	300
25,000-50,000	0.6	300
≥50,000	0.4	300

INDUSTRIAL USE **Table B3.11 for UC = 10**

T (tonnes/year)	f main source	No. of days
<10	0.9	10f.T
10-20	0.75	10f.T
20-100	0.6	5f.T
100-1,000	0.4	300
1,000-10,000	0.2	300
≥10,000	0.1	300

INDUSTRIAL USE **Table B3.12 for UC ≠ 10**

T (tonnes/year)	f main source	No. of days
<10	0.75	5f.T
10-100	0.4	5f.T
100-750	0.4	f.T
750-3,000	0.2	0.5f.T
3,000-25,000	0.2	300
≥25,000	0.1	300

PRIVATE USE **Table B4.3**

Only for UC = 10 (and only for types of dyes used for batch dyeing by industry)

T (tonnes/year)	f main source	No. of days:
<50	0	
50-500	0.000004	300
≥500	0.00002	300

WASTE TREATMENT **Not applicable**

IC = 14: PAINTS, LACQUERS AND VARNISHES INDUSTRY

PRODUCTION **Table B1.2 for non-HPVC**

Table B1.6 for HPVC (default ≥ 7,000)

FORMULATION **Table B2.10 for non-HPVC**

Table B2.3 for HPVC

INDUSTRIAL USE **Table B3.13**

T (tonnes/year)	f main source	No. of days
<10	0.9	20f.T
10-50	0.6	6.667f.T
50-300	0.3	3.333f.T
300-5,000	0.15	300
5,000-25,000	0.1	300
≥ 25,000	0.05	300

PRIVATE USE **Table B4.4**

Only for wastewater!

Only for paints classified as "do-it-yourself"

F main source = 0.002.f private use

T (tonnes/year)	f private use	f main source	No. of days:
< 500	1	0.002	150
≥ 500	1	0.002	300

PRIVATE USE **Table B4.5**

Only for wastewater!

Only for paints classified as "constructions, maintenance", etc.

F main source = 0.002.f private use

T (tonnes/year)	f private source	f main source	No. of days:
<50	0	0	
50-500	0.00002	4.10^{-8}	200
500-2,500	0.0004	8.10^{-7}	300
2,500-10,000	0.002	4.10^{-6}	300
10,000-50,000	0.01	2.10^{-5}	300
≥50,000	0.05	1.10^{-4}	300

WASTE TREATMENT **Not applicable**

IC = 16: ENGINEERING INDUSTRY: CIVIL AND MECHANICAL

PRODUCTION **Table B1.2 for non-HPVC**

Table B1.6 for HPVC (default ≥ 7,000)

FORMULATION **Table B2.8 for non-HPVC**

Table B2.3 for HPVC

INDUSTRIAL USE **Table B3.14**

T (tonnes/year)	f main source	No. of days
<10	1	2f·T
10-50	0.9	f·*T
50-500	0.8	0.4f·T
500-2,000	0.75	0.2f·T
2,000-5,000	0.6	0.1f·T
5,000-25,000	0.5	300
≥25,000	0.3	300

PRIVATE USE **Table B4.5**

WASTE TREATMENT **Not applicable**

IC = 0 (OTHERS)

PRODUCTION **Table B1.2 for non-HPVC**

Table B1.6 for HPVC (default ≥7,000)

FORMULATION **Table B2.8 for non-HPVC**

Table B2.3 for HPVC

INDUSTRIAL USE **Table B3.14**

PRIVATE USE **Table B4.5**

WASTE TREATMENT **Table B5.3**

T (tonnes/year)	f main source	No. of days
<100	0.5	150
100-1,000	0.3	150
1,000-10,000	0.2	150
≥10,000	0.2	150

Appendix II-a: List of synonyms for functions according to ChemUSES (US EPA, 1980)

No.	Use Category	No.	Function (ChemUSES)
1	Absorbents and adsorbents	131	Absorbents
		60	Adsorbents
		213	Dehumidifiers
2	Adhesive, binding agents	302	Adhesives
		143	Binders
		145	Food additives
		92	Spreaders
		165	Stickers
		280	Tackifiers
3	Aerosol propellants	178	Aerosol propellants
4	Anti-condensation agents		
5	Anti-freezing agents	77	Antifreezes
		74	De-icers
		52	Deodorants
		313	Functional fluids
6	Anti-set-off and anti-adhesive agents	104	Abherents
		63	Antiblocking agents
		188	Anticaking agents
		300	Detackifiers
		233	Dusting agents
		144	Parting agents
		7	Soil retardants
7	Anti-static agents	328	Antistatic agents
		89	Electroconductive coating agents
		318	Humectants
8	Bleaching agents	304	Bleaching assistants

No.	Use Category	No.	Function (ChemUSES)
		132	Bleaching agents
9	Cleaning/washing agents and additives	293	Antiredeposition agents
		180	Boil-off assistants
		242	Cleaners
		173	Detergents
		78	Pre-spotting agents
		274	Scouring agents
		261	Shrinkage controllers
		14	Soaping-off assistants
		294	Soil release agents
10	Colouring agents	5	Bloom agents
		86	Colouring agents
		174	Coupling agents (dyes)
		267	Dyes
		20	Fluorescent agents
		248	Lakes
		381	Luminescent agents
		235	Mercerising assistants
		128	Opacifiers
		139	Pearlizing agents
		125	Pigments
		83	Stains
11	Complexing agents	177	Antiprecipitants
		124	Complexing agents
		10	Sequestering agents
12	Conductive agents	161	Electrical conductive agents
		383	Electrode materials
		245	Electrolytes

No.	Use Category	No.	Function (ChemUSES)
		313	Functional fluids
13	Construction materials and additives	324	Case-hardening agents
		355	Concrete additives
		361	Embrittlement inhibitors
		375	Materials for shaping
		250	Reinforcing agents
		349	Water-reducing agents
14	Corrosion inhibitors	230	Antioxidants
		64	Antiscaling agents
		323	Corrosion inhibitors
15	Cosmetics	301	Antiperspirants
		167	Cosmetic ingredients
16	Dust binding agents	26	Dust control agents
17	Electroplating agents	353	Brighteners
		32	Fume suppressants
18	Explosives	179	Detonators
		363	Explosion inhibitors
		158	Explosives
		27	Incendiaries
19	Fertilisers	34	Fertilisers
20	Fillers	351	Fillers (augmentation)
		212	Fillers (patching)
		371	Surface coating additives
		127	Swelling agents
		58	Weighting agents (textile technology)
21	Fixing agents	291	Anticrock agents
		347	Antistripping agents

No.	Use Category	No.	Function (ChemUSES)
		268	Barrier coating agents
		295	Fixatives
		134	Fixing agents (fragrances)
		112	Fixing agents (textile technology)
		227	Mordents
22	Flame retardants and fire preventing agents	25	Fire extinguishing agents
		332	Flame retardants
23	Flotation agents	163	Activators (ore processing)
		190	Flocculating agents
		297	Flotation agents
		360	Modifiers
24	Flux agents for casting		
25	Foaming agents	358	Blowing agents
		133	Chemical blowing agents
		94	Frothers
		50	Physical blowing agents
26	Food/feedstuff additives	214	Acidulants
		66	Feed additives
		80	Sweeteners (taste)
27	Fuels	247	Fuels
28	Fuel additives	329	Antifouling agents
		76	Antiknock agents
		183	Deposit modifiers
		306	Fuel additives
		138	Sweeteners (petroleum technology)
29	Heat transferring agents	72	Coolants

No.	Use Category	No.	Function (ChemUSES)
		313	Functional fluids
		199	Heat transfer agents
		216	Quenchers
		208	Refrigerants
30	Hydraulic fluids and additives	313	Functional fluids
		65	Hydraulic fluids
		256	Transmission fluids
31	Impregnation agents	102	Delustrants
		98	Sizes
		258	Water repellents
		23	Waterproofing agents
32	Insulating materials	254	Acoustical insulating material
		311	Electrical insulating material
		314	Heat insulating materials
		162	Insulating materials
33	Intermediates	146	Inorganic intermediates
		115	Monomers
		290	Organic intermediates
		43	Prepolymers
34	Laboratory chemicals	238	Analytical and product testing
		122	Chelating agents
		107	Deionisers
		373	Extraction agents
		69	Indicators
		325	Oxidation-reduction indicators
		374	Reagents

No.	Use Category	No.	Function (ChemUSES)
35	Lubricants and additives	119	Antiseize agents
		313	Functional fluids
		148	Internal lubricating agents
		195	Lubricant additives
		364	Lubricating agents
		346	Oiliness agents
		249	Penetrants
		312	Slip agents
36	Odour agents	79	Flavours and fragrances
		339	Odorants
37	Oxidising agents	149	Oxidisers
38	Plant protection products, agricultural	166	Animal repellents
		333	Bactericides
		108	Biocides
		97	Decontaminats
		270	Fumigants
		362	Fungicides
		275	Herbicides
		155	Insect attractants
		348	Insect repellents
		330	Insecticides
		252	Nematocides
		253	Pesticides
		264	Rodenticides
39	Biocides, non-agricultural	287	Algicides
		1	Antifouling agents
		140	Disinfectants
		118	Preservatives

No.	Use Category	No.	Function (ChemUSES)
		116	Slime preventatives
40	PH-regulating agents	172	Laundry sours
		266	pH control agents
		191	pH indicators
41	Pharmaceuticals		
42	Photochemicals	122	Chelating agents
		198	Desensitisers (explosives)
		299	Desensitisers (photography)
		182	Developers
		286	Intensifiers (photography)
		285	Light stabilisers
		344	Photosensitive agents
		303	Sensitisers
43	Process regulators	321	Accelerators
		46	Activators (chemical processes)
		239	Activators (enzymes)
		110	Adhesion promoters
		4	Antifelting agents
		352	Antislip finishing agents
		206	Antistaining agents
		194	Antiwebbing agents
		281	Builders
		222	Carbonising agents
		164	Carriers
		19	Catalyst supports
		170	Catalysts
		31	Chain extenders

No.	Use Category	No.	Function (ChemUSES)
		113	Chain terminators
		141	Chain transfer agents
		122	Chelating agents
		114	Coagulants
		278	Coalescents
		357	Coalescing agents
43	Process regulators (continued)	315	Crabbing assistants
		228	Crosslinking agents
		226	Curing agents (concrete)
		369	Curing agents (polymer technology)
		18	Currying agents
		236	Deasphalting agents
		342	Defoamers
		365	Degumming agents
		137	Dehairing agents
		73	Dehydrating agents
		366	De-inkers
		84	Delignification agents
		30	Depolymerisation agents
		367	Depressants
		292	Desising agents
		259	Dispersants
		317	Dryers
		150	Dye carriers
		255	Dye levelling agents
		307	Dye retardants
		211	Dye retention aids

No.	Use Category	No.	Function (ChemUSES)
		341	Enzyme inhibitors
		157	Enzymes
		284	Finishing agents
		337	Formation aids
		331	Fuel oxidisers
		117	Fulling agents
		103	Initiators
		359	Intensifiers (printing)
		171	Kier boiling assistants
		24	Nucleating agents
		96	Peptising agents
		75	Pitch control agents
		121	Polymerisation additives
		209	Polymerisation inhibitors
		21	Prevulcanisation inhibitors
		153	Refining agents
		223	Repulping aids
		136	Retarders
		296	Retention aids
		338	Rubber compounding agents
		51	Scavengers
		326	Solubilising agents
		310	Weighting agents (petroleum technology)
44	Reducing agents	244	Reducers
45	Reprographic agents	225	Toners
46	Semiconductors	202	Semiconductors
		378	Photovoltaic agents

No.	Use Category	No.	Function (ChemUSES)
47	Softeners	269	Bates
		231	Devulcanising agents
		28	Elasticisers
		265	Emollients
		185	Plasticisers
47	Softeners (continued)	29	Softeners
		147	Water softeners
48	Solvents	229	Degreasers
		82	Dewaxing solvents
		373	Extraction agents
		320	Paint and varnish removers
		16	Reaction media
		271	Solvents
49	Stabilisers	277	Anticracking agents
		12	Antifume agents
		129	Antihydrolysis agents
		168	Antiozonants
		230	Antioxidants
		120	Antilivering agents
		282	Antiplasticisers
		160	Antisagging agents
		68	Antisettling agents
		88	Bloom inhibitors
		123	Coupling agents (polymers)
		159	Emulsifiers
		87	Heat stabilisers
		54	Stabilisers
		36	Ultraviolet absorbers

No.	Use Category	No.	Function (ChemUSES)
50	Surface-active agents	41	Antifloating agents
		234	Antifogging agents
		109	Surfactants
		243	Wetting agents
51	Tanning agents	316	Tanning agents
52	Viscosity adjustors	152	Antiflooding agents
		120	Antilivering agents
		343	Antiskinning agents
		221	Gelling agents
		262	Pour point depressants
		272	Thickeners
		334	Thixotropic agents
		240	Turbulence suppressors
		135	Viscosity adjustors
		15	Viscosity index improvers
53	Vulcanising agents	288	Vulcanising agents
54	Welding and soldering agents	101	Brazing agents
		22	Fluxing agents
0	Other	204	Ablatives
		105	Abrasives
		196	Activators (luminescence)
		354	Aerating agents
		47	Air entraining agents
		376	Alloying agents
		90	Anticratering agents
		48	Anticreasing agents
		99	Antifogging agents
		218	Antipilling agents

No.	Use Category	No.	Function (ChemUSES)
		350	Antiskid agents
		6	Blasting abrasives
		70	Bluing agents
		220	Bright dips
		93	Chemical raw materials
		298	Clarifiers
		260	Cloud point depressants
		130	Coating agents
		283	Collectors
		335	Coupling agents (solutions)
		215	Culture nutrients
		81	Deaerating agents
		309	Deblooming agents
		85	Dechlorinating agents
		73	Dehydrating agents
		107	Deionisers
		232	Demulsifiers
		200	Denaturants
		49	Descaling agents
		205	Dewatering aids
		356	Discharge printing agents
		38	Drainage aids
		44	Drilling mud additives
		322	Dry strength additives
		39	Dye stripping agents
		100	Electron emission agents
		340	Eluting agents
		372	Embalming agents

No.	Use Category	No.	Function (ChemUSES)
		186	Encapsulating agents
		57	Enhanced oil recovery agents
		308	Entraining agents
		319	Etching agents
		336	Evaporation control agents
		373	Extraction agents
		207	Fiber-forming compounds
		368	Filtration aids
		56	Flatting agents
		79	Flavours and fragrances
		142	Fluid loss additives
		313	Functional fluids
		193	Greaseproofing agents
		184	Grinding, lapping, sanding
		192	Hormones
		246	Humidity indicators
		210	Hydrotropic agents
		181	Impact modifiers
		380	Incandescent agents
		69	Indicators
		2	Ion exchange agents
		91	Lachrymators
		33	Latex compounding agents
		53	Leaching agents
		156	Leather processing agents
		370	Liquid crystals
		381	Luminescent agents

No.	Use Category	No.	Function (ChemUSES)
		379	Magnetic agents
		67	Mar proofing agents
		289	Metal conditioners
		95	Metal strippers
		37	Metal treating agents
		327	Milling aids
		237	Obscuring agents
		197	Oil repellents
		62	Optical quenchers
		382	Osmotic membranes
		17	Papermaking agents
		55	Phosphatising agents
		203	Phosphorescent agents
		59	Pickling agents
		217	Pickling inhibitors
		251	Plant growth regulators
		176	Plastics additives
		224	Plastics for shaping
		169	Plating agents
		8	Poison gas decontaminants
		3	Polymer strippers
		111	Pore forming agents
		151	Precipitating agents
		106	Protective agents
		45	Radioactivity decontaminants
		374	Reagents
		219	Refractive index modifiers

No.	Use Category	No.	Function (ChemUSES)
		241	Refractories
		154	Resists
		9	Rinse aids
		71	Ripening agents
		187	Rubber for shaping
		201	Rubber reclaiming agents
		189	Rubbing fastness agents
		276	Rust inhibitors
		11	Rust removers
		263	Scrooping agents
		42	Sealants
		98	Sizes
		126	Slime control agents
		305	Soil conditioners
		61	Strippers
		40	Tar removers
		345	Tarnish inhibitors
		13	Tarnish removers
		279	Textile specialities
		257	Vat printing assistants
		273	Wax strippers
		35	Well treating agents
		175	Wet strength additives
		377	X-ray absorbents

Appendix II-b: List of synonyms for functions according to ChemUSES (US EPA, 1980)

No.	ChemUSES Function	Use category EU (No.)
104	Abherents	6
204	Ablatives	55
105	Abrasives	0
131	Absorbents	1
321	Accelerators	43
214	Acidulants	26
254	Acoustical insulating material	32
46	Activators (chemical processes)	43
163	Activators (ore processing)	23
196	Activators (luminescence)	55
239	Activators (enzymes)	43
110	Adhesion promoters	43
302	Adhesives	2
60	Adsorbents	1
354	Aerating agents	0
178	Aerosol propellents	3
47	Air entraining agents	0
287	Algicides	39
376	Alloying agents	0
238	Analytical and product testing	34
166	Animal repellents	38

No.	ChemUSES Function	Use category EU (No.)
63	Antiblocking agents	6
188	Anticaking agents	6
277	Anticracking agents	49
90	Anticratering agents	0
48	Anticreasing agents	0
291	Anticrock agents	21
4	Antifelting agents	43
41	Antifloating agents	50
152	Antiflooding agents	52
234	Antifogging agents	50
99	Antifogging agents	0
1	Antifouling agents	39
329	Antifouling agents	28
77	Antifreezes	5
12	Antifume agents	49
129	Antihydrolysis agents	49
76	Antiknock agents	28
120	Antilivering agents	49, 52
230	Antioxidants	14, 49
168	Antiozonants	49
301	Antiperspirants	15
218	Antipilling agents	55
282	Antiplasticisers	49
177	Antiprecipitants	11
293	Antiredeposition	9

No.	ChemUSES Function	Use category EU (No.)
	agents	
160	Antisagging agents	49
64	Antiscaling agents	14
119	Antiseize agents	35
68	Antisettling agents	49
350	Antiskid agents	0
343	Antiskinning agents	52
352	Antislip finishing agents	43
206	Antistaining agents	43
328	Antistatic agents	7
347	Antistripping agents	21
194	Antiwebbing agents	43
333	Bactericides	38
268	Barrier coating agents	21
269	Bates	47
143	Binders	2
108	Biocides	38
6	Blasting abrasives	0
132	Bleaching agents	8
304	Bleaching assistants	8
5	Bloom agents	10
88	Bloom inhibitors	49
358	Blowing agents	25
70	Bluing agents	0
180	Boil-off assistants	9
101	Brazing agents	54
220	Bright dips	0
353	Brighteners	17
281	Builders	43
222	Carbonising agents	43
164	Carriers	43
324	Case-hardening agents	13
170	Catalysts	43
19	Catalyst supports	43
31	Chain extenders	43
113	Chain terminators	43
141	Chain transfer agents	43
122	Chelating agents	34, 42, 43
133	Chemical blowing agents	25
93	Chemical raw materials	0
298	Clarifiers	0
242	Cleaners	9
260	Cloud point depressants	0
114	Coagulants	43
278	Coalescents	43
357	Coalescing agents	43
130	Coating agents	0

No.	ChemUSES Function	Use category EU (No.)
283	Collectors	0
86	Colouring agents	10
124	Complexing agents	11
355	Concrete additives	13
72	Coolants	29
323	Corrosion inhibitors	14
167	Cosmetic ingredients	15
123	Coupling agents (polymers)	49
174	Coupling agents (dyes)	10
335	Coupling agents (solutions)	55
315	Crabbing assistants	43
228	Crosslinking agents	43
215	Culture nutrients	0
226	Curing agents (concrete)	43
369	Curing agents (polymer technology)	43
18	Currying agents	43
366	De-inkers	43
81	Deaerating agents	0
236	Deasphalting agents	43
309	Deblooming agents	0
85	Dechlorinating agents	55

No.	ChemUSES Function	Use category EU (No.)
97	Decontaminats	38
342	Defoamers	43
229	Degreasers	48
365	Degumming agents	43
137	Dehairing agents	43
213	Dehumidifiers	1
73	Dehydrating agents	0, 34
74	Deicers	5
107	Deionizers	0, 34
84	Delignification agents	43
102	Delustrants	31
232	Demulsifiers	0
200	Denaturants	0
52	Deodorants	5
30	Depolymerisation agents	43
183	Deposit modifiers	28
367	Depressants	43
49	Descaling agents	0
198	Desensitisers (explosives)	42
299	Desensitisers (photography)	42
292	Desizing agents	43
300	Detackifiers	6
173	Detergents	9
179	Detonators	18

No.	ChemUSES Function	Use category EU (No.)
182	Developers	42
231	Devulcanising agents	47
205	Dewatering aids	0
82	Dewaxing solvents	48
356	Discharge printing agents	0
140	Disinfectants	39
259	Dispersants	43
38	Drainage aids	0
317	Dryers	43
44	Drilling mud additives	0
322	Dry strength additives	0
26	Dust control agents	16
233	Dusting agents	6
150	Dye carriers	43
255	Dye leveling agents	43
307	Dye retardants	43
211	Dye retention aids	43
39	Dye stripping agents	0
267	Dyes	10
28	Elasticisers	47
161	Electrical conductive agents	12
311	Electrical insulating material	32
89	Electroconductive coating agents	7
383	Electrode materials	12
245	Electrolytes	12
100	Electron emission agents	0
340	Eluting agents	0
372	Embalming agents	0
361	Embrittlement inhibitors	13
265	Emollients	47
159	Emulsifiers	49
186	Encapsulating agents	0
57	Enhanced oil recovery agents	0
308	Entraining agents	0
341	Enzyme inhibitors	43
157	Enzymes	43
319	Etching agents	0
336	Evaporation control agents	0
363	Explosion inhibitors	18
158	Explosives	18
373	Extraction agents	34, 48
66	Feed additives	26
34	Fertilisers	19
207	Fiber-forming compounds	0

No.	ChemUSES Function	Use category EU (No.)
212	Fillers (patching)	20
351	Fillers (augmentation)	20
368	Filtration aids	0
284	Finishing agents	43
25	Fire extinguishing agents	22
295	Fixatives	21
112	Fixing agents (textile technology)	21
134	Fixing agents (fragrances)	21
332	Flame retardants	22
56	Flatting agents	0
79	Flavours and fragrances	0, 36
190	Flocculating agents	23
297	Flotation agents	23
142	Fluid loss additives	0
20	Fluorescent agents	10
22	Fluxing agents	54
145	Food additives	2
337	Formation aids	43
94	Frothers	25
306	Fuel additives	28
331	Fuel oxidisers	43
247	Fuels	27
117	Fulling agents	43

No.	ChemUSES Function	Use category EU (No.)
32	Fume suppressants	17
270	Fumigants	38
313	Functional fluids	0, 5, 12, 29, 30, 35
362	Fungicides	38
221	Gelling agents	52
193	Greaseproofing agents	0
184	Grinding, lapping, sanding and polishing abrasives	0
99	Heat transfer agents	29
314	Heat insulating materials	32
87	Heat stabilisers	49
275	Herbicides	38
192	Hormones	0
318	Humectants	7
246	Humidity indicators	0
65	Hydraulic fluids	30
210	Hydrotropic agents	0
181	Impact modifiers	0
380	Incandescent agents	0
27	Incendiaries	18
69	Indicators	0, 34
103	Initiators	43
146	Inorganic intermediates	33

No.	ChemUSES Function	Use category EU (No.)
155	Insect attractants	38
348	Insect repellents	38
330	Insecticides	38
162	Insulating materials	32
286	Intensifiers (photography)	42
359	Intensifiers (printing)	43
148	Internal lubricating agents	35
2	Ion exchange agents	0
171	Kier boiling assistants	43
91	Lachrymators	0
248	Lakes	10
33	Latex compounding agents	0
172	Laundry sours	40
53	Leaching agents	0
156	Leather processing agents	0
285	Light stabilisers	42
370	Liquid crystals	0
195	Lubricant additives	35
364	Lubricating agents	35
381	Luminescent agents	0, 10
379	Magnetic agents	0
67	Mar proofing agents	55
375	Materials for shaping	13
35	Mercerising assistants	10
289	Metal conditioners	0
37	Metal treating agents	0
95	Metal strippers	0
327	Milling aids	0
360	Modifiers	23
115	Monomers	33
227	Mordents	21
252	Nematocides	38
24	Nucleating agents	43
237	Obscuring agents	0
339	Odorants	36
197	Oil repellents	0
346	Oiliness agents	35
128	Opacifiers	10
62	Optical quenchers	0
290	Organic intermediates	33
382	Osmotic membranes	0
325	Oxidation-reduction indicators	34
149	Oxidisers	37
320	Paint and varnish	48

No.	ChemUSES Function	Use category EU (No.)
	removers	
17	Papermaking agents	0
144	Parting agents	6
139	Pearlising agents	10
249	Penetrants	35
96	Peptising agents	43
253	Pesticides	38
191	pH indicators	40
266	pH control agents	40
55	Phosphatising agents	0
203	Phosphorescent agents	0
344	Photosensitive agents	42
378	Photovoltaic agents	42
50	Physical blowing agents	25
217	Pickling inhibitors	0
59	Pickling agents	0
125	Pigments	10
75	Pitch control agents	43
251	Plant growth regulators	0
185	Plasticisers	47
176	Plastics additives	0
224	Plastics for shaping	0
169	Plating agents	0

No.	ChemUSES Function	Use category EU (No.)
8	Poison gas decontaminants	0
3	Polymer strippers	0
121	Polymerisation additives	43
209	Polymerisation inhibitors	43
111	Pore forming agents	0
262	Pour point depressants	52
78	Pre-spotting agents	9
151	Precipitating agents	0
43	Prepolymers	33
118	Preservatives	39
21	Prevulcanisation inhibitors	43
106	Protective agents	0
216	Quenchers	29
45	Radioactivity decontaminants	0
16	Reaction media	48
374	Reagents	0, 34
244	Reducers	44
153	Refining agents	43
219	Refractive index modifiers	0
241	Refractories	0
208	Refrigerants	29
250	Reinforcing agents	13

No.	ChemUSES Function	Use category EU (No.)
223	Repulping aids	43
154	Resists	0
136	Retarders	43
296	Retention aids	43
9	Rinse aids	0
71	Ripening agents	0
264	Rodenticides	38
338	Rubber compounding agents	43
187	Rubber for shaping	0
201	Rubber reclaiming agents	0
189	Rubbing fastness agents	0
11	Rust removers	0
276	Rust inhibitors	0
51	Scavengers	43
274	Scouring agents	9
263	Scrooping agents	0
42	Sealants	0
202	Semiconductors	46
303	Sensitisers	42
10	Sequestering agents	11
261	Shrinkage controllers	9
98	Sizes	0, 31
126	Slime control agents	0
116	Slime preventatives	39
312	Slip agents	35
14	Soaping-off assistants	9
29	Softeners	47
305	Soil conditioners	0
294	Soil release agents	9
7	Soil retardants	6
326	Solubilising agents	43
271	Solvents	48
92	Spreaders	2
54	Stabilisers	49
83	Stains	10
165	Stickers	2
61	Strippers	0
371	Surface coating additives	20
109	Surfactants	50
138	Sweeteners (petroleum technology)	28
80	Sweeteners (taste)	26
127	Swelling agents	20
280	Tackifiers	2
316	Tanning agents	51
40	Tar removers	0
13	Tarnish removers	0

No.	ChemUSES Function	Use category EU (No.)
345	Tarnish inhibitors	0
279	Textile specialities	0
272	Thickeners	52
334	Thixotropic agents	52
225	Toners	45
256	Transmission fluids	30
240	Turbulence suppressors	52
36	Ultraviolet absorbers	49
257	Vat printing assistants	0
135	Viscosity adjustors	52
15	Viscosity index improvers	52
288	Vulcanising agents	53
147	Water softeners	47
258	Water repellents	31
349	Water-reducing agents	13
23	Waterproofing agents	31
273	Wax strippers	0
310	Weighting agents (petroleum technology)	43
58	Weighting agents (textile technology)	20
35	Well treating agents	0
175	Wet strength additives	0
243	Wetting agents	50
377	X-ray absorbents	0

Appendix II-c: Input scheme for emission data on substances

1. Characterisation

	Yes	No
High production volume chemical	□	□
Other existing chemical	□	□
New chemical	□	□
Not specified	□	

2. Tonnage

A Produced (t/a): □, □ □ □, □ □ □. □ □ □

B Imported (t/a): □, □ □ □, □ □ □. □ □ □

C Exported (t/a): □, □ □ □, □ □ □. □ □ □

3. Use and stages of the life-cycle

	Yes	No
Production	□	□

		Processing			Production		Formulation		Private use		Recovery	
No.	Fraction	IC	UC	No	Yes	No	Yes	No	Yes	No	Yes	No
1	□ □ □	□ □	□	□	□	□	□	□	□	□	□	□
2	□ □ □	□ □	□ □	□	□	□	□	□	□	□	□	□
3	□ □ □	□ □	□ □	□	□	□	□	□	□	□	□	□
4	□.□ □	□ □	□ □	□	□	□	□	□	□	□	□	□
5	□.□ □	□ □	□ □	□	□	□	□	□	□	□	□	□

N.B. Private use is specified by IC 5 Personal/Domestic; This is the direct use of the substance (or a formulation containing the substance) by the public at large.

If the processing step has not to be considered at the assessment "No" is marked (not applicable for IC 5).

4. Production characteristics

D Main producer (tpa):	□,□ □ □, □ □ □. □ □ □
Not specified:	□

IC 3, UC 33

Non-isolated intermediate	(MC 1a)	□
Isolated intermediate, stored on site	(MC 1b)	□
Isolated intermediate with controlled transport	(MC 1c)	□
Not specified	(MC 1c)	□

Other IC/UC combinations

Continuous production	(MC 1b)	□
Batch process with dedicated equipment	(MC 1c)	□
Batch process with multi-purpose equipment	(MC 3)	□
Not specified	(MC 3)	□

Production capacity of the main source (producer)

E Capacity (t/day)	□ □, □ □ □, □ □ □. □ □ □
F Period (days/year)	□ □, □ □ □, □ □ □. □ □ □
Not specified	□

Specific emission information

Emission	**G**: kg/tonne	**or**	Fraction (**EFcomp-prod**)
Air	□ □ □. □ □ □		**0.** □ □ □
Wastewater	□ □ □. □ □ □		**0.** □ □ □
Soil	□ □ □. □ □ □		**0.** □ □ □
Not specified	□		

5. Formulation characteristics

N.B. For every IC/UC-combination specified in (3) Use and stage of the life-cycle:

Specific information on the scale of formulation

One company (fraction of main source = 1)	□
Fraction of main source (**$F_{ms\text{-}form}$**)	**0.** □ □ □
specified	□

No specific emission information

Dedicated equipment and (very) little cleaning operations	(MC 1b)	□
Dedicated equipment and frequent cleaning operations	(MC 1c)	□
Multi-purpose equipment	(MC 3)	□
Unknown		□

Specific emission information

Emission	**H**: kg/tonne	**or**	Fraction (**EFcomp-form**)
Air	□ □ □. □ □ □		**0.** □ □ □
Wastewater	□ □ □. □ □ □		**0.** □ □ □
Soil	□ □ □. □ □ □		**0.** □ □ □

Content in formulated product

Content:	□ □ □. □ □ □	%, or fraction:	**0.** □ □ □

In case of a given range:

Minimum:	□ □ □. □ □ □	%, or fraction:	**0.** □ □ □
Maximum:	□ □ □. □ □ □	%, or fraction:	**0.** □ □ □

6. Processing characteristics

N.B. For every IC/UC-combination specified in (3) Use and stage of the life-cycle:

Information on the scale of processing

One company (fraction of main source **Fms-proc** = 1)	□
Fraction of main source (**Fms-proc**)	**0.** □ □ □
Not specified	□

Specific emission information

Emission	**I**: kg/tonne	**or**	Fraction (**EFcomp-proc**)
Air	□ □ □. □ □ □		**0.** □ □ □
Wastewater	□ □ □. □ □ □		**0.** □ □ □
Soil	□ □ □. □ □ □		**0.** □ □ □

N.B. For every IC/UC-combinations specific data will be asked to input for release scenarios based on emission scenario documents!

7. Private use characteristics

Specific emission information

Emission	**J**: kg/tonne	**or**	Fraction (**EFcomp-priv**)
Air	□ □ □. □ □ □		**0.** □ □ □
Wastewater	□ □ □. □ □ □		**0.** □ □ □
Soil	□ □ □. □ □ □		**0.** □ □ □

8. Recovery characteristics

Specific information on the scale of recovery

Fraction of product (containing the substance)/substance recovered	**0.** □ □ □
Fraction recovered by the main source	**0.** □ □ □

Specific emission information

Emission	**K**: kg/tonne	**or**	Fraction (**EFcomp-rec**)
Air	□ □ □. □ □ □		**0.** □ □ □
Wastewater	□ □ □. □ □ □		**0.** □ □ □
Soil	□ □ □. □ □ □		**0.** □ □ □

Appendix 7. Guidance document for the use of aquatic model ecosystem studies for biocides

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1. Introduction

Authorization of an active substance requires that "*the biocidal product has no unacceptable effects itself, or as a result of its residues, on the environment*" (Article 19, 528/2012/EC) when the product is used according to the intended purpose. The potential ecological risk of the active substance is assessed by a risk assessment. In the first instance, a base set consisting of standard laboratory studies reflecting worst-case conditions is considered using internationally accepted guidelines (OECD, OPPTS). The predicted no-effect- concentration (PNEC) is calculated from the lowest endpoint derived from such standard acute or chronic laboratory tests using an appropriate assessment factor. The PNEC is compared to the predicted environmental concentration (PEC), which itself is based on realistic worst-case assumptions. In cases where the PEC/PNEC ratio is below 1, the risk is considered acceptable due to the margin established between the concentration at which no relevant ecotoxicological response is expected and the realistic worst case exposure concentration predicted from the biocidal use. In cases where the ratio is above 1, there is insufficient confidence for the absence of unacceptable effects and, an authorisation would require further investigations aiming to render more precisely the predicted no-effect-concentration and/or the expectable exposure situation for the ecosystem of concern. Well designed and scientifically based non-standard refined aquatic studies are considered to be a suitable instrument to derive a more realistic PNEC.

The TGD (2003) provides only very limited guidance on how to design and employ aquatic model ecosystem studies. This resulted in a range of different assessment approaches by the various Member States and a heterogeneous treatment of biocidal active substances. A

harmonized approach is required including a need to transfer knowledge and experience as available for other legislation considering the special situation of biocides.

In the registration procedure of plant protection products in the framework of Regulation 1107/2009/EC (replaces Directive 91/414/EEC) aquatic model ecosystem studies, usually referred to as mesocosm studies, are used more frequently to derive refined regulatory acceptable concentrations (RAC). For the assessment of plant protection products extensive research has been conducted and guidance documents have been issued discussing test design and interpretation of non-standard studies (e.g. CLASSIC edited by Giddings et al. 2002, HARAP edited by Campbell et al. 1999 and ELINK edited by Brock et al. 2010a, draft guidance document on tiered risk assessments for plant protection products, EFSA 2013). In addition, guidance was given for the setting of Environmental Quality Standards published under the Water Framework Directive (2000/60/EC) in which information for the use and design of non-standard studies for refinements is available (TGD EQS 2011). In addition more specific guidance is available on Member State level (Brock et al. 2011).

The integration of methods and decision schemes developed under other legislation will help to foster harmonization for biocides. This can help to generate consistent refinement approaches for the aquatic risk assessment.

The guidance presented here is seen as an extension of the TGD (2003) as it gives further guidance. It is as such intended to supplement the TGD. The approaches outlined in this document are mainly related to the refinement of the risk assessment for parent compounds, but can also be extrapolated to metabolites. The focus of this document is refinement for the $PNEC_{water}$ but general principles can also be applied for the derivation of the $PNEC_{sed}$.

2. Regulatory background and general principles

Member States must only authorize a biocidal product if the product or its residues have no unacceptable effects on the environment. Biocides are divided into different product-types representing different uses. The requirements for the environmental risk assessment are listed in the Annexes of Regulation 528/2012/EC. The available data for different substances can vary considerably. Generally, minimum testing requirements for the aquatic risk assessment comprise a base set of single-species short-term studies for fish, aquatic invertebrate and algae. For most product-types, the base set is extended by chronic studies with these standard species. It is commonly agreed that these studies are conducted according to international accepted guidelines (OECD, OPPTS). The technical guidance document (TGD, 2003) gives advice on testing strategies in cases where the data package is incomplete.

For active substances that are also registered as a plant protection product under Directive 91/414/EEC which is replaced by Regulation 1107/2009/EC much more comprehensive data packages are often available.

The lowest (most sensitive) endpoint is divided by an appropriate assessment factor to derive the PNEC. The size of the assessment factor reflects the uncertainties regarding:

- variation of toxicity data within and between laboratories;
- the variation within and between species;
- potential chronic effects in cases where only acute studies are available and;
- the extrapolation from laboratory to field conditions.

In the TGD (2003) standard assessment factors are established for acute and chronic endpoints available for the different compartments of concern. As the uncertainty is reduced the more data are available, the lower the assessment factor is to be considered, e.g. when long-term toxicity data are available from three species across three trophic levels the assessment factor is reduced to 10, provided that the potentially sensitive species groups are presented in the dataset. Moreover, data on the toxicity to other organisms than the standard species representing as such different trophic levels, taxonomic groups, traits or feeding strategies broaden the knowledge on the substance to be assessed and justify the reduction of the assessment factor.

In the risk assessment, exposure concentrations (i.e. PECs) are divided by the effect concentration (i.e. PNECs) to determine the risk. If the PEC/PNEC ratio is > 1 a potential risk is indicated and refinement of the risk ratio would be required to show a safe use. As such, the refinement can be based upon the further analysis of the PEC on the one side as well as of the ecotoxicological response, the PNEC, on the other side.

For the calculation of PECs, standard approaches considering conservative assumptions are provided by straightforward emission scenarios. The exposure estimation considers the release rate of biocides originating from its use pattern. All potential emission sources and the releases to the receiving environmental compartment(s) as well as the fate of the substance need to be analyzed.

There is some uncertainty how more elaborate data (e.g. field studies) can be used. For communication of potential risks harmonized evaluations across different legislation - some of them assessing the same chemical - are crucial. Therefore, agreement on experiments that can be used to generate input data for models or to refine default values in emission scenario documents are needed as well as refined approaches in modelling require definition as it is done in other areas where chemical risk assessments are performed. For some product-types refined modelling approaches have been developed (e.g. PT8 wood preservatives) but more effort is still needed in this area. Further, the refinement of the release from sewage treatment plants (e.g. elimination studies according to OECD 303a) will in addition help to gain a more realistic impression of exposure. Refinements of PECs by more sophisticated exposure scenarios, however, are not discussed in the context of this document.

The risk assessment performed with base set data is (by design) conservative and so refinements are needed for when a substance do not pass the standard risk assessment. In principle the PEC/PNEC ratio can be refined by:

- using refined toxicity endpoints e.g. from species sensitivity distributions, mesocosm (field) studies etc.;
- using refined emission scenarios.

Goal of all refined risk assessments is that the uncertainty is reduced through an increased amount of information leading to a consistent and meaningful ecotoxicological endpoint that can be used for regulatory purposes. Ecotoxicological observations from tests performed under more representative environmental conditions than standard laboratory tests add on the understanding about the substance of concern respective substance as do further data on other species than the specified base set. In the TGD (2003) guidance is given on the use of species sensitivity distributions (SSD) while other refinement options are not sufficiently addressed. However, other refinement possibilities are available and guidance is needed on how these can be incorporated into current practice. The obvious examples are model ecosystem studies. These experiments that improve the understanding of the ecological response of the aquatic community to a chemical have been found a highly valuable tool in the registration of plant protection products and ample of guidance is available (CLASSIC edited by Giddings et al. 2002, HARAP edited by Campbell et al. 1999, OECD, 2006 and ELINK edited by Brock et al. 2010a).

When a model ecosystem study is needed for the refined assessment it is important that the approach follows the identified area of concern from the assessment of the base set data. The expected exposure profile as well as specific characteristics of the compound (e.g. physical and chemical properties, mode of action on targeted and non targeted organisms, toxicological profile) must lead the test design in order to clarify fields of uncertainty and relevance for the risk assessment.

The final risk assessment should be based upon the overall weight of evidence considering and interpreting all the different lines of evidence (e.g. a laboratory test, a field experiment, an observational field study, information from similar compounds) (see Suter and Cormier, 2011).

3 Model ecosystem studies

3.1 General aspects

3.1.1. Introduction

Model ecosystem studies (in this context referred to as mesocosm studies) are a valuable tool to study effects of chemicals with a greater environmental realism. Mesocosm "*are bounded systems that are constructed artificially with samples from, or portions of, natural aquatic ecosystems, or that consists of enclosed parts of natural surface waters. They usually are characterized by a reduction in size and complexity when compared with their natural counterparts but they include an assemblage of organisms representing several trophic levels*" (EFSA, 2013, page 110). Temperature, light or pH that influence the population dynamics in the ecosystem are naturally established in the test and provide as such a vital base for the responses to the chemical stressor. In contrast to single species tests, semi-field mesocosm and field studies allow for the assessment of a higher number of species and ecological groups, species interactions and secondary effects, endpoints that reflect a higher level of biological organization. Since these studies are performed for a relatively long time also latency of effects can be covered. Limitations of mesocosm studies are a limited number or absence of long-living species as compared to field communities (Beketov et al., 2008) and partly the limited consideration of indirect effects (Von der Ohe et al., 2011).

Information gathered from mesocosm studies can help to minimize the impact on community structure and consequently, ensure long-term functioning of aquatic ecosystems (Figure 19).

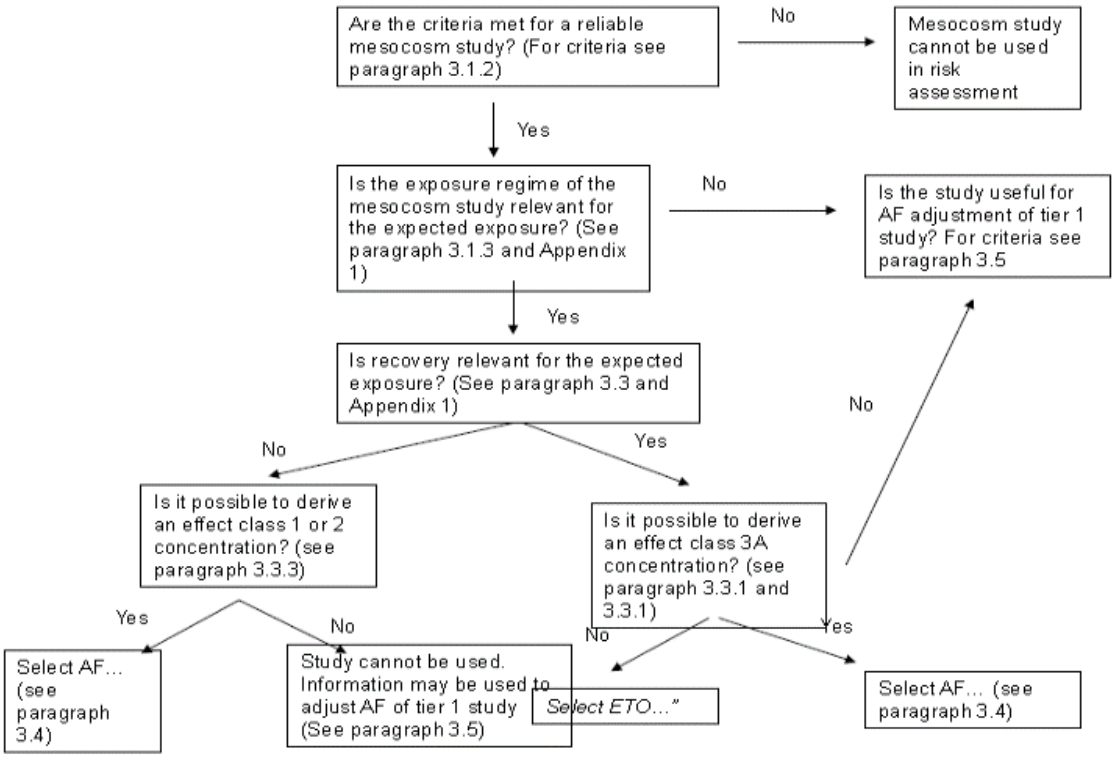

Figure 19: Decision scheme depicting the different assessment steps of a mesocosm study

3.1.2. Criteria for reliability

Based on the general principles of reliability assessment by Klimisch et al. (1997), De Jong et al. (2008) developed extensive guidance on the evaluation of mesocosm studies, which of course can also be seen as guidance for designing and reporting new studies. The following questions should be answered when assessing the quality of the study:

1. Is the test system adequate and does the test system represent a relevant freshwater community?
2. Is the description of the experimental set up adequate and unambiguous?
3. Is the exposure pattern adequately described?
4. Are the investigated endpoints sensitive and in accordance with the working mechanism of the compound?
5. Is it possible to evaluate the observed effects statistically?

Only studies which fulfill these reliability criteria should be used in the assessment. Some of the aspects are further elaborated on below.

EFSA (2013) deals with effects on freshwater ecosystems only, and existing mesocosms performed for PPP authorization address freshwater systems. Little information is present on the representativeness of these studies for marine risk assessments. Differences in pH, salinity, (sensitive) taxa, water refreshment due to tidal exchange, etc., may all contribute to differences in results. It is therefore advised not to use freshwater mesocosm studies as a basis for a marine risk assessment, and vice versa, unless there is scientific evidence that the ecotoxicological response in both types of systems is comparable.

3.1.3 Representative aquatic community

Mesocosm studies should address the potential effects on sensitive species or species groups in a full community. A sufficient number of representatives of taxonomic groups or species with representative biological traits should be present in the test system to provide a result of improved ecotoxicological relevance. Particularly taxa which are expected to be sensitive to the mode of action of the tested substance should be included, e.g. algae and macrophyte species in a study with an herbicide that inhibits photosynthesis, or insects for insecticides. For plant protection products it is specified that "*at least 8 different populations of the sensitive taxonomic group need to be present*" (EFSA, 2013, page 113). This criterion can be transferred to biocides. A number of biocidal actives will have a broader range of potentially sensitive taxa, and similar to EFSA's advice for fungicides, this should be accounted for by including a wider range of non-vertebrate taxa in the mesocosm design. Therefore, in cases where recovery is considered for risk assessment (see 3.1.5 below) it has to be carefully evaluated if potentially vulnerable taxa (e.g. uni- or semivoltine invertebrates with a low dispersal rate and/or macrophytes with a slow growth rate) are sufficiently represented, because recovery of these taxa will be slower than for species with a short life-cycle. The intrinsic sensitivity of insects is not correlated with voltinism (see e.g. Brock et al., 2010a), and there are no indications that slow-growing macrophytes are consistently more sensitive than e.g. algae, but sensitive multi-/bivoltine insects recover faster from insecticide stress than sensitive uni-/semivoltine insects (e.g. Van den Brink et al., 1996; Brock et al., 2009; Liess and Von der Ohe, 2005). In cases where recovery is not considered for risk assessment (indicated as the "ecological threshold option" (ETO)), the (in)ability to recover is not an issue because effects are not accepted at all. EFSA (2013) states that "it needs not to be a problem when sensitive univoltine and semivoltine invertebrates with low dispersal ability or macrophytes with a relatively slow growth-rate are not sufficiently represented in the test systems. Instead, the availability of data on negligible effect concentrations for species sensitive to plant protection products […] may [be] suffice to derive an ETO [= environmental threshold option] -RAC"(EFSA, 2013, page 113). A similar reasoning would apply to biocides.

3.1.4 Exposure

For the design of new studies as well as for the evaluation of existing ones, insight into the predicted exposure profile (PEC-profile, the development of predicted concentrations over time), is a prerequisite for the use of mesocosm studies for risk assessment. For a

straightforward risk assessment, the exposure profile in the mesocosm should be relatively worst case as compared to the PEC-profile in the water body. If exposure in a mesocosm study has been shorter or involved lower concentrations than expected for the proposed use, absence of effects in the mesocosm experiment cannot be used directly to demonstrate that no unacceptable effects will occur in the field situation. To illustrate this, some hypothetical cases are presented below. In Figure 20, on the left hand side, the situation is plotted in which initial exposure in the mesocosm is higher and concentration decline is slower than predicted for the proposed use. Still, no effects are observed in the mesocosm, which may be used as an indication that the proposed use will not lead to unacceptable effects. On the right hand side, the opposite situation is plotted: no effects are observed in the mesocosm, but the proposed use results in a higher peak and longer presence of the substance than considered in the mesocosm.

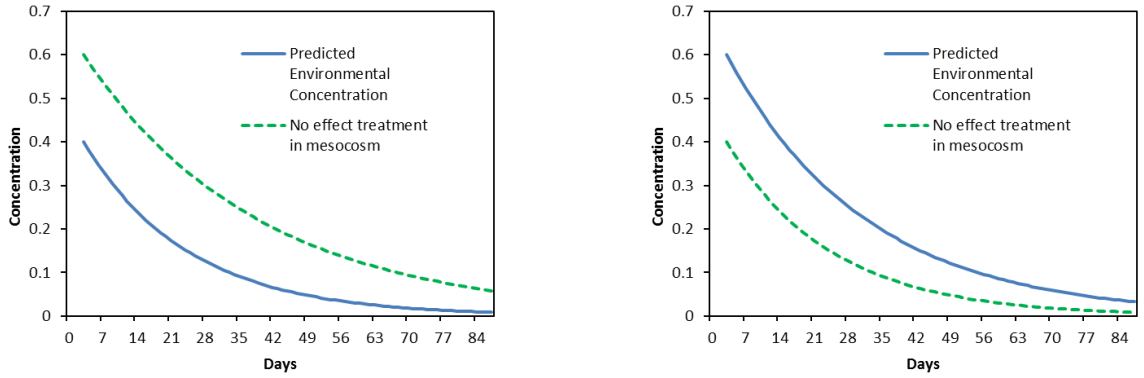

Figure 20: Comparison of the exposure profile in the mesocosm with the predicted exposure for the proposed use. Left: mesocosm is worst case for PEC. Right: mesocosm is best case for PEC.

Figure 21 shows a more complicated situation. On the left hand side, no effects are seen in the mesocosm with a peak concentration that is higher than predicted for the proposed use, but decline in the mesocosm study is faster than in the field. On the right hand side, the initial concentration in the mesocosm is lower than predicted for the proposed use, but the substance has been present in the mesocosm for a much longer time than predicted in the field. In these cases, it is not clear beforehand whether or not the mesocosm represents a worst case. If effects of the substance result from initial exposure during the first days, the mesocosm treatment with a higher initial peak might still be worst case, even if decline later on is faster. If, however, effects are due to prolonged exposure, the difference in decline rate may become more important. In these cases it should be considered if the concentration related to the NOEC-treatment when described in terms of a time weighted average concentration can be used for risk assessment. Further guidance on this is provided in the next chapter.

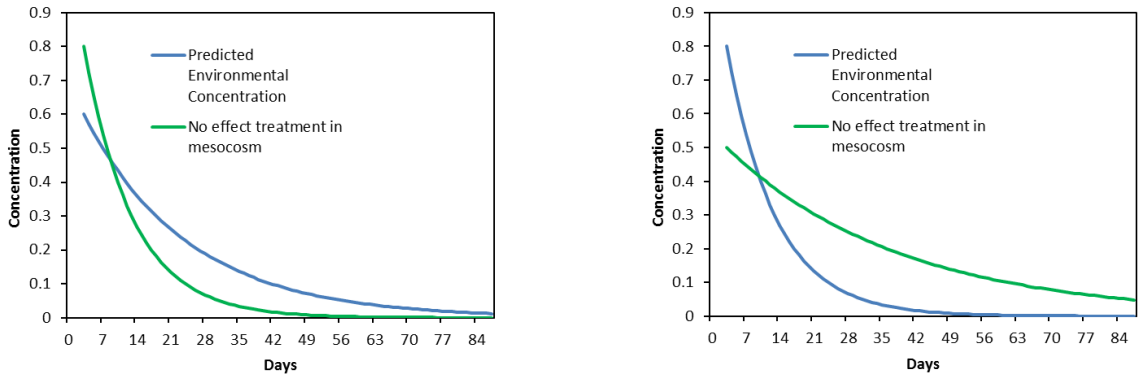

Figure 21: Comparison of the exposure profile in the mesocosm with the predicted exposure for the proposed use. Left: mesocosm is worst case for PEC when considering the peak, but not with respect to concentration decline. Right: mesocosm is not worst case with respect to initial exposure, but the substance has been present for a longer period of time without showing effects.

From these examples, it is clear that knowledge of the PEC-profile is essential both for designing new studies, and to evaluate whether or not an existing mesocosm can be used for the assessment of a different use. It is expected that for biocides authorisation the latter issue is particularly important, since a number of biocidal active substances have already been marketed as plant protection products. The focus of existing studies will often have been at simulating the predicted exposure resulting from plant protection product use, which is characterised by time-variable concentrations (EFSA, 2013). Typical profiles resulting from exposure modelling used for plant protection product assessment are characterised by repeated pulses. The height and duration of the peaks, and the interval between them will depend on agricultural practice, physico-chemical characteristics of the plant protection product, the relative importance of the different routes-of-entry (e.g. drift, run-off, drainage) and the characteristics of the water body (EFSA, 2013). In contrast, for the majority of biocides, predicted exposure will be constant because the emission scenarios consider daily use, discharge to a STP and daily emissions of the STP to the receiving water body. This puts special demands on the mesocosm design, although it does not necessarily mean that only mesocosm studies with constant exposure can be used for risk assessment. Further guidance on this is provided in sections 3.2 and 3.3 of this Appendix. Some PTs may result in non-continuous exposure, i.e. distinct peaks or in some cases irregular peak patterns comparable to those of plant protection products. A summary is given below in Table 54. No ESDs are available for PT 16, 17, and 20. These PTs are therefore not included in the table. Table 57 gives a more detailed overview of the expected exposure patterns per PT in order to facilitate the design and evaluation of the mesocosm studies. Note that Table 54 and Table 57 are meant as a generic overview, and the profile of a specific case may be different. As indicated above, it should always be checked whether the mesocosm study adequately represents the exposure profile resulting from the biocide use. Ihose PTs where emission is indicated as "potentially not continuous", a careful examination of the expected exposure profile is needed to decide on the relevance of the mesocosm design for a particular intended use.

Table 52: Summary of expected exposure patterns for biocide product–types (PT between brackets: probably only in specific cases).

Continuous emissions	Potentially non-continuous emissions
PT 1, 2, 4, 5, 6, 7, 8, 9, 10, 13, 14, 15, 21	(2), 3, (9), 11, 12, 18

3.1.5 Evaluation of endpoints and acceptability of recovery

To draw meaningful conclusions from a mesocosm study it is important that the appropriate endpoints are measured in a sufficient frequency to cover the specific protection goal. The protections goals for biocides have only been phrased in general terms but at present biocide risk assessment generally considers the population in the case of aquatic algae, vascular plants and invertebrates, individuals to populations in the case of vertebrates and populations to functional groups in the case of aquatic microbes. "*This implies that for most organisms at risk that are studied in micro-/mesocosm tests the selected measurement endpoints should relate to relevant population-level endpoints, more specifically the attributes survival/growth and abundance/biomass*" (EFSA, 2013, page 115). To study community level responses, multivariate analyses, parameters like diversity indices as well as endpoints indicative for community processes like dissolved oxygen are recommended. The assessment of reliability of a mesocosm study is described in detail by De Jong et al. (2008) and EFSA (2013). A critical part of the evaluation of mesocosm studies is the statistical analysis of measurement endpoints related to effects. Various univariate and multivariate techniques are available for evaluation of effects at the population and at the community level, to calculate NOECs and LOECs. To ensure that an effect is treatment related and not background variability, information about the statistical power of the NOEC/LOEC values is required. Therefore, EFSA (2013) advises that the minimal detectable difference (MDD) is reported for each measurement endpoint. Calculating the minimal detectable difference (MDD) allows reporting the actual effect which could be determined in the experiment for a given endpoint at a given time. A high MDD means that large changes are not detected as significant, due to e.g. variability in the control or low abundance. For applying the MDD concept to mesocosm experiments it is noteworthy that the MDD is particularly important if no effect is observed, since when a LOEC can be calculated the statistical power apparently is high enough to detect an effect. EFSA (2013) states that the MDD should preferably be lower than 70-90%. However, EFSA (2013) also requires that for at least 8 sensitive taxa a statistical evaluation of the dose-response relationship should be possible, meaning that the MDD should be sufficiently low. The case study with an insecticide that is included in the EFSA guidance shows that indeed low MDDs for sensitive endpoints are possible.

The identification of treatment related responses should not be based on statistical evaluations only, but also on ecotoxicological and ecological knowledge. Single species laboratory data can help to put results of a mesocosm study into perspective and can be considered along with the results from the mesocosm studies. De Jong et al. (2008) and the EFSA (2013) should be consulted for more guidance on statistical analysis and the MDD.

For the reason of a better comparability of studies and their interpretation for the protection level to be achieved, Effect classes as described by de Jong et al. (2008) and adapted by EFSA (2013) should be used to evaluate effects (Table 55). For further details, reference is made to the original report (de Jong et al. 2008) and the PPP guidance by EFSA (2013).

Table 53: Definition of endpoints of mesocosm studies. Classification into Effect classes according to EFSA (2013)

Effect class	Description
0	*Treatment related effects cannot be evaluated*. Due e.g. low abundance and variability the MDD was always larger than 100 % so even very strong effects could not be determined for the endpoint evaluated. If this class is consistently assigned to endpoints that are deemed most relevant for the interpretation of the study, the regulatory reliability of the micro-/mesocosm tests is questionable.
1	*No treatment-related effects demonstrated for the most sensitive endpoints*. No (statistically and/or ecologically significant) effects observed as a result of the treatment. Observed differences between treatment and controls show no clear causal relationship.
2	*Slight effects* Effects concern short-term and quantitatively restricted responses usually observed at individual samplings only.
3A	*Pronounced short-term effects (< 8 weeks, followed by recovery)*

	Clear response of endpoint, but full recovery of affected endpoint within 8 weeks after the first application or, in the case of delayed responses and repeated applications, the duration of the effect period is less than 8 weeks and followed by full recovery[33]. Treatment-related effects demonstrated on consecutive samplings.
3B	*Pronounced effects and recovery within 8 weeks post last application* Clear response of the endpoint in micro-/mesocosm experiment repeatedly treated with the test substance and that lasts longer than eight weeks (responses already start in treatment period), but full recovery of affected endpoint within eight weeks post last application.
4	*Pronounced effect in short-term study* Clear effects (e.g. large reductions in densities of the population) observed, but the study is too short to demonstrate complete recovery within eight weeks after the (last) application.
5A	*Pronounced long-term effect followed by recovery* Clear response of sensitive endpoint, effect period longer than 8 weeks and recovery did not yet occur within 8 weeks after the last application but full recovery is demonstrated to occur in the year of application.

The endpoint (NOEC) from a mesocosm study to be used for biocides risk assessment should preferably be derived on the basis of the treatment that is classified as Effect class 1. However, since Effect class 2 refers to slight effects that are observed on a single occasion, this Effect class might be used also to derive a NOEC from a mesocosm study. Moreover, when more measurement endpoints are assessed on several sampling days (which usually is the case in micro-/mesocosm experiments) that the chance of occurrence of Type II statistical errors may increase (demonstrating a statistical difference when there is not a treatment-related effect). For this reason it could be decided that a single Effect Class 2 response could be seen as the NOEC of the study (Brock et al., 2011), but a higher assessment factor may be applied.

The recovery option is not applicable to product-types that result in continuous exposure. In case biocide emissions lead to a short-term peak on only few occasions during the year e.g. meeting the definition of intermittent release according to the TGD (2003), considering the recovery option might be reasonable. The potential for recovery should be judged in relation to the product specific exposure pattern. Thus, it has to be thoroughly checked if the expected exposure pattern allows for recovery. In the light of harmonization and for registration of active substances on a European level, Effect class 3A endpoints are used for the ecological recovery option. If the PNEC is based on a mesocosm using an Effect class 3A endpoint, special attention should be paid to the representativeness of potential sensitive populations. It is suggested to link the PNEC and the respective covered biocidal use in the list of endpoints. Additional data in relation to the use pattern can be submitted at product authorization stage. Note, that for product authorization on MS level different time periods for recovery might be acceptable (e.g. reduced recovery time in colder areas like in some Nordic countries).

In summary, the results of a properly designed and conducted mesocosm study can thus be used in the effect assessment in two ways (**Figure 22** on the next page):

- by accepting no (or only negligible) population effects (ecological threshold option) or;
- by accepting some population level effects if ecological recovery takes place within an acceptable time period (ecological recovery option); only acceptable if exposure pattern allows for this option.

[33] An endpoint is considered as recovered if the MDD allows statistical evaluation during the relevant recovery period (so excluding MDD class 0) and the conclusion of no statically significant effect between treated systems and controls is not caused by a decline of that endpoint in controls (e.g. at the end of the growing season). If these criteria are violated a higher effect class has to be selected.

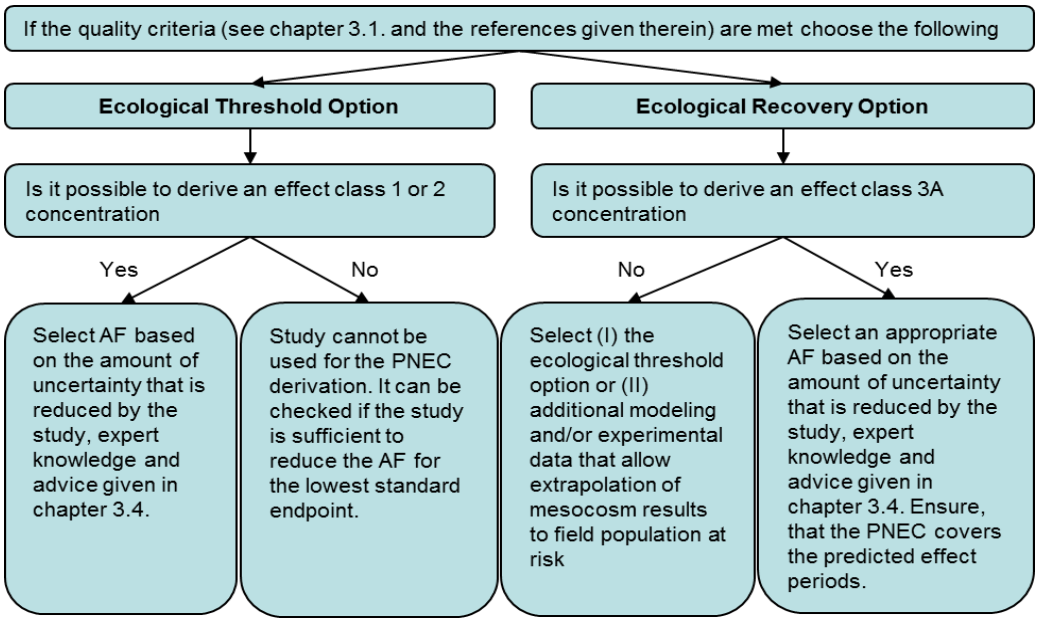

Figure 22: Decision scheme for the derivation of PNECs based on mesocosm studies (EFSA, 2013, page 124; adapted)

3.2 Design of new studies

For the design of mesocosm studies, guidance is given by OECD (2006), EFSA (2013) and in various workshop documents and publications (e.g. CLASSIC edited by Giddings et al. 2002, HARAP edited by Campbell et al. 1999, ELINK edited by Brock et al. 2010a and de Jong et al. 2008) and will not be repeated in detail in this document. In addition to the references given above, the main points given in chapter 3.1 and aspects that are particularly important for biocides should be considered for the design of new studies.

The dose selection should be based on results of the base set data and known effects from literature. Special attention should be given to the anticipated exposure pattern in the field (i.e. the predicted PECs, see 3.1.4 above) and to the question whether recovery can be taken into account or not (see 3.1.5 above). Information from structurally similar compounds can help to properly design the study if the used information is relevant and reliable. Studies which have been peer-reviewed under European or national legislation are a valuable data source. For substances reviewed under Directive 91/414/EEC (replaced by Regulation 1107/2009/EC), the exposure pattern, particularly from tailor-made studies, will often not reflect the exposure pattern resulting from biocidal uses. Nevertheless, these studies can be considered as they provide valuable information, for example on the distribution of sensitivities among species or groups of species.

The active substance should be preferably used as test item. However, for some substances this might not be practicable (e.g. too low water solubility of the active substance). In these cases a formulation may be used as test item. The chosen formulation is preferably the biocidal product that is planned to be authorised. Although a formulation contains several substances, the effects are usually driven by the active substance. In cases for which the tested formulation is not equal to the biocidal product information should be provided to show that the toxicity of the formulation is comparable to the active substance.

Depending on the properties of the active substance it has to be kept in mind that test organisms are exposed to the parent compound as well as to metabolites if these metabolites are stable for a certain time. An appropriate analytical analysis should be conducted so that an assessment of both the exposure and effects of any relevant metabolites can be made. Therefore, if a higher tier study is commissioned and relevant metabolites have been identified

in fate and behaviour studies, these metabolites should be measured in order to include them in the risk assessment

3.3 Evaluation of already available mesocosm studies for biocides

A concept for the re-evaluation of mesocosm studies which were conducted for purposes other than the support of a biocidal registration authorisation (i.e. typically for plant protection products) is developed on the basis of different exposure patterns. In such cases it is important to determine which part of the exposure is most relevant in terms of ecotoxicological effects leading to the ecotoxicologically relevant concentration (ERC).

There are three different kinds of exposure:

- single peak (see 3.3.1 below),
- multiple peak (see 3.3.2 below) and
- continuous exposure (see 3.3.3 below).

As explained in section 3.1.4 of this Appendix a decision should be made whether or not the mesocosm adequately represents the exposure profile resulting from biocide use.

Before listing the recommendations, a general point has to be addressed: effect concentrations can either be expressed as nominal or initial measured or as time-weighted-average (TWA) concentrations. If the TWA approach is used, particular attention should be paid to the time interval over which the TWA is calculated. The time window for the TWA is not necessarily identical to study duration of the mesocosm nor to standard tests in the laboratory, instead it is driven by the ecological response time and the duration of the exposure in the study. It is important to get an understanding of the exposure phase that is most relevant for inducing toxic effects (Brock et al. 2011). The pragmatic approach to base the TWA on the length of the chronic study that triggered the risk was proposed by Brock et al. (2011) in a Dutch national guidance for the derivation of long-term environmental standards. This approach is also used by EFSA (2013) and is seen as being "*most likely being relatively worst case*" (EFSA, 2013, page 49). If scientific data are available that demonstrate that another TWA is more appropriate e.g. information on the ratio between acute and chronic effects, the time to onset of effects or the length of the most sensitive life stage of the organisms at risk, the time window should be shortened or lengthened. If there is reasonable concern that the TWA based on the chronic study that triggered the higher tier study is too short, e.g. if effects in the mesocosm last longer than the duration of the critical chronic laboratory study, it is proposed to base the length of the TWA on the time span during which the most sensitive species in the mesocosm is affected, i.e. from the onset of effects until recovery. This period is derived from the treatment above the NOEC, i.e. above Effect class 2 (see Figure 23) (NOEAEC for plant protection products). This time window is then used to calculate the TWA concentration from the NOEC treatment. In case multiple species are affected then the longest time window should be taken as a basis for the TWA calculation. This approach is only applicable if the mesocosm involves a treatment with recovery of effects within the duration of the study.

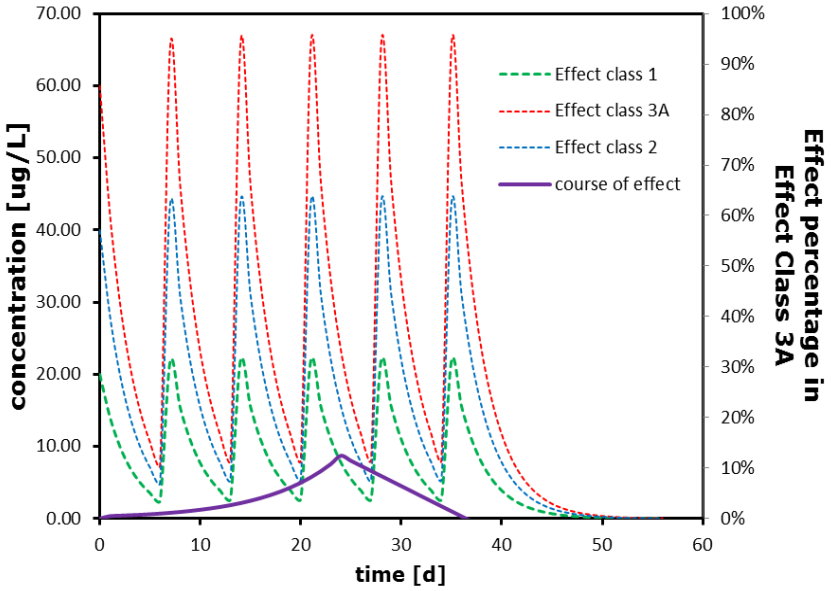

Figure 23: Representation of mesocosm treatments with Class 1, 2 and 3A effects (dotted lines, primary vertical axis) and time course of effects in Effect Class 3A (purple line, secondary vertical axis).

In the eventual case that a reliable mesocosm study cannot be used directly to derive the $PNEC_{water}$, e.g. because the exposure regime is not adequate, it nevertheless needs to be evaluated as the additional information adds on the knowledge of the overall toxicological profile of the compound of concern. For example, mesocosm studies may point at the sensitivity of a taxon that was not included in the laboratory dataset, or mesocosm studies can confirm that a taxon is apparently non-sensitive. Mesocosm data may thus confirm that testing of additional taxa will likely (not) result in lower endpoints. They may reduce the uncertainty when statistical extrapolation methods are applied to laboratory data (Species Sensitivity Distributions (SSD)). This may be a reason to adapt the assessment factor used on laboratory data. It should be realized, however, that when a mesocosm is considered not suitable for PNEC-derivation because the exposure is not relevant for the predicted field exposure, care should be taken when deciding on adapting the assessment factors for a chronic risk assessment based on laboratory studies. In addition, a mesocosm that is judged as not suitable for the surface water risk assessment might still provide useful information for the sediment risk assessment.

3.3.1 Single peak exposure

For studies with single peak exposure, the dissipation time of the substance in water is the first decision criterion.

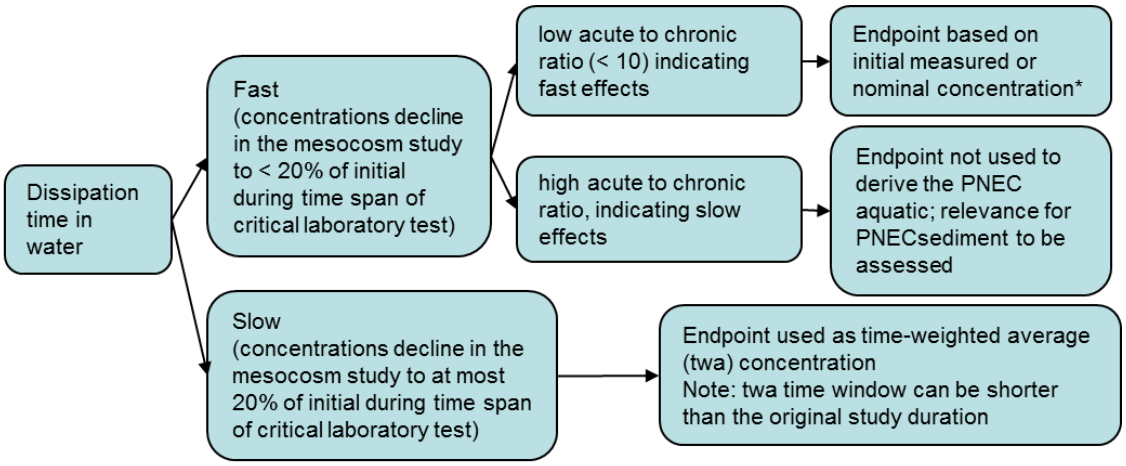

Figure 24: Assessment scheme for single peak exposure studies

For non-continuously released biocides, the initial peak in the treatment which resulted in Effect Class 1 or 2 can be used directly if the peak and decline rate in the study is worst case as compared to those for the field, i.e. if the peak in the mesocosm is higher and the DT_{50} for dissipation from the water phase long enough to cover the exposure that is predicted for the field (see Figure 21, left hand side). When the initial concentration is used for the effects assessment, the PNEC should be compared with the $PEC_{initial}$.

For continuous exposure, it should be judged whether the exposure in the mesocosm study has been long enough to consider the study relevant for the derivation of the PNEC for long-term exposure. For this, Brock et al. (2011) propose that test concentrations between peaks should not decline to <10% of initial. EFSA (2013) gives a more strict criterion for the use of a single pulse mesocosm study for chronic risk assessment, and requires a maximum decline to 20% of initial (i.e. <80% decline) within the time window relating to the duration of the test that triggered the risk assessment. This can be judged from the reported concentrations or using the dissipation time. The minimum required dissipation time can be calculated from the formula $C(t) = C(0) \cdot e^{(-kt)}$, where C(t) is the concentration after t days, C(0) is the initial concentration, k is the decline rate constant and t is the duration of the critical laboratory test.

If the dissipation time in the mesocosm is faster and leads to <20% of initial remaining after the critical time, the acute to chronic ratio (ACR) may be considered. For the calculation of the ACR the ecological group that triggered the mesocosm study is used. For substances with a lower ACR (i.e. < 10) which show a short time-to-onset-of effect, the endpoint can be expressed as the initially measured concentrations or the nominal concentration. Nominal concentrations are used if the measured concentration is between 80-120% of the nominal. Mesocosm studies with substances which dissipate fast but also have a high ACR, indicating that effects assessment is driven by longer/constant exposure, cannot be used directly for the derivation of the $PNEC_{water}$. However, these mesocosm studies might be used for the sediment assessment, when the concentration has been measured in the sediments and benthic organisms have been present in the system in a sufficient number. If the substance that disappeared from the water phase is sorbed to sediment, organic matter or organisms it may still contribute to effects that are treatment related. It has to be checked if analytically determined sediment exposure covers field exposure and if the tested species assemblage is representative.

For slowly dissipating substances that meet the criterion of <80% decline of concentrations within the time window of the critical chronic laboratory test the endpoint is based on the relevant TWA concentrations. The time window for the TWA is not necessarily the same as the duration of the mesocosm study (see above). For instance, Figure 25 on the next page (graph at the top) shows an Effect class 1 mesocosm-treatment where no effects are observed, using

a critical study for PNEC derivation for a 21-day chronic daphnid test. In this example, the initial concentration of the active substance is 100 µg/L, and declines with a DT50 is of 9 days. After 21 days the substance has declined to 20 µg/L (green dashed line). This single peak mesocosm study would meet the criteria as described above, for the use of a single pulse mesocosm study for chronic risk assessment. The NOEC of the mesocosm may be calculated as the 21-day TWA (blue dashed line; 50 µg/L), given that the critical 1st tier test is a 21-day Daphnia study, and in the mesocosm treatment level above the highest treatment with no effects, in other words, above the Effect class 1 NOEC, the time to onset of maximum effects was < 21 days. However, in the case where the treatment level above the level identified as Effect Class 1 NOEC, the time to maximum effect would be of 30 days, then the NOEC of the Effect class 1 treatment should be calculated as the 30-day TWA, and in this case the NOEC would be set to 39 µg/L. As a result, by setting the NOEC to 50 µg/L, it is implicitly assumed that continuous exposure at 50 µg/L will not induce effects. In contrast, if the NOEC is not set at 50 µg/L, the assumption is that effects may occur below this level, even in situations where even at higher concentrations than the TWA no effects were observed, as it is the case in this study. Figure 25 (graph at the bottom) shows an example where the critical test conducted is a 28-day insect study, with a slower decline of the substance in the mesocosm system (DT_{50} of 24 days). In this case, and after 28 days, the actual concentration of the substance in the test is 68.5 µg/L. Thus, the criterion of the substance declining a maximum of 80% from the initial concentration is easily met. In this study, the time to the maximum effect is 35 days, and thus in this situation it could be justified to use the 35-day TWA as the basis for setting a NOEC to 62 µg/L.

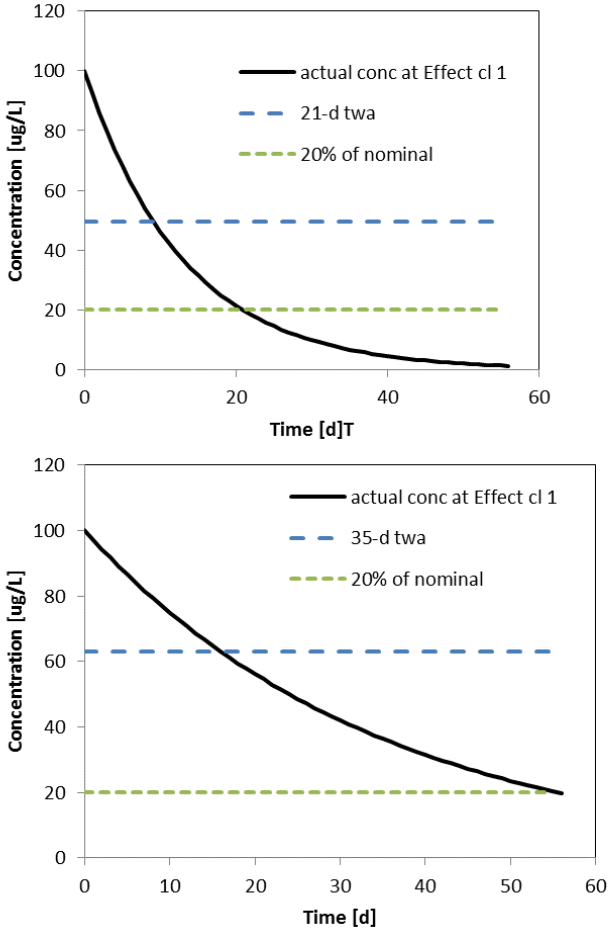

Figure 25: Representation of a chronic daphnid study (21 days) in an Effect class 1 mesocosm system for a single peak exposure treatment in situations where the DT50 is 9 days (graph at the top) and 24 days (graph at the bottom), and where the data can be considered for a chronic risk assessment.

3.3.2 Repeated peak exposure

Repeated pulse studies are considered in a similar way as single pulse studies. If concentrations decline to completely between pulses, the study can in principle not be used for derivation of a PNEC for continuous exposure unless at least 20% of initial concentration is present over the duration used for the TWA time window (if the TWA approach is feasible) of the critical laboratory test. In practice, this will mean that studies, in which concentrations decline completely in between pulses, will be treated as a single pulse study. For rapidly dissipating compounds (i.e. if the DT_{50} of a substance in the mesocosm is shorter than the trigger as calculated above), application has to be repeated before concentrations have dropped to 20 % of initial and application has to be continued until the total application period is long enough to cover at least the duration of the most critical laboratory test.

If a mesocosm study with repeated applications of a fast dissipating compound does not meet the criteria as described above, additional laboratory studies and/or modeling approaches may be used to demonstrate that continuous exposure would not lead to different results than observed in the repeated pulse studies.

For this assessment, results from laboratory studies with a semi-static or continuous design can be compared. For such a comparison, species should be used that are preferably closely related to the sensitive taxon found in the mesocosm. If the endpoints are in a comparable range (factor 3 difference), the endpoint of the mesocosm study can be expressed as a TWA concentration. If the toxicity is not comparable, a further evaluation is needed. This can for example include time-to-event studies or modeling approaches.

Models can provide information on the acute and long-term impacts of substances present over a range of exposure durations and frequencies. Mechanistic effect models may help to integrate the ecological and environmental parameters and thus also increase the understanding of the complex interactions and mechanisms of potential biocide impacts on ecosystems. Toxicokinetic/toxicodynamic models (Ashauer et al. 2011) will help to evaluate the potential long-term impact of non-continuous exposure situations. If modelling approach are used some general rules should be applied across the different models such as 'good modelling practice' and proper documentation of all assumptions, input parameters and modelling steps (Schmolke et al. 2010). An overview of the state of the art with respect to effect modelling, considering toxicokinetic/toxicodynamic modelling, population models, community, food web or ecosystem models, and empirical models can be found in the proceedings of the ELINK-workshop (Brock et al., 2010a). The potential role of ecological population models for pesticide risk assessment and registration was discussed during the LEMTOX-workshop (Thorbek et al., 2010). An EFSA opinion on the use of mechanistic modelling approaches is expected for 2016 (EFSA, 2013).

For repeated peak exposure it is also important to consider the toxicological dependency of these pulses for the life span of the individuals of the sensitive species: If recovery is considered ecological independence (peak intervals are greater than the relevant recovery time of the sensitive populations of concern) has to be evaluated (EFSA, 2013).

Generally, a potential relevance of the study for the sediment risk assessment has to be kept in mind especially for substances that dissipates into sediment and are relatively stable (in) there. An EFSA opinion on sediment risk assessment is expected for 2014 (EFSA, 2013).

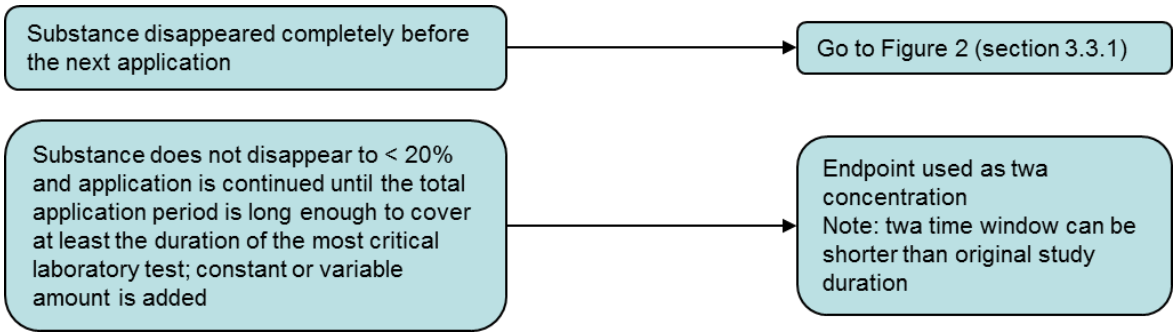

Figure 26: Assessment scheme for repeated peak exposure studies

3.3.3. Continuous exposure

As already indicated before, most biocidal PTs will result in continuous exposure. Mesocosm studies with continuous exposure are rather rare, but if present the derivation of a NOEC from these studies follows the same principle as standard laboratory studies. Nominal concentrations can be used if measured concentrations are between 80 and 120 % of nominal, otherwise actual average concentrations should be used.

Whilst the use of a time weighted average approach may be appropriate in some circumstances it always needs to be considered if it is scientifically valid and supported by sufficient evidence to show reciprocity of effects at relevant concentrations and exposure durations.

3.4 Application of an assessment factor to derive the $PNEC_{water}$

"*The assessment factors reflect the degree of uncertainty in extrapolation from laboratory toxicity test data for a limited number of species to the 'real' environment*" (TGD, 2003 page 93). In the technical guidance document (TGD, 2003) the size of the assessment factor applicable to the endpoint of a mesocosm study is left open. It is only stated that "*the assessment factor to be used on mesocosm studies or (semi-) field data will need to be reviewed on a case-by-case basis*" (TGD, 2003 page 101).

Since mesocosm studies are regarded as an additional step in the risk assessment process which reduces uncertainty, the regulatory trigger values used at assessment of the data from the base set need not necessarily be carried over to the refined risk assessment. Thus, if uncertainty is reduced compared to the preliminary risk characterization, the assessment factor should be reduced.

As stated above the assessment factor has to account for spatio-temporal extrapolation i.e. the mesocosm – field extrapolation. To gain insight into this aspect, Brock et al. (2006) compared the results of mesocosm studies covering ponds, ditches and streams for chlorpyrifos (single peak exposure) and atrazine (multiple peak exposure). Based on endpoints of Effect Class 1 and 2, the spatial and temporal extrapolation of ecological threshold concentrations seems to be possible with relatively low uncertainty. In later work Brock et al. (2008) compared mesocosm experiments in which long-term exposures were simulated and based on these a geographical extrapolation factor was estimated. For their comparison, Brock et al. (2008) used the reported Effect class 1-2 concentrations and calculated the geometric mean, the range between the lowest and highest reported value, and the 95% confidence limits. The difference between the upper and lower 95% confidence limits, indicated as the spread, was used as a measure of variability. The spread in long-term exposure studies was 1.4 for the surfactant dodecyl trimethyl ammonium chloride (C12-TMAC) and 5.4 for the linear alkylbenzene sulfonate (LAS), 1.8 for copper, and 2.5 for atrazine. For short-term pulse studies with chlorpyrifos and lambda-cyhalothrin, the spread was 2.9 and 2.6, respectively. It

should be noted that if Effect class 1 and 2 were both reported, Brock et al. (2008) used the geometric mean of these concentrations for their calculations. In an update, the assignment of Effect classes for the atrazine experiments was slightly revised and data for chlorpyrifos, azinphos-methyl, esfenvalerate, simazine and carbendazim were added (see Brock et al., 2011, Appendix 1; EFSA, 2013; Appendix E). Based on this scientific information, it appears that variability in studies is limited when comparing Effect class 1-2 concentrations, variation between studies increases when higher Effect classes are included in the analysis. The NOEC of a well performed mesocosm study (see 3.1.1) is valid for different local and climatic situations and it was concluded by EFSA (2013) that for short-term pulse studies, a small factor may be sufficient to address remaining variability at the level of Effect Class 1-2. For chronic studies, a factor of 2-3 would be sufficient to ensure that the Effect class 2 concentration in a single study does not overlap with higher Effect classes in other studies. For higher Effect classes, a higher factor may be needed to account for the variability between studies in case only a single mesocosm endpoint is available.

Assessment schemes and approaches for the size of the assessment factor are available under different European legislation. Annual average water quality standards (AA-EQS) as determined under 2000/60/EC are intended to protect water organisms against the occurrence of prolonged to continuous exposure. In the TGD EQS (2011) a rather general approach is presented, and regarding the assessment factor it is stated that "where there is (a) only a single model ecosystem study, and (b) sensitive taxa are included in the study of a compound with a specific mode of action, an assessment factor of 5 would account for variation in the NOECs" (EQS TGD, 2011, page 63). Based on the above presented comparison of mesocosm studies for different types of plant protection products and exposure patterns, EFSA (2013) uses lower assessment factors of 2 to 3 and differentiates between Effect class 1 and 2 for derivation of the RAC. For their justification of assessment factors for the AA-EQS Brock et al. (2011) pointed to the fact that, regulatory acceptable concentrations as determined according to EFSA (2013) are intended to protect water organisms in edge-of-field surface waters. Due to the application pattern of plant protection products the focus is on short-term pulses to prolonged exposure allowing in certain cases recovery of populations. Brock et al. (2011) argue that since EQS values apply to a wider range of water body-types, a higher assessment factor is needed for EQS-derivation. Brock et al. (2011) used the above presented comparison of mesocosm studies, and propose assessment factors of 2 to 4 for Effect class 1, and 4 to 5 for Effect class 2.

Table 54: Assessment factors for a single mesocosm study as proposed under 2000/60/EC and 1107/2009/EC

Effect class	Assessment following Water framework Directive (2000/60/EC)		Regulation of plant protection products (1107/2009/EC)
	(TGD EQS, 2011)	Dutch PPP guidance, (Brock et al., 2011)	(EFSA, 2013)
1: No treatment related effects	annual average AA-EQS: 5 [1)]	2 – 4 [2)]	2 [3)]
2: Slight and transient effects		4 – 5 [2)]	2 - 3 [3)]
3A: Pronounced short-term effects; recovery within 8 weeks after first application or total period of effects < 8 weeks	Not applicable	Not applicable	3 - 4 [3)]

Notes on Table
"where there is (a) only a single model ecosystem study, and (b) sensitive taxa are included in the study of a compound with a specific mode of action, an assessment factor of 5 would

account for variation in the NOECs" (EQS TGD, 2011, page 63). No guidance is given as to whether Effect class 2 may be used for NOEC derivation.

1) "The height of the AF [= assessment factor] is based on expert judgment considering all available lower and higher-tier information. If several adequate micro-/mesocosm studies are available the AF is applied on the highest Effect class 1 or 2 value or a lower AF than reported in the table may be applied" (Brock et al., 2011, page 104).
2) "If several adequate micro-/mesocosm studies or other adequate higher tier studies (e.g. monitoring, relevant population experiments or modelling) are available a lower AF [= assessment factor] should be applied to the RAC derived from the most appropriate micro-/mesocosm study […] for the specific case, considering a weight of evidence approach. If the available micro-/mesocosm studies are of the same quality, the AF may be applied to the geometric mean value of the Effect class 1 or Effect class 2 concentrations derived from the different studies. " (EFSA, 2013, page 128).

Where a range is presented, EFSA (2013) gives some factors that can be considered for justification of a lower AF, apart from having more than one study:

- the number of replicates is higher than the minimum required to achieve acceptable MDDs;
- the number of exposure concentrations tested is larger than the minimum of five concentrations;
- a sufficient pre-treatment period has been included to allow the community to be well-established in the system. Nevertheless, a mesocosm study should always be pre-treated before the test;
- the ecological relevance and richness of species of the community tested is higher than expected for the situation to be assessed;
- more than the minimum 8 populations of sensitive/vulnerable taxa are present with acceptable MDD;
- the exposure concentrations tested are worst-case relative to the predicted exposure scenario (i.e. multiple peaks are tested where a single peak is predicted).

For the selection of an appropriate assessment factor to derive a $PNEC_{water}$ for biocides the proposal by Brock et al. (2011) is followed since this selection of the assessment factors is scientifically justified and was based on published data from mesocosm studies with substances of all indications (i.e. herbicides, fungicides and insecticides) mimicking short-term and chronic exposure, and is considered protective for continuous and non-continuous exposure.

The following assessment factors are proposed based on the discussions at the workshop:

Effect class 1: 2 - 4
Effect class 2: 4 - 5
Effect class 3A: If the recovery option is applicable (for criteria see 3.1.5), an assessment factor of at least 5 would be needed to derive a PNEC from a single Effect class 3A endpoint.

The height size of the assessment factor within the given range is based on expert judgment considering the quality of the study. If several mesocosm studies of comparable quality are available a lower assessment factor may be appropriate or the assessment factor can be based on the highest Effect class 1 or 2 for the environmental threshold option or Effect class 3A for the environmental recovery option. If the recovery option is not applicable, Effect class 3A concentrations may still be used as additional evidence to support Effect class 1 or 2 studies, or to underpin the assessment factor for an Effect Class 1 or 2 endpoints.

4. Summary

For the authorisation of biocides under the BPR Regulation the potential risk to the environment is assessed. In the instance, a base set consisting of laboratory studies reflecting worst-case conditions is considered. If risk is indicated, the assessment can be refined by

refining the effect side using non-standard approaches (e.g. field data or model ecosystem studies). Besides some limitations (e.g. limited number or absence of long-living species as compared to field communities) model ecosystem studies (in this context referred to as mesocosm studies) are a valuable tool to study effects of chemicals with a greater environmental realism. In contrast to single species tests, mesocosm studies allow for the assessment of additional species interactions and secondary effects. Thus, endpoints reflect a higher level of biological organization. Information gathered from mesocosm studies can help to assess the impact on community structure and consequently, ensure long-term functioning of aquatic ecosystems. This guidance is seen as an extension of the TGD (2003) as it gives more and precise information and integrates current research and approaches used under other European legislation (2000/60/EC and 1107/2009/EC) thereby facilitation harmonization.

General guidance on the design of mesocosm studies is given by OECD (2006), EFSA (2013) and in various publications (e.g. CLASSIC edited by Giddings et al. 2002, HARAP edited by Campbell et al. 1999, ELINK edited by Brock et al. 2010a and de Jong et al. 2008). For biocides, special attention should be given to the anticipated exposure pattern in the field and whether recovery can be taken into account or not. An integrated understanding of the used endpoints will facilitate communication and will ease assessment of results. An overview is given which aligns the commonly used abbreviations (e.g. NOEAEC) to the respective Effect classes as described by de Jong et al. (2008).

A concept for the re-evaluation of mesocosm studies which were conducted for purposes other than the support of a biocidal registration authorisation (i.e. typically for plant protection products) is developed on the basis of different exposure patterns: single and multiple peak exposure. The re-evaluation scheme integrates scientific approaches developed and applied under other European legislation (e.g. 2000/60/EC). For studies with one single peak, dissipation time of the substance in water and the time to onset of effect are important criteria that are used to decide on the expression of the endpoint as nominal or time-weighted average value and the applicability of the study as $PNEC_{water}$. For the evaluation of studies with multiple peaks it has to be differentiated between two exposure patterns: (i) the substance disappears between the peaks, (ii) the substance does not disappear completely. If the time span between peaks is longer than the standard laboratory study on the trophic level of interest and the onset of effects were visible before the next peak the mesocosm is evaluated as a single peak mesocosm experiment. If it is shorter, the focal point is whether the toxicity caused by continuous exposure is similar to toxicity caused by repeated exposure. Generally, a potential relevance of a study for the sediment risk assessment has to be kept in mind especially for substances that dissipate into sediment and are relatively stable (in) there.

In the TGD, 2003 the size of the assessment factor is left open. Based on current research and in relation to other European legislation it is proposed to set the assessment factor for a single mesocosm between 2 to 5. The exact size of the factor depends on the used Effect class, the applicability of recovery and the quality of the study. If more data (e.g. several mesocosm studies) are available a lower assessment factor may be applied.

Table 55: Overview of emission patterns per product-type

PT no.	Name	Emission scenario document (ESD)	Scenarios with (indirect) emissions to water	Emission route	Potentially not continuous	Remarks
Main group 1: Disinfectants						
PT 1	Human hygiene	EUBEES RIVM/Haskoning 2004	Private use (based on tonnage or on average consumption)	waste water	N	

PT no.	Name	Emission scenario document (ESD)	Scenarios with (indirect) emissions to water	Emission route	Potentially not continuous	Remarks
			Skin and hand application in hospitals (based on tonnage or on average consumption)	waste water	N	
PT2	Disinfectants and algaecides not intended for direct application to humans or animals	JRC 2011	Industrial and institutional areas	waste water	N	
			Air conditioning	waste water	N	
			Hospital waste			
			Chemical toilets	waste water	N	
		RIVM 2001	Sanitary sector (based on tonnage or on average consumption	waste water	N	
			Room, furniture and objects in the medical sector	waste water	N	
			Instruments in medical sector (endoscopes)	waste water	N/Y	potentially not continuous in case of large replacement interval
			Instruments in medical sector (other instruments)	waste water	N	
			Laundry disinfection	waste water	N	
		OECD 2004/RIVM 2002	Swimming pools	waste water, water	N/Y	potentially not continous in case of draining private pools; relevance not fully clear
PT3	Veterinary hygiene	JRC 2011	Disinfection of animal housings	waste water, slurry, manure	Y	in case of higher tier modelling
			Disinfection of vehicles	waste water	N	
			Teat dips	slurry	Y	id.
			Footwear/animals feet	slurry	Y	id.
			Hatcheries	waste water	N	
PT4	Food and feed area	JRC 2011	Food, drink and milk industry	waste water	N	

PT no.	Name	Emission scenario document (ESD)	Scenarios with (indirect) emissions to water	Emission route	Potentially not continuous	Remarks
			Large scale catering kitchens, canteens., slaughterhouses, etc.	waste water	N	
			Milking parlour systems	waste water	N	
PT5	Drinking water	EUBEES/UBA 2003	Disinfection in distribution system	waste water	N	
Main group 2: Preservatives						
PT6	Preservatives for products during storage	EUBEES RIVM/Haskoning 2004	In-can preservatives; ESD refers to PT8 and 21 for direct emissions to water	waste water, water	N	application phase not continuous, but service life is main driver for risk assessment = continuous
		EUBEES Ineris 2001	Paper coating and finishing PT6, 7 and 9	waste water	N	
PT7	Film preservatives	EUBEES RIVM/Haskoning 2004	Paints and coatings: refers to PT8 for direct emissions to water	waste water, water	N	
		EUBEES Ineris 2001	Paper coating and finishing PT6, 7 and 9	waste water	N	
PT8	Wood preservatives	OECD 2012	industrial use (impregnation and surface treatment) / application	waste water	N	
			industrial use (impregnation and surface treatment) / storage	water via runoff	N	
			in situ application : bridge over pond	water	N	application phase not continuous, but service life is main driver for risk assessment = continuous
			use class 3,1 - external, no ground contact / house	not relevant		
			use class 3,1 - external, no ground contact / noise barrier	waste water	N	
			use class 3,1 - external, no ground contact / bridge over pond	water	N	

PT no.	Name	Emission scenario document (ESD)	Scenarios with (indirect) emissions to water	Emission route	Potentially not continuous	Remarks
			use class 4,1 - external, with ground contact, permanently	not relevant		
			use class 4,2 - external, with water contact, permanently	water	N	
			use class - in seawater, permanently	water	N	
PT9	Fibre, leather, rubber and polymerised materials preservatives	EUBEES Ineris 2001	Leather tanning	waste water	N	
		EUBEES Ineris 2001	Textile processing	waste water	N	
		EUBEES RIVM/Haskoning 2004	Rubber and polimerised materials			
			Rubber	waste water, water	N	
			Plastic	waste water, water	N	
			Textile	waste water, water	Y/N	direct emissions from treated textile to water?
		EUBEES Ineris 2001	Paper coating and finishing PT6, 7 and 9	waste water	N	
PT10	Construction material preservatives	EUBEES Ineris 2002	In-situ treatment (currative) in the city	waste water, water	N	application phase not continuous, but service life is main driver for risk assessment = continuous
			Preservative treatment (in-situ or elsewhere) in the city	waste water, water	N	
PT11	Preservatives for liquid-cooling and processing systems	EUBEES RIVM 2003	Once-through, shock/continuous	water	Y	Only for shock treatment
			Open-recirculating, shcock/continuous	waste water, water	N	
			Closed, shock/continuous	waste water, water	N	
PT12	Slimicides		Paper mill	waste water	N	

PT no.	Name	Emission scenario document (ESD)	Scenarios with (indirect) emissions to water	Emission route	Potentially not continuous	Remarks
		EUBEES RIVM/Haskoning 2003	Offshore oil exploitation (reservoir injection, oil storage systems, etc.)	seawater	N	
			Offshore oil exploitation (workover chemicals, closed drain systems, etc)	seawater	Y	
PT13	Working or cutting fluid preservatives	EUBEES RIVM/Haskoning 2003	Metal working machines	waste water	N	
Main group 3: Pest control						
PT 14	Rodenticides	EUBEES DK EPA 2003	Sewer systems	waste water	N	
			In and around buildings	waste water	N	
PT 15	Avicides	EUBEES 2003	Bait preparation	waste water	N	
			In and around buildings	waste water	N	
PT 16	Molluscicides, vermicides and products to control other invertebrates	No ESD				
PT 17	Piscicides	No ESD				
PT 18	Insecticides, acaricides and products to control other arthropods	OECD 2006	Animal housings and manure storage	waste water, slurry, manure	Y	in case of higher tier modelling
		EUBEES Ineris 2001	Textile processing	waste water	N	
		OECD 2008	Insecticides, acaricides, control arthropods			
			Indoor applications	waste water	N	
			Outdoor applications (urban), rain water	waste water, water	N	
			Outdoor applications rural	not relevant		
			Outdoor application, vector control	water	Y	

PT no.	Name	Emission scenario document (ESD)	Scenarios with (indirect) emissions to water	Emission route	Potentially not continuous	Remarks
			Outdoor application near water pond (biocidal treatment on trees)	water (via drift)	Y	
PT 19	Repellents and attractants	No ESD				
PT 20	Control of other vertebrates	No ESD				
Main group 4: Other biocidal products						
PT 21	Antifouling products	EC 2004	Marina, commercial harbour, shipping lane	water	N	
PT 22	Embalming and taxidermist fluids	EUBEES Ineris 2001	Taxidermy, embalming	waste water	N	

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Appendix 8. Additional guidance from other legislations

In case the guidance provided in this Volume is not sufficient to cover the exposure, effect or risk assessment for a biocidal active substance, e.g. in case of very specific uses or substance properties, the following guidance documents from other legislations could be used as advisory documents:

1. if the chemical is difficult, which implies amongst others hydrophobic, extra guidance is given in OECD aquatic toxicity and difficult substances and mixtures
2. for mixtures, use OECD aquatic toxicity and difficult substances and mixtures
3. Guidance developed within the context of Regulation (EC) No 1907/2006 (REACH)
4. Guidance developed within the context of Directive 91/414/EEC i.e.:

   General guidance for ecotoxicity:

   a. Guidance Document on Aquatic Ecotoxicology under Council Directive 91/414/EEC -
   b. Guidance Document on Terrestrial Ecotoxicology Under Council Directive 91/414/EEC -

   Groundwater modelling guidance documents:

   - FOCUS groundwater scenarios in the EU review of active substances
   - Generic guidance for FOCUS groundwater scenarios

   Assessment of degradation studies

   - Guidance Document on Estimating Persistence and Degradation Kinetics from Environmental Fate Studies on Pesticides in EU Registration

   Risk assessment

   - European Guidance Document on Risk Assessment for Birds and Mammals – working document
   - EPPO Standards - Environmental risk assessment scheme for plant protection products

     Guidance on tiered risk assessment for plant protection products for aquatic organisms in edge-of-field surface waters (EFSA Journal 2013; 11(7):3290)

PART II BIOCIDAL PRODUCTS

5. Introduction to biocidal products

The intention of this document is to provide guidance on how to perform the environmental risk assessment of biocidal products. It should be read in combination with the Guidance on the Biocidal Products Regulation Volume IV Environment - Part B Risk Assessment (active substances).

In accordance with Article 19 of the Regulation (EU) 528/2012 (mentioned in the following as BPR), Member States shall only authorise a biocidal product if it has no unacceptable effect itself, or as a result of its residues, on the environment having particular regard to:

- its fate and distribution in the environment;
- contamination of surface waters (including estuarine and seawater), groundwater and drinking water, air and soil, taking into account locations distant from its use following long-range environmental transportation;
- its impact on non-target organisms;
- its impact on biodiversity and the ecosystem.

In addition, it must not have unacceptable effects on human or animal health through drinking water, food, feed, air, or through other indirect effects. A risk assessment for environmental effects will therefore always be needed before a biocidal product can be authorised.

When assessing the environmental risk of biocidal products, the competent authority must consider the effects arising from the active substance(s) as well as the effects from any substance of concern (including metabolites, and reaction and degradation products where relevant) contained in the product.

Often, biocidal products are multi-component mixtures of one or more active substances and a range of co-formulants that serve different purposes e.g. anti-foaming agents, stabilisers, pigments, emulsifiers, solvents, or diluents. Therefore the overall ecotoxicity of a biocidal product might be significantly different from that of each individual ingredient(s) alone and hence, needs to be assessed during the product authorisation. Article 19(2) of the Biocidal Products Regulation (BPR, 528/2012 EU) states that *"the evaluation […] shall take into account the following factors: […] (d) cumulative effects, (e) synergistic effects."* This is further elaborated in BPR Annex VI (common principles for the evaluation of biocidal products) which states that the risks associated with the relevant individual components of the biocidal product shall be assessed, taking into account any cumulative and synergistic effects.

This guidance aims to provide guidance on how other ingredients should be accounted for during the environmental risk assessment of biocidal products and how mixture effects should be considered when assessing products

This guidance document addresses the identification of SoC in the products, their evaluation and the assessment of the mixture toxicity of products as well as synergistic effects as required by the BPR (and the Biocidal Products Directive (BPD, 98/8/EC) which was replaced in September 2013 by the BPR) by applying a tiered scheme for the consideration of mixture effects during the environmental risk assessment of biocidal products.

In addition the guidance clarifies when new risk assessments have to be performed or the evaluation of the product can rely on the risk assessment presented at the time of active substance evaluation and approval.

For further guidance on the evaluation of microorganisms, refer to the Guidance on Active Micro-organisms and Biocidal Products.

6. Definitions for biocidal products

Representative biocidal product: Biocidal product assessed in the context of active substance approval.

Biocidal product: According to the BPR

Article 3 (1) (a)

any substance or mixture, in the form in which it is supplied to the user, consisting of, containing or generating one or more active substances, with the intention of destroying, deterring, rendering harmless, preventing the action of, or otherwise exerting a controlling effect on, any harmful organism by any means other than mere physical or mechanical action,

any substance or mixture, generated from substances or mixtures which do not themselves fall under the first indent, to be used with the intention of destroying, deterring, rendering harmless, preventing the action of, or otherwise exerting a controlling effect on, any harmful organism by any means other than mere physical or mechanical action.

A treated article that has a primary biocidal function shall be considered a biocidal product.

Substance of concern[34]**:** means any substance, other than the active substance, which has an inherent capacity to cause an adverse effect, immediately or in the more distant future, on humans, in particular vulnerable groups, animals or the environment and is present or is produced in a biocidal product in sufficient concentration to present risks of such an effect.

Mixture toxicity[35]: refers to the combined toxicity and risk to human and animal health, and the environment, from all relevant substances (see **section 10.2.2**) in a biocidal product, including their degradation products and regardless of the underlying mechanism(s) of mixture toxicity (non-interactive or interactive joint action) and taking into account the different environmental, occupational and residential mixture(s) which are formed during all life cycle steps relevant under the BPR.

Synergism/synergistic effects: an effect or toxicity from a chemical mixture which is greater than that expected from non-interactive joint action because one mixture component influences the toxicity of another. The experimentally derived effect of a mixture which is greater than that predicted by concentration addition by a factor of 5 or more should be reviewed and discussed with respect to potential synergistic interactions, as outlined in section 10.2.3[36].

Aggregated effects/exposure[2]**:** refers to the overall exposure to humans and the environment, to the same substance, by emissions during all life cycle steps relevant under the BPR of different products belonging to the same PT or different PTs.

7. Conditions for providing a new risk assessment for the biocidal product

This section aims to clarify in which cases there is a need to perform a (new) risk assessment in the product dossier compared to the evaluation of the respective active substance and its representative biocidal product in the context of the active substance approval.

[34] According to Article 3(f) of the Biocidal Products Regulation (528/2012/EC, BPR)

[35] Document of meeting of representatives of Members States Competent Authorities for the implementation of Directive 98/8/EC concerning the placing of biocidal products on the market (CA-Meeting), CA-July12-Doc.5.2.h

[36] Value derived from the results of several research projects on the mixture toxicity of wood preservative products as a pragmatic proposal [22-24], but might be higher or lower in some cases. If data are indicating synergistic effects, they should be checked carefully regarding the applied methods for the calculation of the prediction of mixture toxicity, the performance of the tests as well as the tested species. Also the criteria given under point 10.2.3 should be taken into consideration to verify synergistic interactions.

- For products consisting of just one active substance mixed with no substances of concern and for which the proposed uses were covered under the evaluation of the representative biocidal product during the active substance evaluation, the assessment of the active substance is sufficient to cover the risks assessment from the product.
- If the uses presented for the biocidal product are different compared to those covered by the representative biocidal product in the assessment report for its active substance(s) or if the concentration of one or multiple active substances in the product is higher compared to the respective assessment report, a risk assessment for each active substance including their metabolites is needed in addition to the assessment of substances of concern and mixture toxicity.
- If new studies with the active substances or the product itself are available triggering changes in the endpoints used for the risk assessment, a new risk assessment is needed.

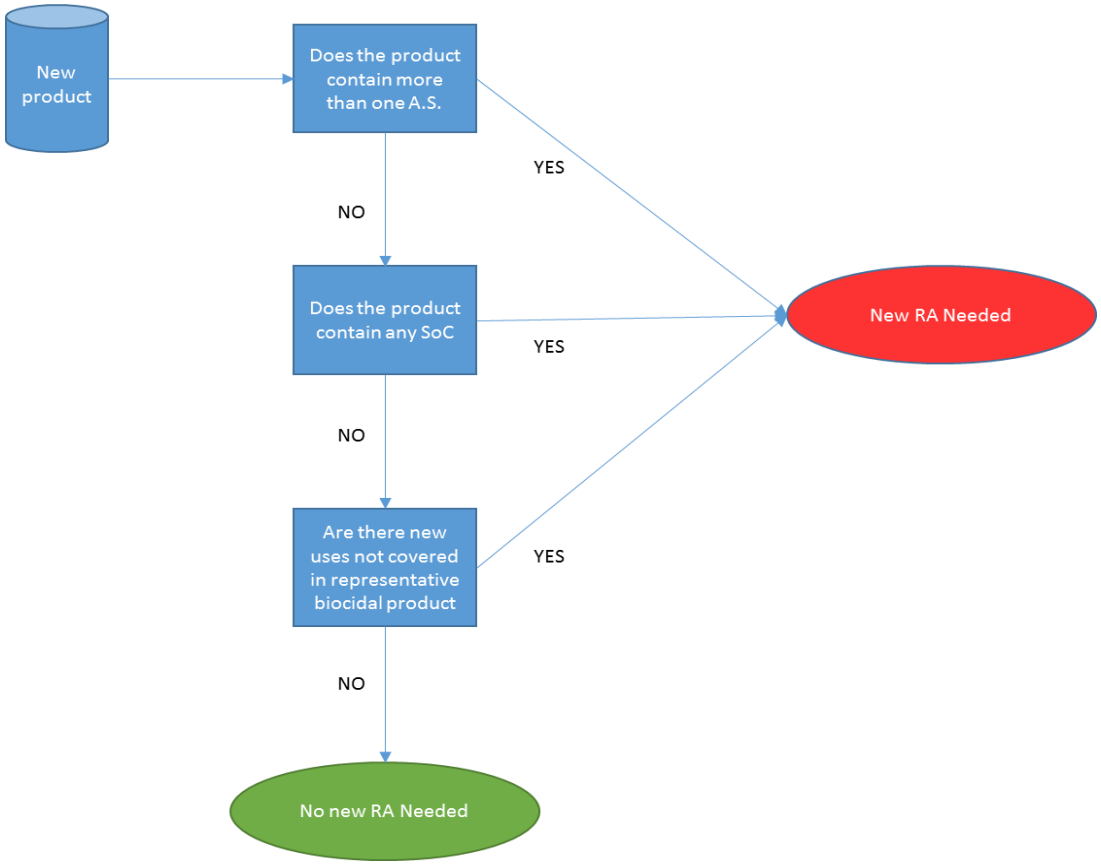

Figure 27: Decision tree for providing risk assessment of a biocidal product in the context of authorisation

Sufficient information on the product and the way it is used has to be submitted by the applicant from which it can be decided whether an exposure of environmental compartments can be expected from the use of the product. Thereby, the procedure is similar to the procedure applied for single substances by taking into account the general principles described in Part I, section 1.1 as well as the related Guidance Documents and Emission Scenario Documents.

If the information provided by the applicant reveals that an exposure of environmental compartments to the products and its components is unlikely, e.g. due to a negligible exposure as the product is only applied in completely closed systems, no environmental risk assessment and consequently no mixture assessment has to be performed. Nevertheless the SoCs would need to be assessed.

The exposure assessment should cover the proposed normal use of the biocidal product, together with realistic worst case scenarios but not releases arising from accidents. Emission scenario documents (ESD) for relevant product-types and/or uses should be followed.

8. Assessment of substances of concern

8.1 Identification of Substances of Concern

Article 3(f) of the BPR specifies that a substance of concern would, unless there are other grounds for concern, normally be:

- a substance classified as dangerous or that meets the criteria to be classified as dangerous according to Directive 67/548/EEC, and that is present in the biocidal product at a concentration leading the product to be regarded as dangerous within the meaning of Articles 5, 6 and 7 of Directive 1999/45/EC, or
- a substance classified as hazardous or that meets the criteria for classification as hazardous according to Regulation (EC) No 1272/2008, and that is present in the biocidal product at a concentration leading the product to be regarded as hazardous within the meaning of that Regulation,
- a substance which meets the criteria for being a persistent organic pollutant (POP) under Regulation (EC) No 850/2004, or which meets the criteria for being persistent, bio-accumulative and toxic (PBT) or very persistent and very bio-accumulative (vPvB) in accordance with Annex XIII to Regulation (EC) No 1907/2006;

That means that a SoC is a co-formulant[37] in a biocidal product which meets at least one of the conditions specified in Article 3(f), i.e. a classified co-formulant present in the biocidal product above the respective specific or generic concentration limit of Directive 1999/45/EC and/or the CLP Regulation and thus, leading to its classification as well as substances meeting the POP, PBT- and vPvB-criteria, respectively

8.1.1 "Other grounds for concern": potential SoCs

However, as it can be seen from Article 3(f), the legal text is vague on what constitutes an SoC on the basis of "other grounds for concern". Therefore, based on the experiences gained during the development of the Transitional Guidance on mixture toxicity assessment for biocidal products for the environment, it is proposed that the following co-formulants present in a biocidal product should be also considered as SoCs in addition to the three cases (three indents) of clearly defined SoCs specified in Article 3(f) (see above):

- Active substances (AS) from other product types (PTs) contained in the product (e.g. in-can preservatives) for which a draft final Competent Authority Report (CAR, with an agreed risk assessment) is available. This criterion identifies other active substances in the biocidal product that act as co-formulants. Those substances should be regarded as SoCs because they potentially affect environmental organisms due to their intrinsic biological activity. They should be considered as SoCs if they are present in the biocidal product at a concentration ≥ 0.1%. This concentration limit is not applicable to PBT- or vPvB- substances and endocrine disrupting chemicals (EDs), as safe concentration limits cannot be derived for those substances. No concentration limit applies to substances that are classified as such. It needs to be checked whether this concentration limit is valid for the respective substance as highly toxic substances may contribute to the overall toxicity of the product even when contained to very small amounts in the product, i.e a co-formulant should be regarded as SoC if the PNEC of the respective substance is lower than the PNEC of the a.s. even though its concentration in the product is below the 0.1% criterion.

[37] Any substance contained in the product other than the active substance declared by the applicant.

However, exemptions are possible under the following condition: the substance is contained in Annex I of the BPR.

- Substances that enhance the effect of the active substance in the product, e.g. synergists. For synergists, information/data shall be provided related to the interaction between the active substance and the synergist, not only for the synergist itself. For such substances, an appropriate evaluation of the risks posed by the active substance in the presence of the synergist rather than an evaluation of the risks posed by the synergist itself should be undertaken. A generic concentration cut-off value for the presence of a synergist in a product, applicable to all synergists cannot be specified. On a case-by-case basis, a synergist should be considered a SoC, if it is present at a concentration that enhances the toxicity of the active substance, as indicated by the available data. Furthermore, the hazard profile, potency and exposure potential of the substance enhancing the effects of the active substance should be taken into account. Further details on the identification of synergists can be found in section 10.2.3. Also diluents, (lipophilic) organic solvents and surfactants like e.g. naptha may influence the toxicity of a mixture by enhancing the bioavailability of the active substance(s) and should therefore be regarded carefully. In principle, all co-formulants need to be checked for a potential influence on the toxicity of the other product components.
- Substances that have been included in the candidate list established in accordance with the REACH Regulation (1907/2006/EC, as amended), Article 57 (f) and 59(1) or fulfil the criteria for inclusion in the candidate list, if not already covered by the criteria of Article 3(f) of the BPR (see above). This criterion will capture, the clearly-defined SoCs specified in Article 3(f) of the BPR as well as endocrine disruptors (EDs) and PBT-substances which are not covered by Article 57 (d-e) of the REACH Regulation.
- Substances which meet two of the criteria for being PBT in accordance with Annex XIII to Regulation (EC) No 1907/2006, as amended.
- Substances for which an Environmental Quality Standard (EQS) has been derived under Directive 2000/60/EC (Water Framework Directive; according to paragraph 67, Annex VI, BPR).

However, exemptions are possible if the substances are contributing only to a very limited extent to the overall toxicity of the mixture (see **section 10.2.2** as well as **Appendix 9**, **Appendix 10** and **Appendix 12**) and are neither EDs nor PBT- or vPvB-substances.

The causes leading to the (non-)classification of a substance as a substance of concern (SoC) need to be documented, i.e. for all substances present in a biocidal product it needs to be checked (and reported) whether they meet one of the criteria described above. It is up to the applicant to provide such an assessment to the evaluating CA.

8.2 Evaluation of identified SoCs and risk assessment

Annex VI of the BPR lays down the common principles for the evaluation of dossiers for biocidal products. The following is stated in Annex VI (BPR) with regard to the evaluation of SoCs contained in biocidal products:

Paragraph 3
In order to ensure a high and harmonised level of protection of human health, animal health and the environment, any risks arising from the use of a biocidal product shall be identified. To achieve this, a risk assessment shall be carried out to determine the acceptability or otherwise of any risks that are identified. This is done by carrying out an assessment of the risks associated with the relevant individual components of the biocidal product, taking into account any cumulative and synergistic effects.

Paragraph 4
A risk assessment on the active substance(s) present in the biocidal product is always required. This risk assessment shall entail hazard identification, and, as appropriate, dose

(concentration) - response (effect) assessment, exposure assessment and risk characterisation. Where a quantitative risk assessment cannot be made, a qualitative assessment shall be produced.

Paragraph 5
*Additional risk assessments shall be carried out in the same manner as described above, on **any substance of concern** present in the biocidal product. Information submitted in the framework of Regulation (EC) No 1907/2006 shall be taken into account where appropriate.*

Paragraph 6
*In order to carry out a risk assessment, data are required. These data are detailed in Annexes II and III and take account of the fact that there are a wide variety of applications as well as different product-types and that this has an impact on the associated risks. The data required shall be the minimum necessary to carry out an appropriate risk assessment. The evaluating body shall take due consideration of the requirements of Articles 6, 21 and 62 in order to avoid duplication of data submissions. Data may also be required on a **substance of concern** present in a biocidal product. For in-situ generated active substances, the risk assessment includes also the possible risks from the precursor(s).*

Paragraph 7
*The results of the risk assessments carried out on the active substance and on the **substances of concern** present in the biocidal product shall be integrated to produce an overall assessment for the biocidal product itself.*

Paragraph 14
*A risk assessment on the active substance present in the biocidal product shall always be carried out. If there are, in addition, **any substances of concern** present in the biocidal product, then a risk assessment shall be carried out for each of these. The risk assessment shall cover the proposed normal use of the biocidal product, together with a realistic worst-case scenario including any relevant production and disposal issue. The assessment shall also take account of how any 'treated articles' treated with or containing the product may be used and disposed of. Active substances that are generated in-situ and the associated precursors shall also be considered.*

Paragraph 15
In carrying out the assessment, the possibility of cumulative or synergistic effects shall also be taken into account. The Agency shall, in collaboration with the Commission, Member States and interested parties, develop and provide further guidance on the scientific definitions and methodologies for the assessment of cumulative and synergistic effects.

Paragraph 16
*For each active substance and **each substance of concern** present in the biocidal product, the risk assessment shall entail hazard identification and the establishment of appropriate reference values for dose or effect concentrations such as NOAEL or Predicted No Effect Concentrations (PNEC), where possible. It shall also include, as appropriate, a dose (concentration) — response (effect) assessment, together with an exposure assessment and a risk characterisation.*

Paragraph 17
*The results arrived at from a comparison of the exposure to the appropriate reference values for each of the active substances and for **any substances of concern** shall be integrated to produce an overall risk assessment for the biocidal product. Where quantitative results are not available the results of the qualitative assessments shall be integrated in a similar manner.*

Effects on the environment

Paragraph 38
*The hazard identification shall address the properties and potential adverse effects of the active substance and **any substances of concern** present in the biocidal product.*

Paragraph 39

*A dose (concentration) — response (effect) assessment shall be carried out in order to predict the concentration below which adverse effects in the environmental compartment of concern are not expected to occur. This shall be carried out for the active substance and for **any substance of concern** present in the biocidal product. This concentration is known as PNEC. However, in some cases, it may not be possible to establish a PNEC and a qualitative estimation of the dose (concentration) — response (effect) then has to be made.*

Paragraph 42
*For each environmental compartment, an exposure assessment shall be carried out in order to predict the likely concentration of each active substance or **substance of concern** present in the biocidal product. This concentration is known as the predicted environmental concentration (PEC). However, in some cases it may not be possible to establish a PEC and a qualitative estimate of exposure then has to be made.*

Paragraph 43
A PEC, or where necessary a qualitative estimate of exposure, need only be determined for the environmental compartments to which emissions, discharges, disposal or distributions (including any relevant contribution from articles treated with biocidal products) are known or are reasonably foreseeable.

Therefore, the BPR requires that a risk assessment is performed for all active substances and SoCs in a biocidal product individually. In addition an assessment of potential cumulative/synergistic effects is required, i.e. also a mixture toxicity assessment (see **section 9**). In doing so, the risk assessment for SoCs should be conducted in the same manner as it is performed for the active substance (see paragraph 5 of Annex VI as cited above). This means, a PEC and a PNEC need to be derived for each SoC for each relevant environmental compartment potentially exposed due to the indented use of the product. However, if a quantitative risk assessment is not possible a semi-quantitative or qualitative assessment can be conducted (see paragraph 4, Annex VI as cited above). This means that, under certain circumstances, it allows applicants to demonstrate that the risk is likely to be acceptable with qualitative arguments or more simplistic calculations (e.g. Tier I exposure assessment). In addition, data waiving is possible for SoCs as it is for active substances.

As stated in Paragraph 6 of Annex VI of the BPR, data are required in order to carry out a risk assessment for AS and SoCs contained in a biocidal product. These data are detailed in Annexes II and III of the BPR and shall be the minimum necessary to carry out an appropriate risk assessment. It needs to be pointed out that it is the responsibility of the applicants to identify SoCs, provide appropriate information/data and perform risk assessments.

As stated above, data for SoCs are only required for the environmental compartments to which emissions, discharges, disposal or distributions are known or likely. It is possible that certain properties of the compound in question mean that the environment is unlikely to be significantly exposed to that substance. In such a situation, qualitative argumentation may be submitted by the Applicant to demonstrate that environmental exposure in a particular compartment would be negligible. Such argumentation should be supported by appropriate data. Examples may include very rapid degradation or dissipation (e.g. by volatilisation and rapid photochemical oxidation in air).

In principle, ecotoxicological fate and behaviour as well as relevant physico-chemical endpoints for SoCs can be derived[38] based on (publicly) available information (e.g. material safety data

[38] For the use of studies that are publicly available the applicable copyright laws should be considered. Further information on issues relating to copyright and the extent of the rights of parties to refer to published data and/or to data whose intellectual property is owned by a third party can be found in the REACH *Guidance on data sharing*, section 3.3.3.8, which applies under the BPR by virtue of the footnote to Article 63(4) of the BPR.

sheets (SDS)[39], EU or international chemical reviews, QSARs, laboratory studies etc.) from which:

1. it can be decided whether a product component has to be regarded as a SoC and
2. a comprehensive risk assessment is possible for the respective SoC.

In case a quantitative risk assessment is not possible, semi-quantitative data may need to be collected. For example: QSAR estimates QSAR-estimates, hazard classification data from classification and labeling according to the CLP Regulation (EC) No 19 1272/2008, data from limit tests or screening studies as well as simple exposure estimates. The Safety Data Sheets (SDSs)[39] for individual co-formulants represent usually the first source of information for the hazard identification on potential SoCs. Information submitted in the framework of the REACH-Regulation (1907/2006/EC) must be taken into account as well, where appropriate. Reference list to be developed.

The decision on which component has to be regarded as a SoC primarily relies on the environmental classification of the component, when available. Therefore emphasis should be put on the selection of the appropriate (i.e. the most reliable) classification: Classification of a substance is either provided by the producer himself (Material Safety Data Sheet), the producer and the authority (via REACH dossier) or the Authority (EU harmonised classification). In case that there are several classifications available the REACH Dossier, Risk Assessment Reports and the harmonised classifications are the preferable sources of substance classification.

In case the data from the SDS[39] are associated with too much uncertainties or the SDS does not contain the required information, useful data can be obtained from a number of specialised databases such as the C&L Inventory, ECHA's dissemination website (database of registered substances under REACH), R4BP 3 (Register for Biocidal Products), Annex VI of the CLP Regulation and cosmetics databases. To identify SoCs, applicants should take into account all available information, including also data in the open, peer reviewed scientific literature and information from predictive approaches such as QSARs (quantitative structure activity relationship available in models like BIOWIN for the estimation of the readily biodegradability and Ecosar for toxicity), read-across from structural analogues and category approaches, etc. cited literature should be provided to the evaluating CAs. The strategy for data search could be based on the information required for the screening criteria for P, vP, B, vB and T as described in Table 11-2 in the PBT assessment guidance from ECHA (*Guidance on Information Requirements and Chemical Safety Assessment Chapter R.11: PBT/vPvB assessment*, Version 2.0 November 2014[40]).

However, it is the applicant's responsibility to make all reasonable efforts to submit the most up-to-date and reliable information and this should be detailed in the submission, along with any letters of access that might be required. It should be noted that wherever data relevant for the assessment are covered by proprietary rights, it is the responsibility of the applicant to obtain the right to use these data and to demonstrate ownership per study.

Only in cases, where sufficient appropriate (ecotoxicological) data cannot be found in the mentioned sources to conduct a comprehensive risk assessment for a SoC, testing of the respective substance should be considered. Thereby, testing should be limited to crucial endpoints and environmental compartments to which emissions, discharges, disposal or distributions are known or reasonably foreseeable. Another option is to directly test the product/environmentally relevant mixture, e.g. in cases where the SoC is not available as pure substance to the applicant (see **section 9.2**).

[39] It is important to note that the validation of data from a SDS is practically impossible. If data from SDS are used for the assessment, this needs to be clearly stated and the uncertainties needs to be addressed. It needs to be checked whether the data from the MSDS can be supported by other kinds of informations (e.g. QSAR estimates, literature data etc.).

[40] This Guidance is currently being updated: [https://echa.europa.eu/guidance-documents/guidance-on-information-requirements-and-chemical-safety-assessment]

9. Generic Options for Mixture Toxicity Assessment

A number of ways to include mixture toxicity in risk assessment have been proposed in literature [1]:

A) Applying a specific mixture assessment factor (MAF): safeguarding against mixture effects by means of a special factor, similar to other uncertainty factors in single substance assessment.
B) Bridging or read-across: drawing conclusions from available data from similar products.
C) Component-based approaches (CBA): calculating the expected joint toxicity from the toxicity data for the individual mixture components by applying corresponding prediction models e.g. Concentration addition (CA) and Independent action (IA).
D) Direct experimental testing of the mixture of concern, i.e. the whole product or the environmentally relevant mixture resulting from the use of the product.

These approaches are more or less suitable for mixture toxicity assessment in a legal context in general and for product risk assessment under the BPR in particular. Using a specific safety factor, e.g. the MAF for mixtures has been dismissed, mainly since it would be difficult to scale such a factor for all different kinds of biocide product types. Bridging is considered as a possible way of building a case but there are clear problems with defining "similar mixtures". Hence, the focus of this guideline is on component-based approaches (CBA) and the direct testing of a chemical mixture.

9.1 Component-based approaches (CBA)

By using mathematical models it is possible to calculate the effect that would presumably be caused by a mixture based on knowledge of the toxicities of the individual mixture components. This is referred to as a component-based approach (in mixture risk assessment). The idea is that by knowing the composition of the mixture under evaluation as well as the hazard profiles for the individual substances of the mixture, it would be possible to predict the effect caused by the mixture without further testing. This is clearly an advantage since it would be impossible to test the vast range of possible mixtures in the environment. Furthermore, the BPR clearly states that unnecessary testing, especially using vertebrate species, should be avoided. A number of methods and models have been suggested in literature for the analysis and assessment of combined effects of substances. However, most of them are based on only two different fundamental concepts for the assessment of the so-called non-interactive joint action (which appears to be the prevalent type of combined effect): Concentration (or Dose) addition (CA) and Independent action (IA), which is sometimes referred to as Response addition (Table 58).

Table 56: The different types of joint action of chemicals and their distinctions

The different types of joint action of chemicals and their distinctions * (after Plackett and Hewlett 1952 [45]; Badot et al 2011 [10])		
Type of combined effect	**Similar joint action**	**Dissimilar joint action**
Non-interactive	Simple similar action Concentration (dose) addition	Simple dissimilar action Independent action, Response addition
Interactive	Complex similar action Synergy, Potentiation (greater than non-interactive effects)	Dependent joint action Antagonism (less than non-interactive effects)

* Interactive joint action denotes the situation where one substance influences the toxicity of another, leading to synergism or antagonism. Such effects cannot be accounted for by CA or IA.

Interactions of components in a mixture can cause either significantly increased (synergistic) or decreased (antagonistic) effects compared with the effects predicted by the reference models (CA, IA, table 58). From the current knowledge such interactions seem to be comparatively rare in general, relatively small and largely confined to mixtures with only few compounds [36]. Furthermore, synergisms are very specific for certain mixtures (compound types, their concentrations and mixture ratios), particular organisms and endpoints. Hence they cannot be incorporated into a general risk assessment scheme, but must be treated on a case-by-case basis. When it comes to pinpointing the causes for synergisms or antagonisms, there are substantial knowledge gaps in the current scientific understanding, e.g. regarding the conditions that might lead to synergistic mixture toxicities or the size that synergisms are likely to be [36] (see **section 10.2.3**).

Both the concepts, CA and IA, build upon mathematical models that can be reasonably transferred to the current understanding of chemical and physiological interactions. In other words, the mathematical models mirror several properties of how chemicals interact with physiological processes. As explained in further detail below, neither concept makes any in-depth assumptions on biology or physiology, nor requires any details on toxicodynamic or toxicokinetic processes. Moreover, for IA, toxicant effects are assumed to be expressed completely independently from each other, which is hardly the case in reality considering that organisms consist of complex interacting subsystems. Taken together, both concepts represent remarkably simple assumptions. Despite this, they have been shown to produce very accurate predictions of mixture toxicity even on higher levels of biological organization such as algal biological communities [3, 6, 7, 9, 15, 16, 29, and 47].

Even though both concepts can be related to toxicological events, they build upon fundamentally different basic principles which sometimes give different results in terms of the predicted effect level. This distinction is clearly important to discuss in the context of risk assessment.

9.1.1 Concentration Addition (CA)

The concept of concentration addition (CA) was first formulated by the German pharmacologist Loewe in 1926 [40].

$$EC_{x,mix} = \left(\sum_{i=1}^{n} \frac{p_i}{EC_{x,i}} \right)^{-1}$$ **Equation 116**

Where *p*i is the proportion of the compound *i* in the considered mixture (ranging between 0 and 1). It is calculated as the concentration of compound *i* in the mixture in relation to the summed concentrations of all compounds that are considered for the mixture assessment. $EC_{x,mix}$ is the concentration of the mixture at a specific effect *x* % for component *i*.

The fraction c/ECx for a compound is termed a "toxic unit" (**Equation 116** below). This represents the concentration of a compound scaled to its potency (e.g. the EC_{50}). The size of the toxic unit can be understood as a measure of how much compound *i* contributes to the mixture effect. A component with a large toxic unit contributes more to the mixture effect than a component with a small toxic unit.

$$TUi = \frac{ci}{ECxi}$$ **Equation 117**

If the sum of toxic units (STU) in a given mixture that provokes x% effect equals 1, the mixture behaves according to CA. Under these circumstances any component in the mixture is replaceable by another compound without changing the overall mixture toxicity, as long as the size of the toxic unit of the replacing compound is equal to the toxic unit of the compound being replaced. This interchangeability is usually interpreted as a combination of two things. First the assumption that the compounds in the mixture do not interact, neither on a physico-

chemical level nor on toxicodynamic or toxicokinetic processes. Secondly, that the compounds have a similar mechanism of action, e.g. by binding to the same receptor site. Inherently, compounds with same mechanism of action would also have an effect on the same endpoint.

9.1.2 Independent action

First described by Bliss in 1939 [13], the concept IA, like CA, assumes that all mixture components have effect on the same integrating endpoint. However, in contrast to CA, IA assumes that the mixture components do not share a common mechanism of action. IA assumes that the components act on different subsystems (e.g. tissues, cells, molecular receptors) of an exposed organism, without any overlap. These affected subsystems must evidently affect the observed endpoint, but independently of each other. Like CA, IA assumes that there are no interactions between the mixture components. The expected mixture effect can thereby be calculated according to the mathematical concept of joint probability of independent events (Equation 117).

$$E(c_{mix}) = 1 - \prod_{i=1}^{n}[1 - E(c_i)]$$ **Equation 118**

According to this equation, n is the number of components, $E(c_i)$ denotes the effect that component i has (on its own, if applied singly) at concentration c, which is the component's concentration in the mixture. This annotation of the IA-equation applies if the effect is scaled 0-1 where 1 means 100 % effect (e.g. 100% mortality). The total concentration of the mixture is called c_{mix}, and $E(c_{mix})$ is thereby the IA-predicted effect of the whole mixture.

In line with what is stated above and the mathematical concept, independent action of the individual compounds in a mixture is commonly interpreted as the compounds having dissimilar mechanisms of action.

9.1.3 Applicability of the models in hazard assessment

Deciding which model would be most accurate in predicting the effect of a given mixture may be difficult and highly dependent on the availability of detailed information on the mechanism of action of the single components. However, such information is rarely at hand, and for most mixtures the very strict requirements of both CA and IA of total similarity or dissimilarity of toxic action is hardly met in reality. It is generally recognized that CA may be used as the default concept of choice for a number of reasons [36]. This discussion is only described very briefly here. A more comprehensive overview can be found in the State of the Art Report on Mixture Toxicity by Kortenkamp and co-workers [36] and the EU-Commission's Expert Panel's opinion on mixture toxicity assessments (SCHER, SCCP, SCENHIR, 2012 [50]).

By comparing predicted mixture toxicity to actual tested mixtures it has been shown that for most tested mixtures, CA predicts higher mixture toxicity than IA, and CA is much less likely to underestimate the effect of a given mixture [1]. For a precautionary predictive risk assessment regime it would not be appropriate to use a concept where there is a potential of underestimating the risk. Furthermore, it could be shown, that CA is also applicable for mixtures composed of strictly dissimilarly acting compounds, especially as the difference of predicted effects between CA and IA are usually small [18], at least when studying integrating endpoints such as mortality. Finally, for pragmatic reasons, CA is much more applicable since it can be used with single datapoints or single substance data, such as EC_{50}- or NOEC-values whereas IA requires more detailed effect information, typically in the low effect range.

As recommended by the EU Commission in 2012 [19] on the basis of numerous scientific reports and opinions (EU Commissions report on the State of the art on mixture toxicity [36], the EU-Commission´s Expert Panel (SCHER, SCCP, SCENHIR, 2012 [50]) as well as several other publications, CA is the preferred concept for estimating mixture toxicity from chemical mixtures, at least in the absence of adequate mode of action information. Moreover, by using CA, the currently available data for active substances can be used without major alterations since EC_{50}- and NOEC- values can be used as input data for the various models building upon

the CA concept (see **section 10.3**) and additional testing is minimized. Furthermore, the CA concept is likely to not underestimate the risk from the evaluated mixture.

9.2 Whole mixture testing

In certain cases, whole mixture testing may be the only viable option (see **sections 10.2.2**, **10.2.3** & **10.3.4**, **Figure 28-Figure 32**). This situation may occur when it is suspected that a component in the mixture acts as a synergist, and may cause an interactive type of joint action for which CA (or IA for that matter) is an invalid assumption (see above, table 58). Whole mixture testing could be used in such situations.

Another cause for choosing to perform whole mixture testing would be that even higher tier effect modeling predicts unacceptable risk (see point 10.3, Figures 28-32). It should be noted, however, that it is stated in the BPR that unnecessary vertebrate testing should be avoided and the employed strategy for refinement of the risk assessment should acknowledge this by choosing invertebrate or algal species to demonstrate the applicability of the concept (and extrapolate to vertebrate/fish). Therefore, testing should always be the last option. If testing is conducted, the most sensitive species as indicated by the single substance data should be tested.

If the whole mixture testing approach is chosen, careful consideration should be taken to determine the most relevant mixture to be tested ("relevant mixture") on a case-by-case basis and it is recommended that the test design is agreed with the Competent Authority before tests are conducted. In some cases, where the environment is directly exposed to the formulated product, testing of the product might be useful. However, in most cases, the environment is exposed to a mixture that is different from the original composition of the product. For a few product types it might be expected, that all components end up in the environment, but in different relative amounts than given in the original product composition. For the vast majority of the product types it can be assumed, that the composition changes radically before release into the environment with regard to both the ratio and the concentration of the mixture components, leading to an environmental mixture which is considerably qualitatively different from the product, for instance after solvents have evaporated. For certain product types, e.g. PT08 (wood preservatives) or 21 (antifoulings), leachate testing might then be indicated and a useful risk assessment option. For other product types it might be adequate to calculate and design a mixture depending on expected environmental fate and behaviour of the various components, before performing whole mixture testing ("surrogate mixture", see **sections 10.2.2** & **10.3.4**).

If the whole mixture testing is performed it should be checked wether the experimentally derived effect of mixture is greater than that predicted by CA by a factor of 5 or more and if this is the case, it should be reviewed and discussed with respect to possible interactions, as outlined in **section 10.2.3**.

10. Tiered Approach for biocidal products

Based on the existing generic options for mixture assessment described in the literature (see above) a tiered approach for the mixture assessment in the environmental risk assessment (ERA) of biocidal products was developed.

This approach accommodates (i) different data situations, acknowledging that the initially available data might be quite different for the various product-types covered by the BPD / BPR, (ii) optimises resource usage, (iii) limits biotesting as far as possible and (iv) ensures adequate protection of the environment. It mainly builds on using component-based approaches (CBAs) based on the concept of Concentration addition (CA) for mixture toxicity prediction, which is either approximated by summing up PEC/PNEC ratios or implemented as sums of Toxic Units (STU). These component-based approaches should be complemented by the direct testing of the product or the ecologically relevant mixture only where essential ("relevant mixture ", see points 10.2.2 & 10.3, Figures 28-32). This is already stressed in the BPR (Annex III), because

it reduces the need for further (vertebrate) testing and also facilitates the re-use of existing data for individual (active) ingredients, a factor likely to be increasingly important in the future as the BPR requests data sharing between applicants. However, the direct testing of the mixture of concern should be regarded as a straight forward approach for the assessment of the mixture toxicity in principle, especially if synergistic interactions are indicated (see **section 9**, & **10.2.3**), although there might be limitations (see **section 10.3.4**). The reason for preferring whole mixture data is that such data capture any interactions that may occur between the mixture components e.g. synergistic effects as well as contributions from compounds that have not been considered in the mixture toxicity predictions or for which ecotoxicity information is lacking (e.g. formulation additives, see **section 9.2**). If such data are available and sufficient for a comprehensive risk assessment, the ERA will be based on the mixture as whole, comparable to the ERA for single substances (see **section 10.3**, **Figure 28**).

In the following the terms "mixture" and "relevant mixture" are used for the product itself and the ecologically relevant mixture, respectively.

The competing concept of Independent action (IA) was assessed as not being suitable for incorporation into a tiered approach without explicit confirmatory studies, as it might otherwise lead to an underestimation of the actual environmental risk, especially when assessing mixtures with components present below effect levels. In addition, IA would lead to higher data demands compared to CA. However, if the applicant can prove that IA adequately describes the toxicity of a given product by submitting appropriate data, e.g. information about the MoAs and the concentration-response relationships of the mixture components, these data should be taken into account for mixture toxicity assessment and assessed according to expert judgment.

10.1 Requested input data for a component-based approach

The minimum requested set of data for a component-based assessment consists of (i) reliable and complete information on the product composition, (ii) basic data[41] for all ingredients on which it can be decided whether a substance has to be regarded as a SoC or relevant for mixture assessment (see **section 8**) as well as (iii) at least the PEC/PNEC ratios for the compounds identified as relevant for mixture assessment and (iv) information on the occurrence of synergistic interactions between the product components (see section 10.2.3).

In the following the consecutive tiers of the approach are described, which are also depicted in decision trees in Figures 28-32 for a better traceability. Case studies applying the tiered approach on products from different product-types (PTs) can be found in **Appendix 12**.

10.2 Screening Step

10.2.1 Identification of the concerned environmental compartments

Sufficient appropriate data have to be submitted from which it can be decided whether an exposure of environmental compartments can be expected from the application of the product and if so, which environmental compartments are likely to be at risk. Thereby, the procedure is similar to the procedure applied for single substances by taking into account the general

[41] Ecotoxicological-, Fate and Behaviour- as well as relevant physico-chemical end-points should be derived for the product components based on available information (e.g. laboratory studies, material safety data sheets, EU or International chemical reviews, QSARs. etc). All reasonable efforts should be made to submit the most up to date and reliable information and this should be detailed in the submission, along with any letters of access that may be required. As only semi-quantitative data are needed for this purpose, e.g. QSAR-estimates, hazard classification data from classification and labeling according to the CLP Regulation (EC) No 1272/2008, censored toxicity data (e.g. from limit tests) or simple exposure estimates should be sufficient in the first step.

principles described in the Technical Guidance Document [28) and the Technical Notes for Guidance on Product Evaluation [27] as well as the related Guidance Documents and Emission Scenario Documents.

If the data provided reveal that an exposure of environmental compartments to the products and its components is unlikely, e.g. due to a negligible exposure as the product is only applied in completely closed systems, no ERA and consequently no mixture assessment has to be performed.

In case an exposure of the environment due to the application of the product is possible, it has to be checked whether there is a direct release of the product or a release of a modified mixture into environment and if so, which components are likely to be released. Also the physico-chemical properties of the product components influencing the environmental fate have to be evaluated. It is possible that for some of the mixture components the intrinsic substance properties indicate that the environment is unlikely to be significantly exposed to these substances. In such a situation qualitative argumentation may be submitted to demonstrate that environmental exposure in a particular compartment would be negligible. Such argumentation should be supported by appropriate data. Examples may include very rapid degradation or dissipation (e.g. by volatilisation and rapid photochemical oxidation in air, see also **section 10.2.2** and **Appendix 9**).

A definition of a time-scale for indirect releases is only possible on a case-by-case basis and should be discussed in relation with the respective Emission Scenario Document (ESD) as this information is highly dependent on the actual use of the biocidal product.

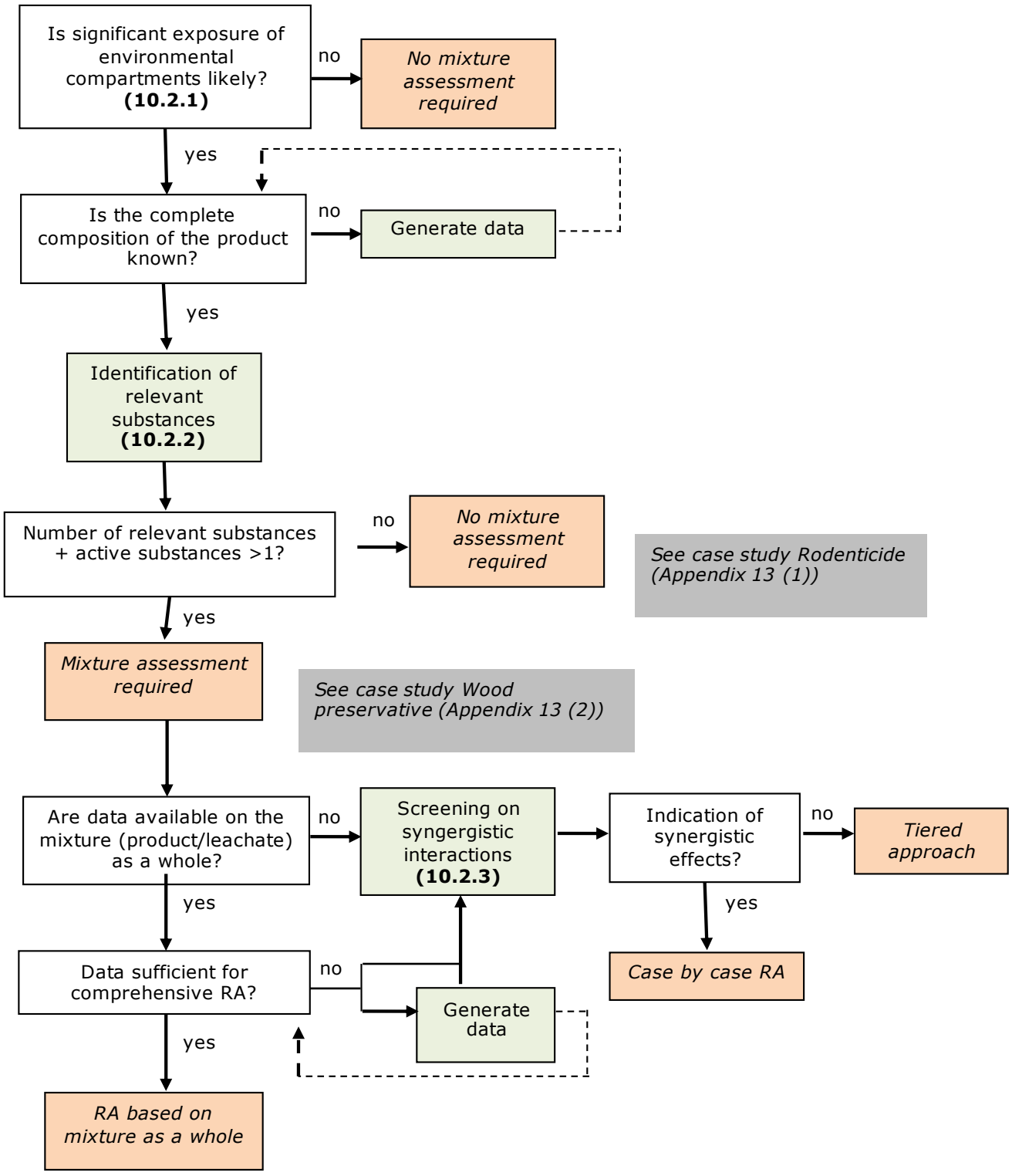

Figure 28: Decision tree for the Screening Step (point 3.2, RA = risk assessment).

If this procedure reveals that an exposure of environmental compartments is likely due to the application of the product, it has to be checked, in the next steps, whether a mixture assessment is required for the product. For this purpose the complete composition of the product will be required (see sections 10.1 and 10.2.2).

10.2.2 Identification of substances relevant for mixture assessment

The default approach is that all ingredients originally present in the biocidal product are considered as a priori relevant for a mixture risk assessment. Qualitative or quantitative argumentation taking into account, e.g., the composition of the mixture to which the environment is exposed, or expected relative contribution to an additive mixture effect, may be employed to demonstrate that some ingredients can be safely disregarded whilst still allowing an adequate assessment of the risk of the mixture. Further guidance on this is given below.

Any component based approach requires that all "relevant" components of a mixture are included in the assessment, i.e. biologically active chemicals that are present at sufficiently high concentrations and are contributing to the overall toxicity of the respective mixture [1]. Obviously, if relevant compounds besides the active substance(s) are not considered in a component-based mixture toxicity assessment, the calculated risk will be an underestimation of the actual risk of the biocidal product. It is, however, impossible to provide a general estimate of the magnitude of such an underestimation, as this depends on the concentration and toxicity of the compounds that are not included in the assessment. Therefore, special care has to be taken to ensure that all relevant ingredients are included in a component-based assessment of a biocidal product.

If there is no confidence that all relevant substances are included in the assessment or if no (ecotoxicological) information is at hand for some of the ingredients, the only effect assessment options are either the direct biotesting of the substances, for which no information is available or the direct biotesting of the biocidal product and/or the resulting environmental mixture, respectively. The direct testing of the "relevant mixture" should be regarded as a straight forward approach for the assessment of the product toxicity in principle, especially in cases where synergistic interactions are indicated (see sections 10.2.3, 10.3.4).

Likewise, in case of testing a "surrogate mixture", i.e. a mixture supposed to represent the product because it is impossible to test the product as it is (see above & section 10.3.4), it has to be ensured that all relevant substances are included in this mixture.

What are 'Relevant Substances' in a typical biocidal product?

The following substances are regarded as relevant for mixture assessment:

1) Active substances.
2) Substances of concern (SoC), see section 8 of this guidance)

It has to be emphasised again, that special care has to be taken to ensure that all relevant substances are included in a component-based assessment of a biocidal product, because otherwise the risk for environment resulting from the application of the product may be underestimated. If no or insufficient (ecotoxicological) information is at hand for all ingredients to decide whether a substance is relevant for mixture assessment, the only effect assessment option is the direct biotesting either of the respective substance(s) or of the biocidal product and the resulting environmental mixture, respectively. If a mixture cannot be assessed in its entirety, because of e.g. insoluble pigments or other ingredients making a direct testing of the product unfeasible, it is also possible to assess generic mixtures of the relevant substances („surrogate mixture", see above & section 10.3.4). If the assessment reveals, that there are several relevant substances (>1) contained in the product, a mixture assessment is required for the respective product under consideration. It has to be checked then, whether mixture data, i.e. product tests or leachate toxicity tests, are already available and whether these data are sufficient for a comprehensive environmental risk assessment (ERA). If such data are at hand and are sufficient for a comprehensive ERA, the risk assessment (RA) will be based on the mixture data as a whole, comparable to the ERA for single substances (see section 10.3.4).

If the available mixture data are not sufficient for RA, there are several options to continue: The first option is to provide the missing data for the RA, whereas the second option is to proceed with the tiered approach. If it can be concluded from the available mixture data, that no synergistic interactions are likely to occur between the product components, it can be

proceeded as described under point 6.3. If this conclusion is not possible, it is recommended to continue with the next step of the tiered approach. It is also recommended to continue with the next step of the tiered approach if mixture data are lacking (see section 10.2.3).

10.2.3 Screen on synergistic interactions

Synergistic interactions describe the combined effect of two or more substances as stronger than expected from non-interactive joint action because the mixture components are influencing each other's toxicity (see section 9.1). The interactions may vary according to the relative concentration level and the biological targets as well as the route(s), timing and duration of exposure (including the biological persistence of the mixture components). Several different types of interactions are described in literature [20, 31, 50, 55]:

- Chemical-chemical interactions: chemicals are reacting together directly to form another compound or a complex which is more toxic (or less toxic) than the parent compounds or enhances (or weakens) their toxicity
- Toxicokinetic interactions: chemicals modifying the absorption, distribution or elimination of others or chemicals competing for active transport mechanisms (uptake, clearance) leading to an increase (or decrease) in the internal dose of a compound compared to the level that occur if no interactions occurred.
- Metabolic interactions: chemicals modifying the metabolism of other mixture components due to e.g. enzyme induction, enzyme inhibition or saturation of an enzyme by the presence of other substrates.
- Toxicodynamic interactions: interactions between the biological responses resulting from exposure to the individual chemicals, e.g. resulting from similar targets (e.g. ligand-receptor interaction).

Concentration addition (CA), as well as Independent action (IA), is based on the assumption that the compounds in a mixture do not interact, neither chemically nor in their toxicokinetic / toxicodynamic phases (see section 9.1, ref. 1, 2, 4, 55). Although cases where the observed mixture toxicity deviated significantly from the expected additivity, indicating synergisms, are comparatively rare in general and for biocides in particular [1, 4] , several examples can be found in the literature (see **Appendix 3**). In this context it has to be distinguished between intended synergisms, i.e. the intended use of synergists (e.g. PBO) in products to enhance the efficacy of the a.s. in the target-organisms, and un-indented synergistic interactions between the product components. In both cases a careful evaluation of the available data is indispensable for the risk assessment process (see below).

Synergism is mainly reported for mixtures with a few (usually two) compounds, which is exactly the situation that is relevant for many biocidal product, which contain typically two or more active ingredients. For biocides they are mainly described for antifouling substances (e.g. 37, 60) and essential oils in combination with pyrethrins and other insecticides (e.g. 33, 48, 56) as well as for ergosterolbiosynthesis-inhibting (EBI) fungicides in combination with pyrethroid insecticides, organophosphates or neonicotinoids (17, 43, 51, 55, see also **Appendix 11**). For example, the combination of zinc-pyrithione and copper shows a clearly higher toxicity than predicted by CA in a range of bioassays such as diatoms, worms or amphipods, partially due to the formation of copper-pyrithione by trans-chelation of zinc-pyrithione with copper [11, 37]. Mixtures of organophosphates and carbamates (insecticides) were consistently more toxic to fish than predicted by CA, despite their similar mechanisms of action [39]. This is most likely caused by the inhibition of organophosphate biotransformation to their inactive dicarboxylic acid derivates by carbamates. Further examples can be found in **Appendix 11**.

Synergism is, besides other factors, highly dependent on: (i) the ratio and (ii) the concentrations of the mixture components, (iii) the presence of other chemicals, (iv) the species in which synergism is to be expected as well as (v) the mode of action of the substances [34, 38, 39, 58], these factors should be taken into account when deciding whether

synergism is relevant for a product under consideration. Furthermore, it should be taken into account whether there are direct emissions to water and soil or whether a modified mixture is introduced into the environment. For additional effective substances such as synergists in a product formulation, independent sources of information, e.g. from the intentional use aspects would need to be considered.

It is therefore proposed that sufficient and reliable data has to be submitted from which it can be decided whether synergistic interactions are unlikely to occur between the product components. The following aspects should be considered within the decision-making process:

- Are known or indented synergists or components declared as synergists present in the product?
- Are substances present in the product which are contained in one of the tables in **Appendix 11**? For the substances in the tables in **Appendix 11** potential synergistic effects are reported in the peer-reviewed literature. These publications should be seen as indications for possible synergisms of the shown substances and be taken into account during the decision making process. However, they should be analysed in more detail for this purpose, e.g. regarding the additive effects analysed in the study, the tested concentrations, mixture ratios and the concentration-dependence of interaction as well as the tested organisms and endpoints.
- Are synergisms known or reported elsewhere in literature for one of the product components? If so, for which group of organisms, endpoints and concentrations (incl. number and ratios) are synergistic effects reported? Which conclusions can be drawn from these data for the product under consideration? Are the deviations from CA covered by the AF applied on the single substance data or are the data sufficient to derive an additional assessment factor to cover the observed synergistic interactions as suggested by [17], [20] and [55]? For which compartments are the synergistic effects reported? Are these likely to be at risk due to the application of the product?
- Are there any structural similarities for one or more of the product components with known synergists ("structural alerts" e.g. methylenedioxyphenyl group, piperamides, furanocoumarins, [12, 42, 48])?
- Can one or more product components significantly enhance the uptake of other components [50]?
- Can one or more product component inhibit significantly the excretion/clearance of other components [50]?
- Do one or more of the product components exert their toxic action via the formation of an active metabolite(s) and may one or more of the components induce the metabolising enzymes that may be involved in the formation of these active metabolites [50]?
- Can two or more product components act on different enzymes in an important metabolic pathway [50]?
- Can two or more product components act on different elements of cellular protection mechanisms or cellular repair mechanism [50]?

The assessment of the possible interaction requires expert judgement and hence needs to be considered on a case-by-case basis in a weight-of-evidence approach. If there are any indications of synergistic effects, which cannot be explained by the available data or are not manageable by e.g. additional safety factors, the only option is the direct testing of the product or of the ecologically relevant mixture for a comprehensive environmental risk assessment as synergisms are not predictable with the available methods in a systematic fashion, especially under the data situation given for biocidal products and their components [1, 2, 20, 21, 55].

If there are no indications for synergistic effects, it is recommended to proceed with the next step of the tiered approach (see section 10.3).

10.3 Tiered assessment scheme

In the following, the consecutive tiers of the tiered assessment scheme are described, which are also depicted in decision trees in Figures 1-5 for a better traceability. Case studies applying the tiered approach on products from different product types (PTs) can be found in **Appendix 12**. The assessment scheme is based on a series of four tiers that begins with simple and conservative screening steps and moves to higher tiers as necessary (Figure 29):

- Tier 1: PEC/PNEC-Summation,
- Tier 2: Modified Toxic Unit Summation (TUS)separated for trophic levels,
- Tier 3: StandardToxic Unit Summation (TUS) separated for trophic levels,
- Tier 4: Experimental testing.

Each of the higher tiers involves a less conservative and more accurate assessment than the previous tiers but requires also more resources, including additional exposure and toxicity data. Two different approaches for the Toxic unit summation are proposed to acknowledge the fact, that not for all relevant substances of a biocidal product homogenous data sets are available.

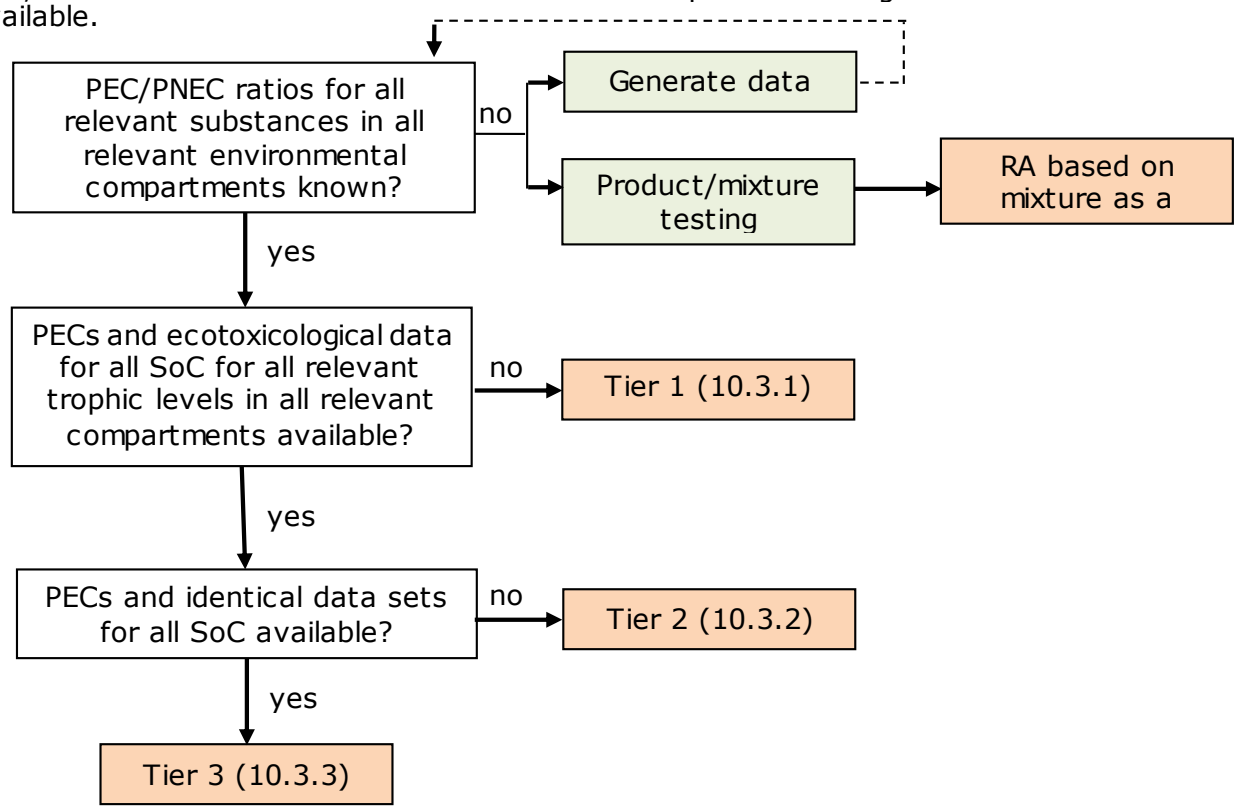

Figure 29: Decision tree for the tiered approach (point 3.3, PEC = Predicted Environmental Concentration, PNEC = Predicted No Effect Concentration, RA = risk assessment).

The tiers must not be performed step by step for a respective product, e.g. in case the data for tier 3 are available in the beginning, the assessment can be started with tier 3 (see Figure 29). Dependent on the data availability for all of the product components which were identified as relevant substances in the previous steps (see section 10.2.2) it should be proceeded with the different tiers of the assessment scheme: If at least the PEC/PNEC-ratios are available for all relevant substances for all relevant compartments and scenarios it is recommended to start with tier 1. If ecotoxicological data and PEC-values are available for all relevant substances for all relevant trophic levels for all relevant compartments and for all relevant scenarios it is recommended to start with tier 2. In case identical ecotoxicological data sets are available for all relevant substances for all relevant species and all relevant compartments, it is recommended to start with tier 3 (see Figure 29).

As outlined above, the tiered approach is based on the concept of Concentration addition (CA, point 2). For the practical application of CA in a regulatory context, a number of different approaches have been suggested in the literature [1]. For pragmatic reasons, these CA-based regulatory approaches usually include simplifying or additional assumptions, and hence they deviate more or less from the principal assumptions that are inherent to the original concept of CA. As a result, such CA-based approaches may differ with regard to both the suitability for specific assessment purposes and the quantitative mixture toxicity estimates that are derived from their application. Several types of pragmatic deviations or simplifications are at hand, for which four are relevant for the use of CA-based approach in biocidal products authorisation:

- No strictly identical (eco-)toxicological endpoint (selection of test species, exposure conditions, exact testing criteria and methodology) for all relevant substances,
- Use of NOEC- instead of EC_x-values,
- Assessment factors included in the single substance toxicity data (e.g. PNEC),
- Assumption of parallel concentration response curves for all mixture components.

As input data, the original concept of CA requires effect concentrations that refer to the same biological effect in the same species under identical test conditions. For the regulatory use as developed here, however, pragmatic simplifications and assumptions are unavoidable. This refers to the merging of data for different test conditions, endpoints and species and to the use of NOEC values as surrogate for quantitative estimates of low effect concentrations. In any case, the potential additional errors that may be introduced by such deviations from the original concept should be made transparent and where possible, should be removed in a stepwise manner [1].

10.3.1 Tier 1

If the PEC/PNEC ratios are available for all relevant ingredients, the risk quotient of the product can be simply estimated by their sum:

$$RQ_{\text{Product}} = \sum_{i=1}^{n} \left(\frac{PEC}{PNEC} \right)_i \qquad \textbf{Equation 119}$$

Summing up PEC/PNECs is mentioned in the Technical Notes for Guidance as one option for biocidal product assessment (ECB, 2002 [27]). However, it should be pointed out that **Equation 118** is fundamentally different from the concept of Concentration addition (CA), as the PNECs from the various compounds might be based on data from completely different endpoints and species. Hence Equation 118 violates one of the fundamental assumptions of CA, that all individual toxicity data refer to same biological endpoint and organism. Consequently, the use of PEC/PNEC sums derived from a set of different species and endpoints are only recommended for first-tier CA assessment in the opinion on mixture toxicity assessment as put forward by the EU scientific committees [50]. It can be proven that Equation 118 provides a conservative approximation of CA [4]. Furthermore, it is a major

advantage of the PEC/PNEC sum (Equation 118) that it can be applied even if different amounts of data are available for the different compounds in the product, for example when an extended data set including chronic ecotoxicity data is at hand for the active ingredient, but only base-set data are available for the other substances of concern. For a more detailed discussion on the use of PEC/PNEC sums see [4].
Should Equation 118 indicate reasons for concern ($RQ_{Product}$ >1), the following options exist:

(i) a refinement of the PEC- and/or PNEC-values by providing additional information on the exposure and/or hazard characterisation of the compounds, especially those that dominate the sum of PEC/PNECs,

(ii) continue with tier 2 , i.e. the application of CA in the form of a modified Toxic Unit Summation for each trophic level separately if homogenous data sets for the relevant substances are notavailable,

(iii) continue with tier 3, i.e. the application of CA in the form of the standard Toxic Unit Summation for each trophic level separately(in cases where homogenous data sets are available for all relevant substances),

(iv) direct testing of the mixture of concern (tier 4),

(v) the definition of effective Risk Mitigation Measures (RMM).

If the aforementioned options are not applicable the only remaining option is the non-authorisation of the product (Figure 30).

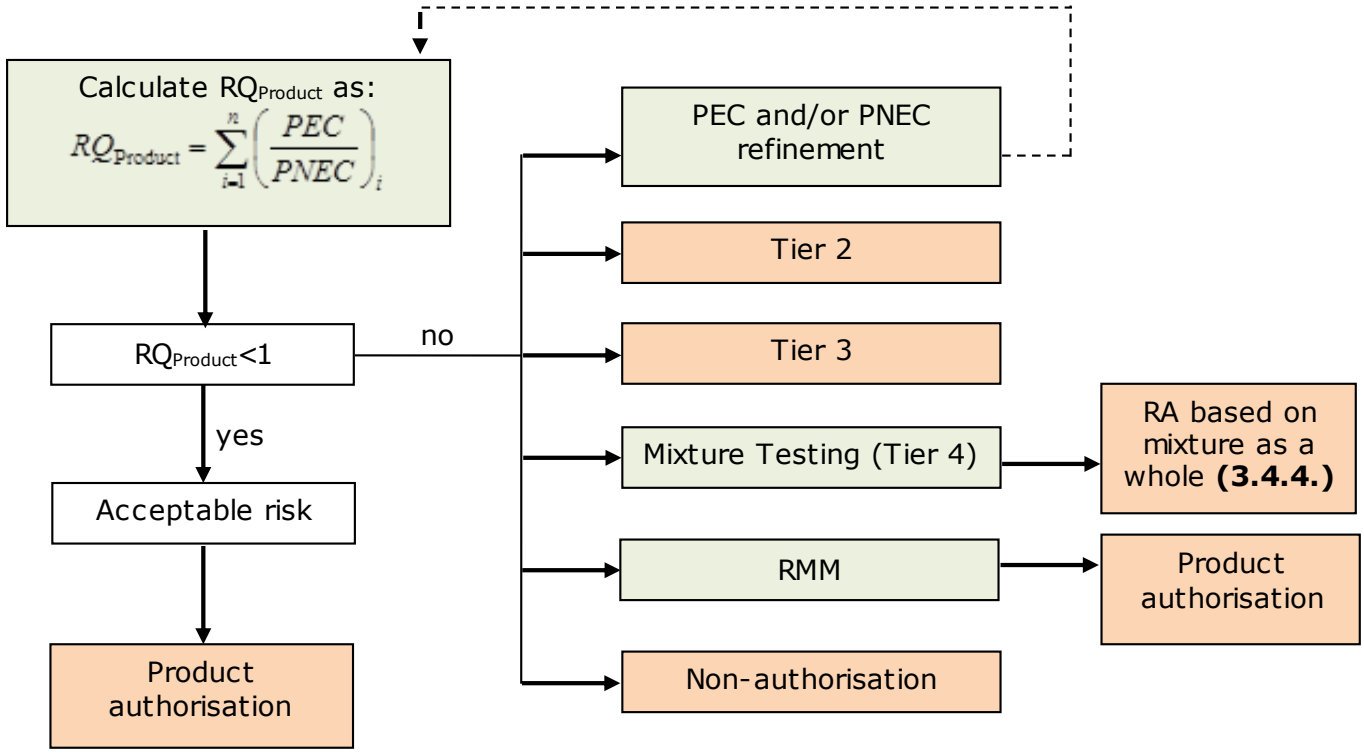

Figure 30: Decision tree for tier 1 (PEC/PNEC-Summation, point 3.3.1, PEC = Predicted Environmental Concentration, PNEC = Predicted No Effect Concentration, RA = risk assessment, RMM= Risk Mitigation Measures, $RQ_{Product}$ = Risk Quotient of the Product).

The refinement in tier 2 and tier 3 consists of looking separately at the combined risk from all relevant substances towards each separate trophic level, by calculating the Sum of Toxic Units (STU) for each trophic level. Two approaches are presented: First, a modified Toxic Unit Summation (TUS) which can take into account varying data sets for the relevant substances (tier 2) and secondly, the standard TUS as described by Backhaus and Faust [4] for cases

where homogeneous data sets are available for all relevant substances.

10.3.2 Tier 2

If ecotoxicological data and PEC-values are available for all relevant substances for all relevant trophic levels in all relevant compartments and for all relevant exposure scenarios, but the amount of available data varies from substance to substance, the risk quotient of the product can be calculated by applying the following equation:

$$RQ_{\text{Product}} = \max \sum_{i=1}^{n} \left(\frac{PEC}{ECx / AF} \right)_i$$ **Equation 120**

where EC_x[42] is the effect concentration that affects x% of the exposed organisms and is calculated for each trophic level and each relevant substance, separately. The AF is the same Assessment factor used for calculating the PNEC of the respective substance (see tier 1). This means that for each substance, the same AF is used consistently.In this tier the trophic levels of the respective compartment are assessed separately, e.g. separate risk-ratios are calculated for all relevant substances for algae, dahnids and fish. In this approach it is preferred to compare the same types of endpoints, e.g. chronic effects for same trophic level. However, if chronic data are not available for all substances acute effects can be included in the calculation as well. This method is a more realistic approach than tier 1, as it combines effects for each trophic level; however it requires several more data and calculations. The difference to tier 3 is that the same data sets for all relevant substances might not be available and hence, it would not make sense to use a common AF for all relevant substances as used in Equation 120. The modified toxic unit equation (Equation 119) should be used with caution. It gives the opportunity to include different types of effect values and AFs, which in itself is a violation of the CA assumption of similar endpoints. For each substance, the AF used to derive the substance PNEC is used to calculate the RQ for the different trophic levels, regardless of whether the effect concentrations are similar to that used for the PNEC derivation of the substance. For example, if the PNEC for substance X is based on a fish NOEC and an AF 100, and you only have an EC_{50} for e.g. algae, the AF used to calculate the contribution of substance X's toxicity towards algae would also be 100. Since you cannot know whether the chronic toxicity towards algae would be higher than towards fish, this represents some uncertainty. On the other hand, if the data set had contained chronic data for both fish and algae, the overall AF would be lower (less conservative). Furthermore, if a higher AF is used on those endpoints that are acute, regardless of the AF used for the PNEC derivation of the substance, the basis for tiers 1 and 2 are no longer the same and hence tier 2 might not represent a meaningful refinement.

If there are acute endpoint values with low AFs in the equation, the uncertainty they bring to the resulting $RQ_{Product}$ should be considered. If an RQ for a trophic level is close to 1 and a low acute endpoint value with a low AF is included in the STU for that trophic level, the uncertainty might be too high and extra justification or a higher tier might be warranted.

It is recommended to use tier 2 in cases where identical data sets are not available for all relevant substances and hence a standard toxic unit summation (TUS, tier 3) is not possible, because a common overall AF (the prerequisite of the TUS) cannot be applied. Tier 2 is similar to the Standard TUS regarding separate evaluation of each trophic level and the use of the RQ for the trophic level which is most at risk (the highest RQ). The only difference between the two tiers is that tier 2 gives the opportunity to use different AFs for each relevant substance (Equation 119). If identical data sets are available for all relevant substances and hence a common AF can be used, the two tiers give the exact same result. An example of the application of Equation 119 can be found in **Appendix 12**.

Therefore, going from tier 2 to tier 3 is only a refinement option, when additional data are

[42] lowest EC_{50}-, LC_{50}- or NOEC values for the same endpoint and *preferably* (not necessarily) the same exposure setting and the same species.

provided for the relevant substances for which less data are available. Tier 2 is applied in the first place, when identical data sets are not available for all relevant substances and the TUS-approach is not possible as no common AF can be used. To do a Standard TUS with substances with dissimilar data sets, it would be necessary to disregard some of the data and only use what is common for all substances, e.g. acute data. If chronic data for some substances are disregarded and only acute data with a common AF of 1000 are used (i.e. it is pretended that for some substances the data sets are smaller than they actually are), it is likely to end up with higher RQ's and a more conservative result than in tier 1. Hence, tier 3 would not be a refinement if applied to these unbalanced data. This is the reasoning behind proposing tier 2, i.e. a modified toxic unit approach, where it is possible to take into account the differing data sets and AFs for the different substances. In case identical data sets are available, the tier 2 calculations would be identical to the tier 3 (TUS) calculations.

If in Tier 2 (Equation 119) the criterion for an acceptable risk for the environment is still not met, i.e. $RQ_{Product} > 1$, the following options exist:

(i) a refinement of the PEC- and/or EC_x-values by providing additional information on the exposure and/or hazard characterisation of the compounds,
(ii) the application of CA in the form of the standard toxic unit summation (TUS) for each trophic level separately (tier 3). In cases where homogenous data sets are already available for all relevant substances, it is recommened to start the assessment directly with tier 3 (see above & **Figure 29**).
(iii) direct testing of the mixture of concern (tier 4), or
(iv) the definition of effective Risk Mitigation Measures (RMM).

If the aforementioned options are not applicable the only remaining option is the non-authorisation of the product (Figure 31).

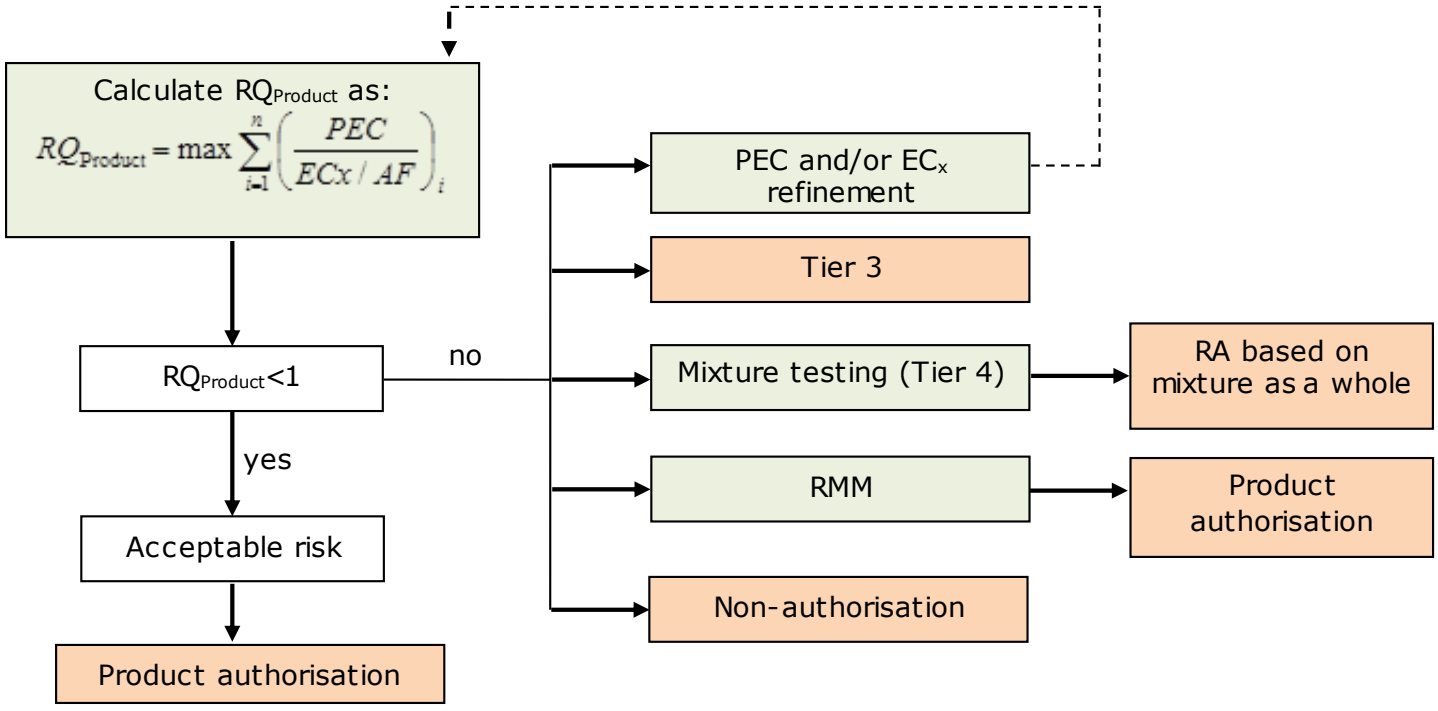

Figure 31: Decision tree for tier 2 (Modified Toxic Unit Summation, point 3.3.2, AF = Assessment Factor, EC_x = Effect Concentration that provokes an x%-effect in the exposed organisms, PEC = Predicted Environmental Concentration, RA = risk assessment, RMM= Risk Mitigation Measures, $RQ_{Product}$ = Risk Quotient of the Product).

10.3.3 Tier 3

In case identical ecotoxicological data sets are available for all relevant substances for all relevant species and all relevant compartments, the risk quotient for the product can be assessed by calculating the sum of Toxic units (STU) for each trophic level / group of organisms and every of *m* ecotoxicological endpoints (e.g. daphnia immobility, fish mortality, algae growth) separately for every component *i* of the mixture:

$$RQ_{Product} = \max(STU_{endpoint1}, STU_{endpoint2}, ..., STU_{endpointm}) \times AF$$

$$RQ_{Product} = \max\left(\sum_{i=1}^{n} \frac{PEC_i}{ECx}_{i,j}, \sum_{i=1}^{n} \frac{PEC_i}{ECx}_{i,j}, ..., \sum_{i=1}^{n} \frac{PEC_i}{ECx}_{i,m}\right) \times AF \quad \textbf{Equation 121}$$

AF denotes the resulting assessment factor, as used for calculating the PNEC of the respective substance (see tier 1). PEC/EC_x is a toxic unit.

Of the calculated STU, one for each endpoint, the highest is used for calculating the risk quotient. The assessment factor is selected depending on the amount of available data according to the rules set up in the Biocidal Products Regulation Volume IV Environment - Part B Risk Assessment Part I Active substances.

Equation 120 is only a rearrangement of Equation 119, in that the AF is placed outside the brackets, allowing same AFs to be used for each involved substance. If a common AF is used for all substances, the equations 119 and 120 give identical results. In equation 120 the maximum STU is calculated first (toxic unit = PEC/EC_x) before it is multiplied by an AF. In Equation 119, these two steps are combined.

The Standard Toxic Unit Summation (TUS) is a more strict application of CA, than PEC/PNEC summation (Tier 1) and the Modified TUS (tier 2), and requires that same species and endpoint are used for the different mixture components. For example: daphnia acute test data are combined with other daphnia acute test data and fish reproduction data with fish reproduction data etc. This leads to a calculated risk quotient for a given environmental compartment that is based on the most sensitive organism group for the evaluated mixture. A prerequisite for using the standard toxic unit summation (TUS) is that the ecotoxicological dataset for the evaluated mixture is balanced for all relevant substances, i.e. data from a specific endpoint can only be used if there are data for the same endpoint for all relevant substances. For example, the availability of only the base set of acute toxicity for all substances would enable a common AF on the effect concentrations. Likewise, similar chronic data for all relevant substances would allow using a reduced AF.

If there are chronic data available for some substances, but not for others, the dataset would be unbalanced and those data could not be used since that would violate the assumption of similar endpoints. In that case, the extra chronic data would have to be disregarded and only the common acute data could be used. The problem in this case is that in tier 1 (PEC/PNEC summation), imbalanced data sets are not an issue as the PNECs can be derived using different AFs. To disregard chronic data and hence use a higher AF for a substance in tier 3 than in tier 1 could in some cases be more conservative, and it can result in an RQ in tier 3 which is higher than in tier 1. Therefore, a modified toxic unit summation approach could be considered for cases with unbalanced data sets (tier 2, see above), or further data have to be provided for the relevant substances for which less data are available

The maximum STU indicates which endpoint for which species is expected to be most sensitive to the biocidal product in question and is hence used for the final assessment, i.e. by applying the corresponding AF the RQ for the product is calculated.

It can be proven that the risk quotient that results from summing up PEC/PNECs (Equation. 118) is always equal or higher than the maximum STU according to Equation 120, provided that the same data is used as a basis for the PEC/PNEC summation and Toxic unit summation.

Their precise relationship depends on the ecotoxicological profiles of the compounds in the mixture. In case of dissimilar profiles, the ratio between the application of Equations 118 and 120 approaches the theoretical maximum of *m* (number of considered endpoints). If the compounds have almost the same ecotoxicological profiles (which can be expected e.g. for a mixture of simple organic solvents), then the risk quotients from both equations become identical.

The maximum ratio between the risk quotients (RQs) of tier 1 and tier 3 of *m* (number of species-specific ecotoxicological endpoints) provides a convenient decision criterion on whether the detailed data collection or production in order to conduct a refined assessment based on the RQ of tier 3 (Equation 120) might influence the regulatory outcome: if the RQ of tier 1 is higher than *m*, the RQ of tier 3 will always be above 1, i.e. indicate reason for concern. In such cases it is not constructive to proceed with the tiered approach and alternatives such as the direct testing of the product /or the ecologically relevant mixture or effective Risk Mitigation Measures should be taken into account. In case the aforementioned options are not applicable the only remaining option is the non-authorisation of the product.

Employing eq. 6 requires that data for all relevant compounds are available for all endpoints, as it would otherwise be impossible to determine the maximum of all organism- and endpoint-specific STUs and an appropriate overall assessment factor (AF). This makes an application of Equation 120 – although it most closely follows the conceptual idea of CA – rather demanding.

A risk quotient exceeding one might be caused by the mixture toxicity overestimation that results from the application of CA to a mixture of not entirely similarly acting compounds. Details on how to estimate this possible overestimation are provided by Junghans and colleagues [35] and Backhaus and colleagues [4]. The direct testing of the biocidal product or the ecologically relevant mixture might provide additional insight, given that a substantial risk overestimation by CA is possible, which depends on the number of involved compounds, their toxicity and ratio in the mixture. Otherwise there would be a clear indication for a reason for environmental concern, which would call for appropriate risk management strategies

If the tiers still indicate an unacceptable risk for environment, the only risk assessment option is the direct biotesting either of the biocidal product, if there is a direct release of the product into environment or of the ecologically relevant mixture in case the composition of the product changes radically before release to environment as the ultimate option for clarification (tier 4). If the direct biotesting of the mixture of concern, i.e. the product and/or the ecologically relevant mixture is not possible and other options such as a further refinement of the single substance data or the definition of effective RMMs are not applicable, the only remaining option is the non-authorisation of the product (Figure 32).

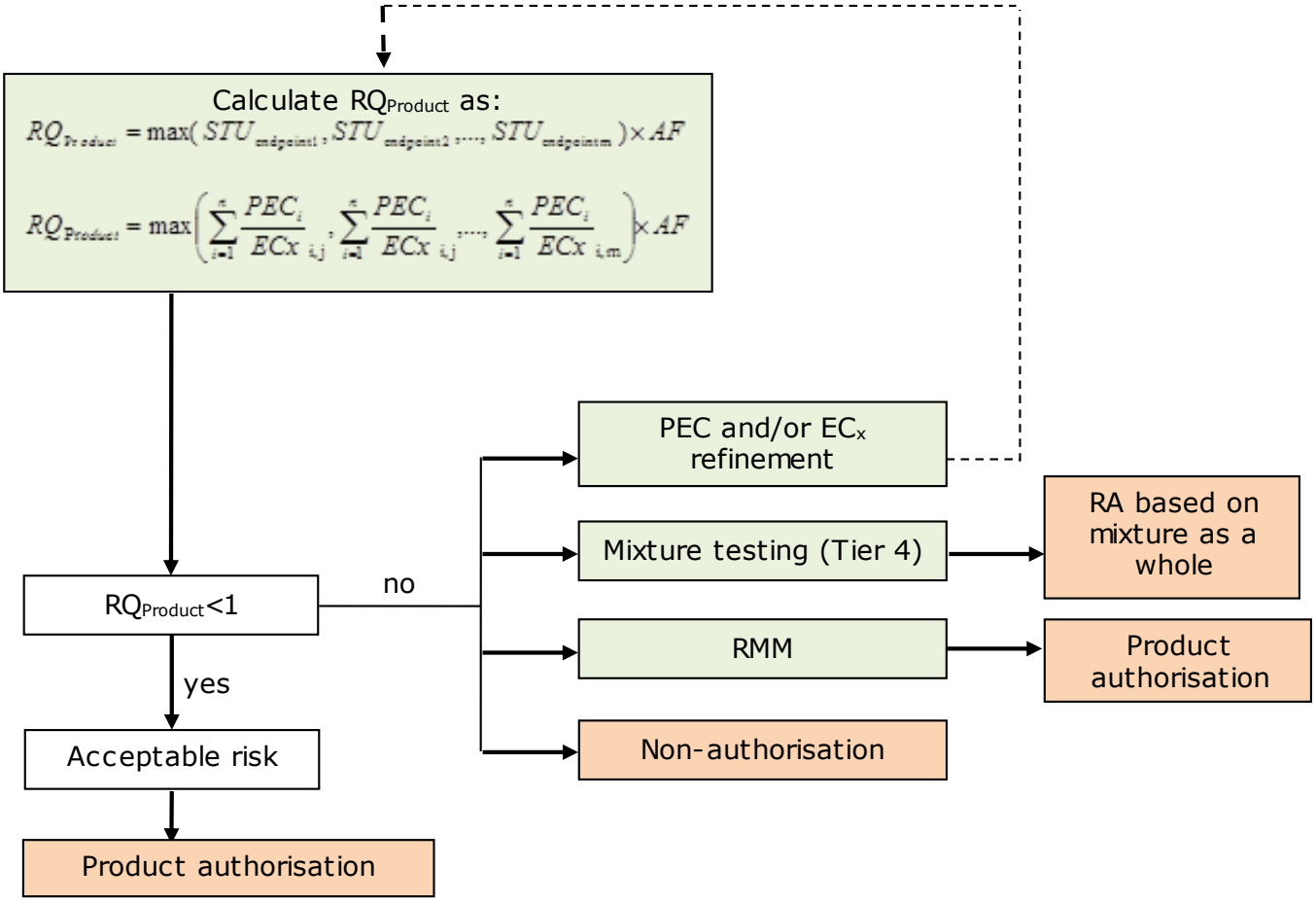

Figure 32: Decision tree for tiers 3 and 4 (Standard Toxic Unit Summation and Mixture Testing, point 3.3.3, AF = Assessment Factor, EC_x = Effect Concentration that provokes an x%-effect in the exposed organisms, PEC = Predicted Environmental Concentration, RA = risk assessment, RMM= Risk Mitigation Measures, $RQ_{Product}$ = Risk Quotient of the Product, STU = Sum of Toxic Units)

10.3.4 Tier 4

Tier 4 should be used if data on the whole "relevant mixture", i.e. product tests or tests with the ecologically relevant mixture are not already available. These tests should only be employed in situations, where well-founded suspicions for synergistic interactions require clarification, or as last option where results of predictive modelling (tiers 1-3) indicate unacceptable risks for environment (see also section 9.2). In these cases the most sensitive species from the single substance data should be tested.

It should be kept in mind that the PEC and PNEC have to be estimated based on the same concentration of constituents.

Effects Assessment

Direct testing of the whole product is not straight forward in principle. Eventhough it does in principle not require any specific methodology and can hence use the same experimental outline as the tests of an individual chemical, in reality there are other parameters that should be considered before engaging in such studies (e.g. lack of guidance for endpoint derivation). In general terms, further guidance on testing on mixtures would be highly desirable in the future.

The BPR states that tests with vertebrate animals can only be conducted as a last resort, i.e.

when alternative testing and assessment methods have been exhausted. Tests on vertebrate animals are to be carried out only where the purpose and use of a product so requires and such tests cannot be repeated for the purposes of the BPR. In addition to the obligation to inquire about previously submitted tests (Article 62(2) BPR), an applicant may also consult the relevant competent authority with regard to the testing on vertebrates that the applicant proposes to carry out (see Annex III BPR). Furthermore, the long term testing of a biocidal product might be of only limited informative value (although it is feasible, as it could shown by Coors et al., 2012 [24]) as the results may be difficult to interpret and use for regulatory purpose. The composition of the product might change already during the exposure in the biotest system, as the different chemicals might have a different stability and distribution between the different compartments in the test (e.g. biota, headspace, aqueous media, soil, sediment). Changes in the chemical composition of the initial mixture are most likely even more pronounced if environmental fate and distribution processes are taken into consideration. Such processes can be accounted for by testing the ultimate, environmentally relevant mixture instead of the original product. For example, it might be more relevant to test the leachate of a wood preservative than the original product. It could be shown in two research projects for several test organisms, that the leachates are clearly less toxic than the original product [20], providing an opportunity to lower the risk for a respective product by providing leachate toxicity data. The validity of the toxicity data for the risk assessment then strongly depends on a thorough definition of the underlying exposure scenario. However, there are currently also no agreed guidelines at hand in the EU for the testing of such "realistic" mixtures (e.g. leachates).

If the solubility of the product or the environmentally relevant mixture in water is low or reduced, the OECD Guidance document No. 23 on Aquatic Toxicity Testing of Difficult Substances and Mixtures [42] should be followed. If it is technically not feasible to test the mixture in its entirety, because of e.g. insoluble pigments or other ingredients making a direct testing of the product unfeasible, it is also possible to assess generic mixtures of the relevant substances („surrogate mixture") by combining the substances identified as relevant for mixture assessment in a ratio similar to that of the product or the ecologically relevant mixture.

By experimental testing of a given mixture of substances, both effect concentrations and NOEC values can be determined in the same way as this is usually done for single substances. Therefore, no knowledge either about the composition of the mixture e.g. nature, number or concentration ratio of the components must be known for testing nor toxicity data for the individual components or their mechanism of action.

When testing mixtures the procedures applied are similar to the procedures applied for single substances by taking into account the general principles described in the Technical Guidance Document [28) and the Technical Notes for Guidance on Product Evaluation [27] as well as the related Guidance Documents and Emission Scenario Documents. Risk quotients for mixtures can be derived from such experiments if in the exposure situation in the environment the concentration ratio of mixture components is comparable to that in the experiments. However, it should be kept in mind, that due to distribution and transformation processes in the environment, the mixture to which the non-target organisms may be exposed is only conditionally comparable with the original composition of the product [1]. But, as such mixture data encompass any effects due to interactions that may occur between the mixture components, e.g. synergistic interactions as well as contributions from compounds that have not been considered in the mixture toxicity predictions or for which ecotoxicity information is lacking (e.g. formulation additives), the risk assessment will be based on the mixture as a whole if the data are available, rather than on the sole prediction of the mixture toxicity by using the concept of Concentration addition or pragmatic approaches of this concept, i.e. PEC/PNEC-summation.

It is difficult to suggest a generally applicable testing scheme for products and ecologically relevant mixtures also in terms of the test design (i.e. species, test duration, test concentrations etc.). Therefore, it is recommended to assess each mixture carefully and base decisions regarding testing on expert judgement in agreement with the Competent Authority.

Exposure Assessment

According to the Technical Notes for Guidance on Product Evaluation (TNsG, chapter 5.2 Risk assessment for products, [27]) the calculation of a PEC for the whole product should be possible when there is a direct release of the product to environmental compartments:

"For products for which a direct exposure of a given compartment is possible, test results with whole products can be taken into account. A PEC and a PNEC can be derived for the whole product and a corresponding risk characterisation can be performed for the product:

$(PEC/PNEC)_{product} = PEC_{product}/PNEC_{product}$

The approach is usually not possible throughout a risk assessment for all compartments.

That means that currently:

- $PEC_{product}$ can be calculated for the first receiving compartment if direct release of the whole product takes place. In this case $PEC_{product}$ could be calculated referred to as dilution in the receiving compartment (no degradation can be considered). The amount of product used will be taken into account in the respective equations in the ESDs whenever possible. A risk assessment based on the tested mixture (product) would be in this case, possible.
- There is no agreed methodology available to calculate $PEC_{product}$ if there is an indirect release into environmental compartments e.g. via STP or by distribution between water and sediment, as no partition coefficients for products are available. In this case, a risk assessment based on the tested mixture (product) is currently not possible.
- There is no agreed methodology available to calculate $PEC_{product}$ if there is direct release of a part of the product e.g. as a leachate into environmental compartments. Even if it is possible to analyse all relevant substances in a leachate, the composition of the leachate often vary with time. In this case, a risk assessment based on the tested mixture (leachate) is currently not possible.

It is recommended to review the relevant emission pathways of the application of the biocidal product with regard to direct releases before doing mixture testing.

A more comprehensive summary of the scientific background of the mixture toxicity assessment and the outlined strategy can be found in Altenburger et al. (2012) [1] and Backhaus et al. (2012, [5]).

Appendix 9. Workshops on mixture toxicity 2012-2013: Draft proposal for the identification of relevant substances for mixture assessment

NOTE to the reader:
Owing to the recent consultation to update this guidance it has been noted that the information on the identification of relevant substances for mixture assessment in Appendices 9 and 10 describes outdated methodology and the guidance in section 10.2.2 of this guidance (version 2.0) should be followed. This will be reviewed and aligned at the next update.

What are 'Relevant Substances' in a typical biocidal product?

The discussions during the Workshops on mixture toxicity assessment raised the following issues regarding relevant substances:

- Relevant substances for mixture assessment cannot be restricted to active substances (a.s.) of biocidal products only;
- Relevance relates to effects to non-target organisms in environmental risk assessment and not to the purpose of the products use;
- In case of lack or insufficiency of data conceptually there is always the product testing as the ultimate option to gain a satisfactory assessment answer;
- The definition may refer to substances of concern (SoC) as used in BPD and BPR or it may relate to an understanding of relevance in general.
- There may be other components to be considered by default that do not fall under the current SoC definition.

There was a broad agreement among the vast majority of attendees on regarding SoCs as relevant for the calculation of the mixture toxicity.

It was agreed at the follow-up workshop at TM III/2012 to regard the following substances as relevant for mixture assessment:

1) Active substances.
2) Substances of concern.
3) Active substances from other PTs. However, it should be considered under which conditions exemptions are possible (e.g. substances contained in Annex I of the new regulation or substances contributing only to a very limited extent to the overall toxicity of the mixture, see below).
4) Other ingredients which do not fall under one of the aforementioned categories but might be relevant for mixture assessment like e.g. known synergists should be considered as well on a by-case basis.

Therefore, it is proposed that active substances and SoCs have to be regarded as relevant for mixture assessment *per se*. For all other product components ecotoxicological, fate and behaviour as well as relevant physico-chemical endpoints should be derived based on available information (e.g. laboratory studies, material safety data sheets, EU or international chemical reviews, QSARs etc.) from which it can be decided whether a product component has to be regarded as relevant substance for the mixture toxicity assessment. It is the applicants responsibility to make all reasonable efforts to submit the most up to date and reliable information and this should be detailed in the submission, along with any letters of access that might be required. As only semi-quantitative data are needed for this purpose, e.g. QSAR-estimates, hazard classification data from classification and labeling according to the CLP Regulation (EC) No 1272/2008, data from limit tests or screening studies as well as simple

exposure estimates should be sufficient in this first step.

In addition, a research project funded by the German Federal Environment Agency [24] revealed, that the calculation of the relative toxic units (TU) of the single product components as also recommended by Backhaus & Faust (2012) [4] might be a helpful tool to decide whether *active substances from another PT, or other ingredients which are neither a.s. nor SoC* must be regarded as relevant substance for mixture assessment together with the a.s. and the SoC, provided that toxicity estimates comparable to those of the a.s. and SoC are available for these substances.

The calculation of the individual TU (for each trophic level separately) is based on the concentration of the substances in the product (c*i*) and the available toxicity estimates, i.e. equi-effective concentrations of the single substances, such as the EC_{50}-values ($EC_x i$,[43] Equation 121):

$$TUi = Ci/EC_x i \qquad \textbf{Equation 122}$$

Hence, the calculation of the TU is independent of any biological testing of the products or the leachates and can therefore be done ahead of experimental investigations to indentify the relevant mixture components and target the testing where relevant [24]. Finally, the relative TU (rel TU) is calculated as depicted in Equation 122 and indicates how much each mixture component contributes to the overall expected toxicity (see also **Appendix 10** & **Appendix 12**):

$$\text{rel } TUi = (TUi/\Sigma TU)/100 \qquad \textbf{Equation 123}$$

As the relative TU depends on the overall composition of the product, the concentration of the respective substance in the product as well as their toxicity, no threshold values can be given for the rel TU. Therefore, the decision on whether a substance is relevant for the assessment of the mixture toxicity is subject to expert judgement.

Another possibility to assess the influence of the individual components on the overall toxicity of the mixture is the Maximum Cumulative Ration (MCR) as proposed by industry:

NOTE to the reader:
The MRC document is at the end of this Appendix

Inert compounds (e.g. water, non-soluble pigments) are chemicals that do not show any toxic effects, even at excessive concentrations and do not interact with other chemicals present. Hence, they do not have an impact on the mixture toxicity assessment and can be ignored, as both concepts assume that they do not contribute to the overall toxicity of the product, unless there are indications that they influence the toxicity of the other mixture components [3]. However, inert compounds need to be clearly differentiated from compounds that are not an active ingredient *per se*, (i.e. they are not inherently toxic to exposed organisms), but still are biologically active. Piperonyl butoxide (PBO) for example would fall into this group, as the compound itself is not biocidal, but increases the toxicity of other biocides e.g. pyrethrins, pyretroids or carbamates by inhibiting their cytochrome P450-driven metabolisation [32, 41,53]. Such "synergists" might lead to serious toxicity and risk underestimations, and hence have to be considered specifically in a case-by-case manner.
Also diluents, (lipophilic) organic solvents and surfactants like e.g. naptha may influence the toxicity of a mixture by enhancing the bioavailability of the active substance(s) [24, 27] and should therefore be regarded carefully.

[43] lowest EC_{50}- or LC_{50}-values for the same endpoint and *preferably* (not necessarily) the same exposure setting and the same species.

It is possible that certain properties of the compound in question mean that the environment is unlikely to be significantly exposed to that substance. In such a situation qualitative argumentation may be submitted by the Applicant to demonstrate that environmental exposure in a particular compartment would be negligible. Such argumentation should be supported by appropriate data. Examples may include very rapid degradation or dissipation (e.g. by volatilisation and rapid photochemical oxidation in air) or negligible exposure e.g. when only used in completely closed systems.
It has to be emphasised again, that special care has to be taken to ensure that all ingredients toxic for the environment are included in a component-based assessment of a biocidal product, because otherwise the risk for environment resulting from the application of the product is underestimated. If no or not sufficient (ecotoxicological) information is at hand for all ingredients, to decide whether a substance is relevant for mixture assessment the only effect assessment option is the direct biotesting either of the respective substance(s) or of the biocidal product and the resulting environmental mixture, respectively. If a mixture cannot be assessed in its entirety, because of e.g. insoluble pigments it is also possible to assess generic mixtures of the relevant substances ("surrogate mixture").

NOTE to the reader: MRC document

The Maximum Cumulative Ratio (MCR) a Tool for the Investigation of Risks Associated with and Individuals' Concurrent Exposures to Multiple Chemicals

Introduction

Humans are constantly exposed to multiple chemicals from multiple sources. However, regulatory programs often evaluate risks on a chemical-by-chemical basis and do not require the consideration of cumulative exposures. The Maximum Cumulative Ratio (MCR) is a tool for investigating the magnitude of the toxicity received by a receptor that is missed if a cumulative risk assessment is not performed (Price and Han, 2011).

The objective of the publication is to present the MCR concept, derivation and interpretation. In a second step, the MCR was applied to the case studies presented during the mixture toxicity workshop on the environmental mixture toxicity assessments from biocidal products at the TMIII 2012.

The Maximum Cumulative Ratio (MCR)

The Maximum Cumulative Ratio is an index quantifying the significance of cumulative toxicity to a receptor compared to the toxicity from individual components (Junghans et al., 2006). As described in Price and Han (2011) it can be calculated based on an individual receptor's hazard quotients (HQs) of the individual chemicals and hazard index (HI)[44]. The value of MCR for an individual human/organism exposed to a mixture of comprised of *n* chemicals in an environmental media is calculated by:

$$HQ_i = \frac{C_i}{RV_i}$$

$$HI = \sum_{i} HQ_i$$

$$MCR = \frac{HI}{\max HQ_i}$$

where C_i is the concentration of the i^{th} chemical in the media to which an individual is exposed and RV_i is the health based reference value of chemical *i* (expressed as a concentration). HQ_i is the hazard index of the individual's exposure to the i^{th} chemical. *HI*, is the sum of the

[44] The MCR can also be applied to environmental receptors (Price et al. 2012b).

individual's HQs. The MCR of the individual's exposure to the mixture is the ratio of the *HI* of the mixture to the maximum of the hazard quotients of the individual components max *HQi*.

As noted by Konemann (1981) this ratio is bounded by 1 and *n*. An MCR value close to 1 means that one chemical is responsible of all of the mixture's toxicity. Exposures to mixtures of chemicals with equal toxicities would have an MCR of *n*. Price et al. (2012) describe how the MCR and the HI can be use to classify mixture exposures into four groups (Table 1), each one requiring a different risk management strategy (Price et al 2012b).

The MCR methodology has been used to investigate the potential human health effects of environmental mixtures of plant protection products in surface waters on human health (Price and Han, 2011), mixtures of chemicals in ground water wells (Han and Price, 2011), mixture of chemicals measured in surface water and waste water treatment effluents (Price et al. 2012b) and cumulative exposures to dioxin like chemicals (Han and Price, 2012).

The MCR can be used in assessments of risks from combined exposures to multiple chemicals in a number of ways. First, the values of the MCR and HI can be used to assign the individual's mixture exposures into the four groups. Each of these groups requires a different risk management approach. In addition, the categories help identify those mixtures where the cumulative assessments are most needed (Group IIIB), and the specific chemicals that drive such mixtures. This approach can be helpful in the evaluation of "real world" mixtures that occur from multiple sources (surface water, indoor air, diet, etc.) that involve large numbers of chemicals and highly variable exposures.

Table 1: Classification of mixtures according MCR and HI (Price et al., 2012a)

Group	Values of MCR, HI, and Max HQ_i that define the groups	Description
Group I	$\mathrm{Max}HQ_i > 1$ and $\left(\frac{HI}{MCR} > 1\right)$	Mixtures containing at least one chemical in concentration that poses a health risk. The risk would have been identified also in a chemical-by-chemical assessment.
Group II	$HI < 1$	Mixtures of low concern
Group IIIa	$MCR < 2,$ $HI > 1$ and $\mathrm{Max}HQ_i < 1$	Mixtures containing one chemical responsible for most of the mixture's toxicity that should be prioritized for further investigation. A chemical-by-chemical assessment would have not identified this mixture as of concern, since max $HQ_i < 1$.
Group IIIb	$MCR > 2,$ $HI > 1$ $and\ \mathrm{Max}\,HQ_i < 1$	Mixtures with no single chemical standing out for its toxicity but of concern for combined effects. A chemical-by-chemical assessment would have not identified this mixture as of concern.

Second, the approach can be a part of a decision tree for the evaluation of mixtures (Price et al., 2012a,b). Finally the MCR can be used to determine which types of formulations are most

in need of cumulative assessments (fall into Group I or III) and whether there are characteristics which predict the need for cumulative assessments.

In summary, the MCR is a descriptor of the influence of individual components on the overall toxicity of a mixture. The MCR is a useful tool for prioritization of mixtures for higher tier risk assessments and risk management.

Integration of MCR approach to the case studies presented at TMIII

The case studies presented during the mixture toxicity workshop on the environmental mixture toxicity assessments from biocidal products were reviewed and reworked to include the prioritization tool. The goal is to provide an example and discuss key conclusion to be drawn in the tiered approach.

Steps to derive the MCR

The Hazard quotient for a single substance is calculated as following:

$$HQ_i = \frac{c_i}{RV_i} \quad ,$$

where the RV_i is an endpoint (EC_{50} of NOEC) or the PNEC, and c_i is the concentration measured in the sample or the Predicted Environmental Concentration (PEC)

Under the REACH legislation, the HQ is commonly named the risk characterization ratio (RCR), which is derived as the ratio of the PEC/PNEC.

The risk assessment of a mixture is based on a response addition assumption, hence the HQ of the individual substance should be <1 to justify further considerations.

As described earlier, the Hazard Index (HI) is the cumulative risk of the component in a mixture, which is derived as the sum of the substance specific HQ:

$$HI = \sum_{\mathrm{i}} HQ_i$$

The Maximum Cumulative Ratio (MCR) is derived by dividing the HI, by the HQ of substance having the maximum contribution

$$MCR = \frac{HI}{\max HQ_i}$$

Example 1

The product characteristics were presented with the following information on ecotoxicity endpoints and predicted exposure concentration (PEC) (Table2).

Table 2 : Hazard and PEC of a three component formulation

Species	Hazard endpoint	Substance 1	Substance 2	Substance 3
Fish	EC50 (mg/L)	0.01	4.3	0.0027
	NOEC (mg/L)	0.00407	0.43	0.00056
Daphnia	EC50 (mg/L)	0.42	0.31	0.0052
	NOEC (mg/L)	0.00265		0.00063
Alga	EC50 (mg/L)	15	0.058	0.0016
	NOEC (mg/L)	1		0.00034
AF	-	10	100	10

PNEC	(mg/L)	0.00027	0.00058	0.00003
PEC surface water	(mg/L)	0.00004	0.00015	0.0000272
HQ (PEC/PNEC)	**-**	**0.15**	**0.26**	**0.8**

TIER 1:

The risk of the mixture calculated based on the assumption of response additivity is:

$$HI=\Sigma\ HQ= 0.15+0.26+0.8= 1.21$$

The highest HQ in the mixture is 0.8; therefore the MCR can be derived as following:

$$MCR = 1.21/0.8= 1.51$$

The risk analysis (HI) and the MCR analysis indicates that the mixture may be of concern however contains one chemical responsible for most of the mixtures' toxicity. Based on the MCR analysis further supports that the third component of the mixture is driving the exposure assessment; hence a refinement of the risk assessment should primarily focus on the exposure or hazard characterization of this component.

TIER 2:

The Tier 2b is a toxic unit approach; hence it is suggested to apply the MCR approach as following.

The ratio of the PEC and the RV_i is calculated for each trophic level and each substance. The RV_i is either the EC_{50} or the NOEC when available. The TU approach should sum contribution to the mixture effect based on the same RV_i (common endpoint). In consequence, the RV_i chosen for each trophic level is a common denominator. When NOEC were available for all substances, this endpoint was chosen as the reference value, else the EC_{50} was selected.

Table 3 presents the calculated TU and the RV_i:

Tier 2b	RVi	Substance 1	Substance 2	Substance 3
		TU=PEC / RV_i	**TU=PEC /** RV_i	**TU=PEC /** RV_i
Fish	NOEC	0.01	0.0003	0.05
Invertebrate	EC_{50}	0.0001	0.0005	0.01
Alga	EC_{50}	0.000003	0.0026	0.02

Table 4 presents the sum of the toxic units, the highest TU, as well as the MCR derived from the TU calculations.

	Sum of TU	max TU	MCR
Fish	**0.059**	0.05	1.21
Invertebrate	**0.006**	0.01	1.11
Alga	**0.020**	0.02	1.15

The MCR indicates that a substance in this mixture is a clear driver of the mixture risk assessment at each trophic level. In this case, the trophic level approach confirms that substance 3 is the main driver of the toxic unit assessment. In this specific example, substance 3 is the driver for fish, invertebrate and alga, however this analysis could indicate that a

substance with a specific mode of action is the driver of the assessment for a unique trophic level (i.e. primary producers).

The TU approach was carried out for each trophic level individually. The application of an assessment factor would be needed to extrapolate the result of TU assessment at each trophic level to ecosystem effect.

Examples 2 and 3.

The risk assessment of these mixtures was not reiterated, as both mixtures have a component which has an HQ greater than 1, concluding to potential risk at a single substance level. The single substance risk assessment should be refined before addressing any product assessment.

Conclusion

In this communication, we present the concepts of the Maximum Cumulative Ratio (MCR) as a prioritization tool in mixtures risk assessment. The MCR consists of a simple additional calculation step of a quantitative risk assessment for mixtures, which allows to differentiate between situation, where one chemical responsible for most of the mixture's toxicity or where there is concern for a combined effect. To illustrate the concept, the MCR calculation was applied to case studies presented at the TMIII. In the first product describe one substance was identified as a key driver of the mixture's risk in the two tiered approach. The other products contained a substance which would require further refinement in the exposure and or hazard assessment at the single substance level prior any mixture risk assessment.

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Appendix 10. Workshops on mixture toxicity 2012-2013: Sample calculation relative Toxic Unit

NOTE to the reader:
Owing to the recent consultation to update this guidance it has been noted that the information on the identification of relevant substances for mixture assessment in Appendices 9 and 10 describes outdated methodology and the guidance in section 10.2.2 of this guidance (version 2.0) should be followed. This will be reviewed and aligned at the next update.

Underlying data for the substances indentified as relevant for mixture toxicity assessment:

Substance	Active substance	Preservative	Solvent
Content in the product [w/w%]	0.5	6.5	83.1
Algae (E_rC_{50}(72h)	0.0052 mg/L	9 mg/L	695 mg/L
Daphnid (EC_{50}(48h)	0.003 mg/L	5 mg/L	700 mg/L
Fish (LC_{50}(96h))	0.0012 mg/L	7 mg/L	850 mg/L

Based on these data the TU are calculated for all three product components according to Equation 121 ($TU_i = C_i/EC_{x}i$):

Substance	Active substance	Preservative	Solvent	ΣTU
TU Algae	96.2	0.72	0.12	97.0
TU Daphnid	166.7	1.30	0.12	168.1
TU Fish	416.7	0.93	0.10	417.7

Finally, the relative TU are calculated according to Equation 122 ($rel\ TU_i = (TU_i/\Sigma TU)/100$):

Substance	Active substance	Preservative	Solvent
Relative TU Algae	99.13	0.74	0.12
Relative TU Daphnid	99.16	0.77	0.07
Relative TU Fish	99.76	0.22	0.02

According to this calculation only the active substance has to be regarded as relevant for mixture toxicity assessment as the a.s. accounts for more than 99% of the toxicity of the mixture in algae, daphnid and fish in this theoretical example.

Appendix 11. Synergisms

Table 57: Intended Synergisms

Synergistic interaction reported for	Organisms for which synergism are reported	Reference
Bacillus thuringiensis Berliner & Endosulfan	Cotton boll worm (*Helicoverpa armigera*)	46
Copper & Formaldehyd	Micro-organisms	49, 54,
Copper & isothiazolone	Micro-organisms	49
Formaldahyd & Isothiazolone	Micro-organisms	49
Propiconazol & λ-cyhalothrin	Honeybee (*Apis mellifera*)	43
Copper & CPT	Bacteria (*Vibrio fischeri*)	59
Copper (pyrithione)& ZPT	Bacteria (*Vibrio fischeri*), Diatoms (*Thalassiosira pseudomona*), polychaete larvae (*Hydroides elegans*), amphipods (*Elasmopus rapax*), brine shrimp (*Artemia salina*)	11, 38, 60
Copper & Dithiocarbamates	Ciliates (*Colpidium campylum*)	14, 57, 59,
Copper & Diuron	Bacteria (*Vibrio fischeri*), marine algae (*Chaetoceros gracilis*), brine shrimp (*Artemia salina*)	37, 38, 60
Copper & Irgarol	Bacteria (*Vibrio fischeri*), marine algae (*Chaetoceros gracilis*)	37, 60
Copper & Sea Nine 211	Bacteria (*Vibrio fischeri*)	60
Copper & Ziram	Bacteria (*Vibrio fischeri*)	60
Deltamethrin & Carbaryl	Snail (*Lymnaea acuminata*)	25
Diuron & ZPT	Marine algae (*Chaetoceros gracilis*), brine shrimp (*Artemia salina*)	37, 38
Diuron & cadmium	marine algae (*Chaetoceros gracilis*)	37
Dithiocarbamates & heavy metals	*not reported*	57
EBI-fungicides & insecticides (pyrethroids, organophosphates, neonicotinoids)	Microorganisms *(Vibrio fischeri), i*nvertebrates *(Daphnia magna, Apis mellifera)*	17, 44, 51, 55
Isoproturon & Cypermethrin & Difufenican	*not reported*	55
Isoproturon & Cypermethrin & Pendimethalin	*not reported*	55
Isoproturon & Cypermethrin & Trifluralin	*not reported*	55

Synergistic interaction reported for	Organisms for which synergism are reported	Reference
Isoproturon & Fenvalerate & Pendimethalin	*not reported*	55
Isoprotuon & Delthamethrin & Diflufenican	*not reported*	55
Irgarol & Cadmium	Marine algae (*Chaetoceros gracilis*)	37
Irgarol & Diuron	Bacteria (*Vibrio fischeri*), green algae (*Selenastrum capricornotum*), marine algae (*Chaetoceros gracilis*) crustaceans (*Daphnia magna*)	30, 37
Irgarol & TCMTB	Bacteria (*Vibrio fischeri*), green algae (*Selenastrum capricornotum*), crustaceans (*Daphnia magna*)	30
Irgarol & Chlorthalonil	Bacteria (*Vibrio fischeri*), green algae (*Selenastrum capricornotum*)	30
Irgarol & DCF	Bacteria (*Vibrio fischeri*), crustaceans (*Daphnia magna*)	30, 60
Thiacloprid & Tebuconazole	Bees (*Apis mellifera*)	51
ZPT & Irgarol	Marine algae (*Chaetoceros gracilis*)	37
ZPT & cadmium	Marine algae (*Chaetoceros gracilis*)	37
Zinc pyrithione & Ziram	Bacteria (*Vibrio fischeri*)	60
Irgarol & TCMTB & Dichlofluanid	Green algae (*Selenastrum capricornotum*), crustaceans (*Daphnia magna*)	30
Zinc pyrithione & Copper pyrithione & Chlorothalonil	Brine shrimp (*Artemia salina*)	38
Zinc pyrithione & Copper pyrithione & Chlorothalonil	Nrine shrimp (*Artemia salina*)	38

Table 58: Un-intended Synergisms

For the substances depicted in the table potential synergistic effects are reported in the peer-reviewed literature. These publications should be seen as indications for possible synergisms of the shown substances and be taken into account during the decision making process. However, they should be analysed in more detail for this purpose, e.g. regarding the tested concentrations, mixture ratios and the concentration-dependence of interaction as well as the tested organisms and endpoints.

Synergistic interaction reported for	Organisms for which synergism are reported	Reference
Bacillus thuringiensis Berliner & Endosulfan	Cotton boll worm (*Helicoverpa armigera*)	46
Copper & Formaldehyd	Micro-organisms	49, 54,
Copper & isothiazolone	Micro-organisms	49
Formaldahyd & Isothiazolone	Micro-organisms	49
Propiconazol & λ-cyhalothrin	Honeybee (*Apis mellifera*)	43
Copper & CPT	Bacteria (*Vibrio fischeri*)	59
Copper (pyrithione)& ZPT	Bacteria (*Vibrio fischeri*), Diatoms (*Thalassiosira pseudomona*), polychaete larvae (*Hydroides elegans*), amphipods (*Elasmopus rapax*), brine shrimp (*Artemia salina*)	11, 38, 60
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Copper & Irgarol	Bacteria (*Vibrio fischeri*), marine algae (*Chaetoceros gracilis*)	37, 60
Copper & Sea Nine 211	Bacteria (*Vibrio fischeri*)	60
Copper & Ziram	Bacteria (*Vibrio fischeri*)	60
Deltamethrin & Carbaryl	Snail (*Lymnaea acuminata*)	25
Diuron & ZPT	Marine algae (*Chaetoceros gracilis*), brine shrimp (*Artemia salina*)	37, 38
Diuron & cadmium	marine algae (*Chaetoceros gracilis*)	37
Dithiocarbamates & heavy metals	*not reported*	57
EBI-fungicides & insecticides (pyrethroids, organophosphates, neonicotinoids)	Microorganisms *(Vibrio fischeri),* invertebrates *(Daphnia magna, Apis mellifera)*	17, 44, 51, 55
Isoproturon & Cypermethrin & Difufenican	*not reported*	55
Isoproturon & Cypermethrin & Pendimethalin	*not reported*	55
Isoproturon & Cypermethrin & Trifluralin	*not reported*	55
Isoproturon & Fenvalerate & Pendimethalin	*not reported*	55
Isoprotuon & Delthamethrin & Diflufenican	*not reported*	55
Irgarol & Cadmium	Marine algae (*Chaetoceros gracilis*)	37

Synergistic interaction reported for	Organisms for which synergism are reported	Reference
Irgarol & Diuron	Bacteria (*Vibrio fischeri*), green algae (*Selenastrum capricornotum*), marine algae (*Chaetoceros gracilis*) crustaceans (*Daphnia magna*)	30, 37
Irgarol & TCMTB	Bacteria (*Vibrio fischeri*), green algae (*Selenastrum capricornotum*), crustaceans (*Daphnia magna*)	30
Irgarol & Chlorthalonil	Bacteria (*Vibrio fischeri*), green algae (*Selenastrum capricornotum*)	30
Thiacloprid & Tebuconazole	Bees (*Apis mellifera*)	51
ZPT & Irgarol	Marine algae (*Chaetoceros gracilis*)	37
ZPT & cadmium	Marine algae (*Chaetoceros gracilis*)	37
Zinc pyrithione & Ziram	Bacteria (*Vibrio fischeri*)	60
Irgarol & TCMTB & Dichlofluanid	Green algae (*Selenastrum capricornotum*), crustaceans (*Daphnia magna*)	30
Zinc pyrithione & Copper pyrithione & Chlorothalonil	Brine shrimp (*Artemia salina*)	38
Zinc pyrithione & Copper pyrithione & Chlorothalonil	Nrine shrimp (*Artemia salina*)	38

Appendix 12. Workshops on mixture toxicity 2012-2013: Case Studies

NOTE to the reader:
Owing to the recent consultation to update this guidance it has been noted that the agreed methodology for identification of relevant substances for mixture assessment described in the case studies in Appendix 12 is outdated and the guidance in section 10.2.2 of this guidance (version 2.0) should be followed. This will be reviewed and aligned at the next update.

Case Study 1: PT14, Rodenticide

Screening Step

1. Identification of the concerned environmental compartments

The ready-to-use baits (wax blocks) are used for the control of rats and mice indoors and outdoors (in and around buildings, open areas, waste disposal sites) and in sewers in secure and tamper resistant covered applications (bait stations, other secured coverings). The use in the sewer system may lead to contamination of surface waters and sediment through sewage water and STP. No or significantly lower contamination of surface water is expected from the other proposed uses of the product.

The exposure of soil organisms to the product by direct contamination of soil may occur following use in and around buildings. It is also possible that soil may become exposed following the spreading of sewage sludge from a sewage treatment plant that has been exposed to the product used in sewers. There is also a risk for primary and secondary poisoning of non-target organisms. An exposure of the environment towards the product is likely (surface water, sediment, soil).

2. Identification of Relevant Substances

The composition of the product is given in Table 59.

Table 59: Composition of the biocidal product

Ingredient	Content in the formulation [w/w%]	Classification	Relevant substances of concern
Active substance	0.005	Acute Tox. 1 (H310, H330), Acute Tox. 2 (H300, H330); Repr. 1A (H360); STOT RE 1 (H372); Aquatic Acute 1 (H400), Aquatic Chronic 1 (H410)[45]	X
Flour	60.88	not classified	-
Paraffin	26.80	not classified	-
Cereals	6.00	not classified	-
Sugar	3.00	not classified	-
Co-formulant	2.38	not classified	-
Colouring agent	0.68	not classified	-
Co-formulant	0.195	not classified	-

[45] The translation between DSD and CLP classification needs to be checked.

Preservative	0.04	not classified	-
Aroma	0.02	not classified	-

X: substance relevant for mixture assessment; -: substance not relevant for mixture assessment

The biocidal product contains no substances of concern or other ingredients bearing an environmental classification or otherwise a potential hazard for environment.

Beside the active substance, the product contains a preservative. This substance is notified as an active substance under the BPD for several PTs and should therefore be considered as a relevant substance for mixture toxicity assessment. However, the preservative is not classified for environment and from the available ecotoxicological data it can be concluded, that the preservative is less toxic for environmental organisms than the active substance.

Furthermore, a comparison of the toxic units of the a.s. and the preservative according to Equations 121 and 122 (**Appendix 9**), for the aquatic and the soil compartment revealed, that mainly the a.s. is the risk driver of the product toxicity for the aquatic compartment (see Table 62 & 63).

Table 60: Toxicity data for the a.s. and the preservative for the aquatic and the soil compartment.

Substance	Active substance	Preservative
Content in the product [w/w %]	0.005	0.04
Aquatic compartment		
Algae (E_rC_{50}(72h), [mg/L]	0.51	480
Daphnid (EC_{50}(48h), [mg/L]	0.52	982
Fish (LC_{50}(96h)), [mg/L]	0.064	>1000
Soil compartment		
Earthworm (LC_{50}(14d), [mg/kg dw]	>100	>5000

Table 61: Relative toxic units (individual TU in % of the sum of TU) for the a.s. and the preservative with regard to aquatic organisms.

	Active substance	Preservative
Algae	99.16	0.84
Daphnid	99.58	0.42
Fish	99.95	0.05

Table 62: Relative toxic units (individual TU in % of the sum of TU) for the a.s. and the preservative with regard to soil organisms.

	Active substance	Preservative
Earthworms	13.8	86.2

Based on expert judgment it can be concluded that the preservative is not a relevant substance for mixture assessment.

→ Besides the active substance, no other ingredients bearing an environmental classification

or otherwise a potential hazard for environment are contained in the product according to the composition provided by the applicant and the material safety data sheet.

3. Screen on synergistic interactions

→ There are no indications for synergistic effects for the product or its constituents in the literature.

4. Conclusion

→ Consequently, the environmental risk assessment for the product is based on the active substance and no mixture assessment is needed.

Case Study 2: PT08, Wood preservative

Screening Step

1. Identification of the concerned environmental compartments

The screening step revealed that an exposure of environment is likely. According to the intended use of the product and the applied RMMs only an exposure of the soil_compartment is likely.

2. Identification of Relevant Substances

Besides the four active substances, no other ingredients bearing an environmental classification or otherwise a potential hazard for environment are contained in the product according to the composition provided by the applicant and the material safety data sheet.

3. Screen on synergistic interactions

There are no indications for synergistic effects for the product or its constituents in the literature.

4. Conclusion

Consequently, the environmental risk assessment for the product is based on the four active substances and a mixture assessment is needed.

Tiered assessment scheme

Table 63: Available terrestrial ecotoxicity data and PECs for soil for the four a.s. contained in the product.

a.s.	Effect concentration [mg/]			AF	PNECsoil [mg/kg]	PECsoil [mg/kg]	PEC/PNEC
	Plants	Earthworms	Microorganisms				
1	EC_{50} = 30.0	LC_{50} = 800	EC_{50} = 120.0	1000	0.03	0.01	0.33
2	EC_{50} = 5.0	NOEC = 0.05	EC_{50} = 7.0	50	0.001	$8.5*10^{-5}$	0.085
3	EC_{50} = 22 NOEC = 5.0	NOEC = 0.4	NOEC = 6.0	10	0.04	0.035	0.875
4	NOEC = 1.0	NOEC = 20.0	EC_{50}= 30.0	50	0.02	0.01	0.50

red: values used for PNEC-derivation

Tier 1

$$RQ_{\text{Product}} = \sum_{i=1}^{n}\left(\frac{PEC}{PNEC}\right)_i$$

$RQ_{product}$ = 0.33 + 0.085 + 0.875 + 0.50 = 1.79

→ unacceptable risk for environment

Tier 2

$$RQ_{\text{Product}} = \max \sum_{i=1}^{n} \left(\frac{PEC}{ECx/AF} \right)_i$$

Table 64: Plants

a.s.	PEC [mg/kg]	Effect concentration [mg/kg]	AF	EC_x/AF	$PEC/(EC_x/AF)$
1	0.01	EC_{50} = 30.0	1000	0.03	0,333
2	$8.5*10^{-5}$	EC_{50} = 5.0	50	0.1	0,00085
3	0.035	NOEC = 5.0	10	0.5	0,07
4	0.01	NOEC = 1.0	50	0.02	0,5

$RQ_{product}$ = 0.33 + 0.00085 + 0.07 + 0.5 = 0.904

→ acceptable risk for environment

Table 65: Earthworms

a.s.	PEC [mg/kg]	Effect concentration [mg/kg]	AF	EC_x/AF	$PEC/(EC_x/AF)$
1	0.01	LC_{50} = 800.00	1000	0.8	0.0125
2	$8.5*10^{-5}$	NOEC = 0.05	50	0.001	0.085
3	0.035	NOEC = 0.4	10	0.04	0.875
4	0.01	NOEC = 20	50	0.4	0.025

NOTE: $RQ_{product}$ = 0.125 + 0.085 + 0.875 + 0.025 = 0.9975

→ acceptable risk for environment

Table 66: Microorganisms

a.s.	PEC [mg/kg]	Effect concentration [mg/kg]	AF	EC_x/AF	$PEC/(EC_x/AF)$
1	0.01	EC_{50} = 120	1000	0.12	0,083
2	$8.5*10^{-5}$	EC_{50} = 7.0	50	0.14	0,00060
3	0.035	NOEC = 6.0	10	0.6	0,058
4	0.01	NOEC = 30	50	0.6	0,017

$RQ_{product}$ = 0,083 + 0,00060 + 0,058 + 0,017 = 0.16

→ acceptable risk for environment
→ highest $RQ_{earthworm}$ = 0.9975
→ acceptable risk for soil for all three trophic levels
→ no need to proceed with Tier 3 or 4
→ analogous procedure for all other relevant compartments

11. References

NOTE to the reader

This list of references has been taken from TGD 2003 and supplemented.

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EUROPEAN CHEMICALS AGENCY
ANNANKATU 18, P.O. BOX 400,
FI-00121 HELSINKI, FINLAND
ECHA.EUROPA.EU