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GUIDANCE

Guidance on information requirements and Chemical Safety Assessment

Chapter R.16: Environmental exposure assessment

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Guidance on Information Requirements and Chemical Safety Assessment
Chapter R.16: Environmental exposure assessment

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DOCUMENT HISTORY

Version	Changes	
Version 1.0	First edition	May / July 2008
Version 2.0	Redrafting the section about the general workflow of exposure estimation: The workflow for environmental exposure assessment has been completely redrafted (R.16.1.2). A diagram has been introduced to better illustrate it. First tier assumptions and the iteration/refinement alternatives are also shown. The diagram is consistent with the text and makes clear references to other chapters of the IR-CSA Guidance. Many of the changes in this section and in the whole guidance have been triggered by the need to make the guidance R.16 more relevant for release estimation under REACH, and, in particular, consistent with its general approach which aims to make registrants describe the conditions of safe use. Reworking chapter structure and headings. In particular: The exposure assessment workflow (R.16.1.2) and general principles (R.16.2: local assessment, regional assessment and time frame) have been described first, before the release estimation, fate, distribution and exposure estimation sections. In the previous guidance, these introductory principles were spread across several paragraphs. Both, in the release estimation and in the exposure estimation parts, a clear distinction has been made between first tier assumptions and refinement options for the eventual iteration. The different options for refinement have been listed in two separate paragraphs, one for release estimation (R.16.3.5) and the other for exposure estimation (R.16.8). In the previous version of the guidance, they were spread across different paragraphs. Revision of scenarios for the local assessment Two different scenarios for the local assessment have been introduced. The "Industrial setting" scenario (R.16.2.1.1) describes the releases from industrial point sources. The "Wide dispersive use" scenario (R.16.2.2) describes releases derived from consumers, professional and service life uses. Since releases to water from wide dispersive uses are associated with a municipal sewage treatment plant, they can be assessed as a point source at the local scale. A scenario for outdoor wide dispersive uses, based on releases onto an urban paved surface, collection into a public sewer and treatment in a sewage treatment plant (STP) has been added. A method has been provided to attribute a default tonnage for wide dispersive uses at a local scale. Since all releases to water from each identified wide disperse use will by default enter into the same sewage system, combined risk should be considered. In previous versions of the guidance, the local scenario for wide disperse	May 2010

uses was less visible, and there was no suggestion to add up all disperse uses at the local scale for assessing combined risks.

Tonnage attribution

Default conservative assumptions are now clearly described for the definition of a tonnage for each identified use and at local (R.16.3.2), regional and continental scale (R.16.3.3). If market data or information from downstream users is available, the registrant can overwrite these default values.

Operational conditions described in the exposure scenario

The parameters determining the release rate in the local scenario are expressed in a way now suitable for describing operational conditions in exposure scenarios under REACH (e.g. daily and annual use at an industrial site and daily wide dispersive use, see chapter R.16.3.2). Compared to the previous version of the guidance, the parameters themselves have not changed.

Continental release estimation

A sub-paragraph has been inserted to illustrate the method for calculating the releases at the continental scale starting from the tonnage at EU level, the regional tonnage and the same release factors used at the local and regional scale (within R.16.3.3). No content changes with respect to TGD (2003).

Review of the chapter on Measured data (R.16.4):

The previous paragraph, focused on environmental concentrations, has been expanded to also consider release measurements. The consistency need with RMM/OC, as described in the exposure scenario, has been stressed.

Review of fate, distribution and exposure estimation sections (R.16.5).

This section has undergone minor revisions mainly aimed at avoiding duplication with concepts already mentioned in the previous paragraphs and ensuring consistency with the new release estimation part.

The Appendix A.16.1 has been updated

The link between environmental release categories (ERCs) and the release estimation is limited now to default release factors. All other defaults that may be applied in a tier 1 default assessment have been removed for reasons of consistency.

Two new ERCs, ERC 12A and ERC 12B, related to industrial processing of articles with abrasive techniques have been introduced.

Release factors for direct regional releases onto industrial soil (ERCs 1-7) have been introduced, to be taken into account for regional exposure estimates.

The description of some other ERCs has also been slightly refined, including the explanation on the associated default release factor The following default release factors have been changed:

- ERC 4 to air: 100% instead of 95%;
- ERC 8D to soil: 20% instead of 1%;
- ERC 9A to water: 5% instead of n/a.;

	▪ ERC 10A to water: 3.2% instead of 0.16 × Tservice.	
Version 2.1	Corrigendum: Replacing references to DSD/DPD with references to CLP. Implementing minor recommendations for nanomaterials from the RIP-oN3 report. Implementing further minor editorial changes/corrections (notably to correct over-zealous replacements of "preparation" by "mixture" in some contexts in version 2).	October 2012
Version 3.0	Full update of the guidance to address and implement the latest developments in projects related to exposure scenarios (ESs), chemical safety reports (CSRs) and Chesar (ECHA's application to help companies carry out their chemical safety assessments (CSAs) and prepare their CSRs and ES for communication in the supply chain) and the practical experience in implementing the principles for a chemical risk assessment. The general approach and principles for the environmental exposure assessment remain generally the same but the structure of the guidance has been completely revised. The new structure aims at presenting the information relevant for carrying out an environmental exposure assessment in a more complete, coherent and user friendly way and better correspond to the logic of the safety assessment as laid down in the REACH legislation. The focus of the guidance has been enlarged by moving from exposure estimation to exposure assessment. In this respect, the section on release estimation has been expanded by further elaborating existing information. In the core body of the guidance, the standard assessment approach and underpinning principles are described. Technical details and calculations, which are generally embedded in the exposure estimation tools, and relevant information for refined assessment, are moved to the appendices. The update covers the following main issues: • Redrafting of the introductory chapter R.16.1 to present an overview of the assessment approach and main principles; new subchapters on the definition of the scope of the assessment and the environmental targets with a new figure to illustrate the identification of the scope of the assessment. Added reference to contributing activities (CAs) and contributing scenarios (CSs) and description on their role in exposure assessment. Added link to waste life cycle stage assessment and reference to Chapter R.18. • New chapter R.16.2 on the relevant information to carry out a release assessment. The chapter illustrates the key elements: definition of conditions of use (including estimation of tonnage for widespread uses, tonnage for uses at industrial sites and tonnage for regional estimation) and available estimation methods. The chapter is based on existing information in original 16.3 and Chapter R.13. Section on site-specific information expanded with considerations on use of measures data. Furthermore relevant considerations on article service life have been expanded incorporating information from R.17 and adding an equation for the calculation of	February 2016

		substance quantity. Information on use of Specific Environmental Release categories (SPERCs) expanded. Added specific considerations for releases from waste life-cycle stage and link to Chapter R.18. • New chapter R.16.3 on the Biological Sewage Treatment Plant, its role as an RMM and in the standard default assessment. The chapter is based on existing information in original 16.6.5. Added clarification about the version of SimpleTreat currently implemented in EUSES and described in the Guidance not being the latest one. Indication that different more up to date sub-models exist and EUSES update needs have been identified. • New chapter R.16.4 on exposure estimation: illustration of the existing methods for a default assessment, descriptions of the relevant distribution and fate processes and a general overview of PEC estimation for each environmental compartment (including humans via environment). The chapter is based on existing information in original 16.5 and 16.6. • New chapter R.16.5 on the use of the outcome of the exposure assessment for risk characterisation and link to Part E. • New chapter R.16.6 on the summary of the elements relevant for a standard and refined assessment. • Deletion from Appendix 16-1 of the tables 16-21 and 16-22 describing the ERCs (reference is provided to the updated guidance R.12). Modification of release factor for water for ERC 8C from 1% to 30% (or 5%, depending on whether the activity is water based or not) as the original figure had been set omitting a variety of relevant processes. For water-based activities the new figure is aligned with Table A4.1 (textile dyeing) and for non-water-based activities with Table A4.5 (use of paints) of TGD Part II (EC, 2003). The release factor for ERC 8F has been adjusted accordingly (relevant only regarding non-water-based activity). Addition of new ERC12C. • Deletion of original Appendix 16-2 on the overview of Emission Scenario Documents and provision of references to updated lists available on the web. • New Appendix 16-3 collecting all the calculations embedded in the available model to estimate fate and distribution parameters and the predicted environmental concentration (PEC) in each environmental compartment. The new Appendix collects existing information originally spread throughout original chapters of R.16.5 and R.16.6. • New Appendix 16-4 on detailed regional assessment and relevant calculations (reorganisation of information originally covered in 16.6.6.8). • New Appendix 16-5 providing more information on existing models (EUSES and some other tools such as CHARM or the ECPA LET). • New Appendix 16-6 on release estimation from articles. Information relevant for the environment previously	

	addressed in Chapter R.17 has been updated and moved to this Appendix. • New Appendix 16-7 on selection and evaluation of measured data. Information originally covered in Chapter R.16.4 updated and moved to this Appendix. • Substitution of term "wide dispersive" by "widespread" for better alignment with R.12. • Correction of identified errors in the equations carried over from the original version of the Guidance. • Update of scientific references and creation of new unique list at the end of the guidance.	
Version 4.0	The following changes have been introduced in this version: • Adaptation of the text to clarify that the estimation tool EUSES, is currently maintained by ECHA in Chesar Platform (R.16.1.1, , R16.4.1.2, Appendix A.16-4) • In the calculation of the PEC local sediment, the PEC regional is considered as a background concentration for the local scale (A.16-2.3.4) • Adaptation of equations to consider the natural background concentration for inorganics for (sea)water and (sea) water sediment and soil compartments (A.16-2.3.3, A.16-2.3.4, A.16-2.3.5, A.16-2.3.6) • Update of the version of SimpleTreat from 3.0 to 4.0 (R.16.3.2) • Introduction of the differentiation of the sediment and suspended matter partition coefficients between freshwater and seawater (A.16-2.2.1) • Introduction of the Arrhenius equation for calculating the half-lives (DT50 values) of the (bio)degradation processes (A.16-2.2.2) • Update of the standard factors derived from OPS gaussian emission model (A.16-2.3.2) • Adaptation of the text to harmonise the use of 'agricultural soil' to refer to the arable land and grassland together • Introduction of the release and exposure model to be used in case of direct releases to agricultural soil (A.16-2.4) • Introduction of model to account for removal in the sewer (A.16-2.3.1) • Removal of obsolete chapters and respective references in the text (Appendix A.16-2 and section A.16-5.2) • Conversion factor for suspended matter added (A.16-2.1)	XXX 2024

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PREFACE

This document describes the information requirements under REACH Regulation with regard to substance properties, exposure, use and risk management measures, and the chemical safety assessment. It is part of a series of guidance documents that are aimed to help all stakeholders with their preparation for fulfilling their obligations under the REACH Regulation. These documents cover detailed guidance for a range of essential REACH processes as well as for some specific scientific and/or technical methods that industry or authorities need to make use of under the REACH Regulation.

The original version of the guidance documents was drafted and discussed within the REACH Implementation Projects (RIPs) led by the European Commission services, involving stakeholders from Member States, industry and non-governmental organisations. The European Chemicals Agency (ECHA) updates these guidance documents following the Consultation procedure on guidance. These guidance documents can be obtained via the website of the European Chemicals Agency (http://echa.europa.eu/web/guest/guidance-documents/guidance-on-reach).

This document relates to the REACH Regulation (EC) No 1907/2006 of the European Parliament and of the Council of 18 December 2006[1] and its amendments until the publication of this guidance.

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[1] 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 (OJ L 396, 30.12.2006).

Convention for citing the REACH Regulation

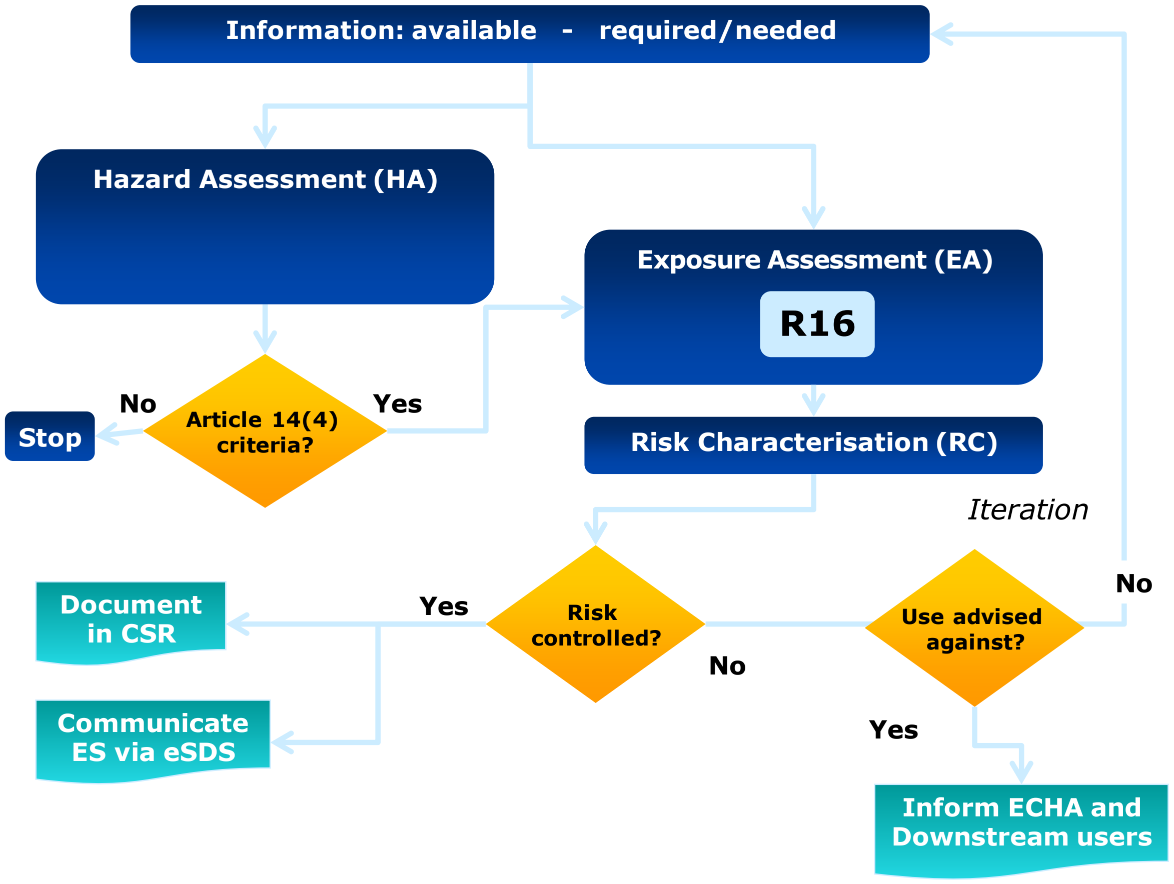
Where the REACH Regulation is cited literally, this is indicated by text in italics between quotes.

Table of terms and abbreviations

See Chapter R.20

Pathfinder

The figure below indicates the location of Chapter R.16 within the Guidance Document.



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R.16. ENVIRONMENTAL EXPOSURE ASSESSMENT

R.16.1 INTRODUCTION

R.16.1.1 Aim of this guidance

This document provides guidance on how to carry out environmental exposure assessment in the context of REACH. REACH requires, according to Article 14(4), exposure assessment and subsequent risk characterisation to be carried out for substances subject to registration, which are manufactured or imported in quantities equal to or greater than 10 tonnes/year, and where the substance meets any of the criteria to be classified as hazardous.

More specifically, this guidance document deals with:

- The description of the conditions of use and the related estimation of the releases to air, wastewater, surface water, and soil at local and regional scale;
- Fate and distribution of the releases in biological sewage treatment plants and environmental compartments (air, soil, surface water, sediment, biota);
- Calculation of exposure concentrations/doses for, respectively:
    - Environmental compartments, in terms of predicted environmental concentrations (PECs), at both local and regional scales, covering both direct exposure of organisms and exposure via the food chain for predators;
    - Humans via the environment in terms of inhalation (intake via air) and human daily intake of the substance through drinking water, fish, leaf crops, root crops, meat and dairy products, at local and regional scales.

Most of the current guidance on environmental exposure estimation has been developed for organic substances. Metals and metal compounds present particular issues (natural background and historical releases, speciation, adsorption/desorption behaviour, differences in bioavailability) which require specific adaptations when performing the exposure assessment. These issues are considered in the Appendix A.7.13-2 of the *Guidance on Information Requirement and Chemical Safety Assessment* (IR&CSA)[2].

The approach for exposure estimation presented in this Guidance follows the approach and methodology used in EUSES (European Union System for Evaluation of Substances, Vermeire et al. 1997). EUSES is a decision-support system for the evaluation of the risks of substances to humans and the environment. The system is based on the EU Technical Guidance Documents (TGDs; EC-TGD, 2003) for the risk assessment of new and existing substances and biocides. EUSES is currently owned and updated by ECHA. EUSES is, from 2024, completely reimplemented in the ECHA chemical risk assessment tool named Chesar Platform[3].

The final outcome of exposure assessment under REACH is the description of the conditions for safe use (exposure scenarios). The exposure assessment comprises an assessment of the expected exposures of identified targets under the actual or anticipated conditions of use. These exposure levels are used to characterise the risks by comparing them with the outcome of the hazard assessment.

Note: In line with EUSES, the current document systematically distinguishes between releases before the "biological" sewage treatment plant (STP), i.e. the releases from the use-process as such - with or without particular measures to prevent losses and/or to treat emissions onsite -

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[2] The full Guidance on IR&CSA is available at http://echa.europa.eu/guidance-documents/guidance-on-information-requirements-and-chemical-safety-assessment.

[3] Chesar Platform available at: https://chesar.echa.europa.eu/.

and releases (if needed) after the biological STP. Biological refers to both the municipal STP and the industrial STP (which has by default a similar setting as the biological municipal STP). The "biological treatment" is modelled by SimpleTreat in EUSES, and refers to biodegradation and associated mechanisms to remove substances from the water pathway (e.g. adsorption and sedimentation, volatilisation, etc. See section R.16.3 for further information). Reference to application of sludge to agricultural soil is also systematically associated to the biological STP. Other types of wastewater treatment are considered under risk management measures (see section R.16.2.2.3).

Note: Exposure assessment under REACH should in principle cover the releases from the waste life stage, i.e. treatment of waste from manufacture or use of the substance or treatment of articles at the end of their service life. In particular when the treatment of waste (aiming at final disposal or recovery) may lead to releases that are significantly higher than those from other life cycle stages, the registrant should perform an exposure assessment. Such assessment is not addressed in the current guidance but *in Chapter R.18 of the Guidance on IR&CSA*.

R.16.1.2 Workflow for environmental exposure assessment

The environmental exposure assessment is built upon the following previously performed processes: collection of information on relevant **substance properties** (physical-chemical, fate as well as (eco)toxicological properties), hazard assessment and **mapping of uses**.

Substance properties such as vapour pressure, water solubility, molecular weight, octanol-water partition coefficient, melting point and biodegradability have an impact on the fate of the substance in the environment and are therefore needed as a minimum for the environmental exposure estimation.

Mapping of uses consists of identifying all the uses of the substance including realistic information on the corresponding conditions of use. This can be efficiently done by retrieving information from sector *use maps*. Such use maps provide a harmonised description of the main uses relevant for a sector and information on typical conditions of use[4].

The whole exposure assessment is therefore built upon the definition of the life-cycle stages of the substance giving rise to release/exposure (see *part D* and *Chapter R.12 of the Guidance on IR&CSA*) and the identification of the covered uses for each life-cycle step. Once this framework has been completed, the release and exposure estimations can start.

The exposure assessment consists of the following steps:

1. Determination of **operational conditions (OCs)** and **risk management measures (RMMs)**, including, for example, the amount of the substance, availability of filters, scrubbers, municipal sewage treatment plants etc.; OCs and RMMs constitute the "conditions of use" (see section R.16.2.2);

2. **Release estimation** consisting of the determination of the local and regional release rates for each use (section R.16.2), starting from the appropriate release factors and the tonnage assigned to any identified use and taking into account a realistic effectiveness of the RMMs assumed to be in place;

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[4] Use maps can be developed by suppliers or downstream user sector associations; for more details see guidance Chapter R.12 and the ECHA use maps library (https://echa.europa.eu/csr-es-roadmap/use-maps/use-maps-library). The full list of ECHA Guidance documents is available at http://echa.europa.eu/guidance-documents/guidance-on-reach.

3. **Environmental distribution and fate** and **exposure estimation**. The distribution and fate of a substance in the environment (section R.16.4.2 and A.16-2.2) is assessed at local and regional scale. Consequently, predicted environmental concentration (PEC) values for each environmental compartment and the daily intake of humans via the environment (section R.16.4.3 and for further details Appendices A.16-2.3 and A.16-2.4) are derived at local and regional scales. A single overall PEC is derived for (top-) predators (section R.16.4.3.8) based on local and regional contributions. PEC values for the sewage treatment plant are calculated at the local scale (section R.16.3 and R.16.4.3.1 and Appendix A.16-2.3.1).

Exposure assessment can be an iterative process. If the **risk characterisation** (see section R.16.5 for general principles and Part E for details) indicates that the applied risk management measures and operational conditions are not adequate to control risks occurring from the manufacture and all identified uses (Risk Characterisation Ratio, RCR > 1), the exposure assessment may need to be refined. This refinement is possible at every step in the workflow.

The following flowchart (Figure R.16-1) illustrates the steps to carry out a complete chemical safety assessment for the environment. The part of the overall process covered by this Guidance document is included in the grey box. Where to find guidance on the remaining steps is also indicated.

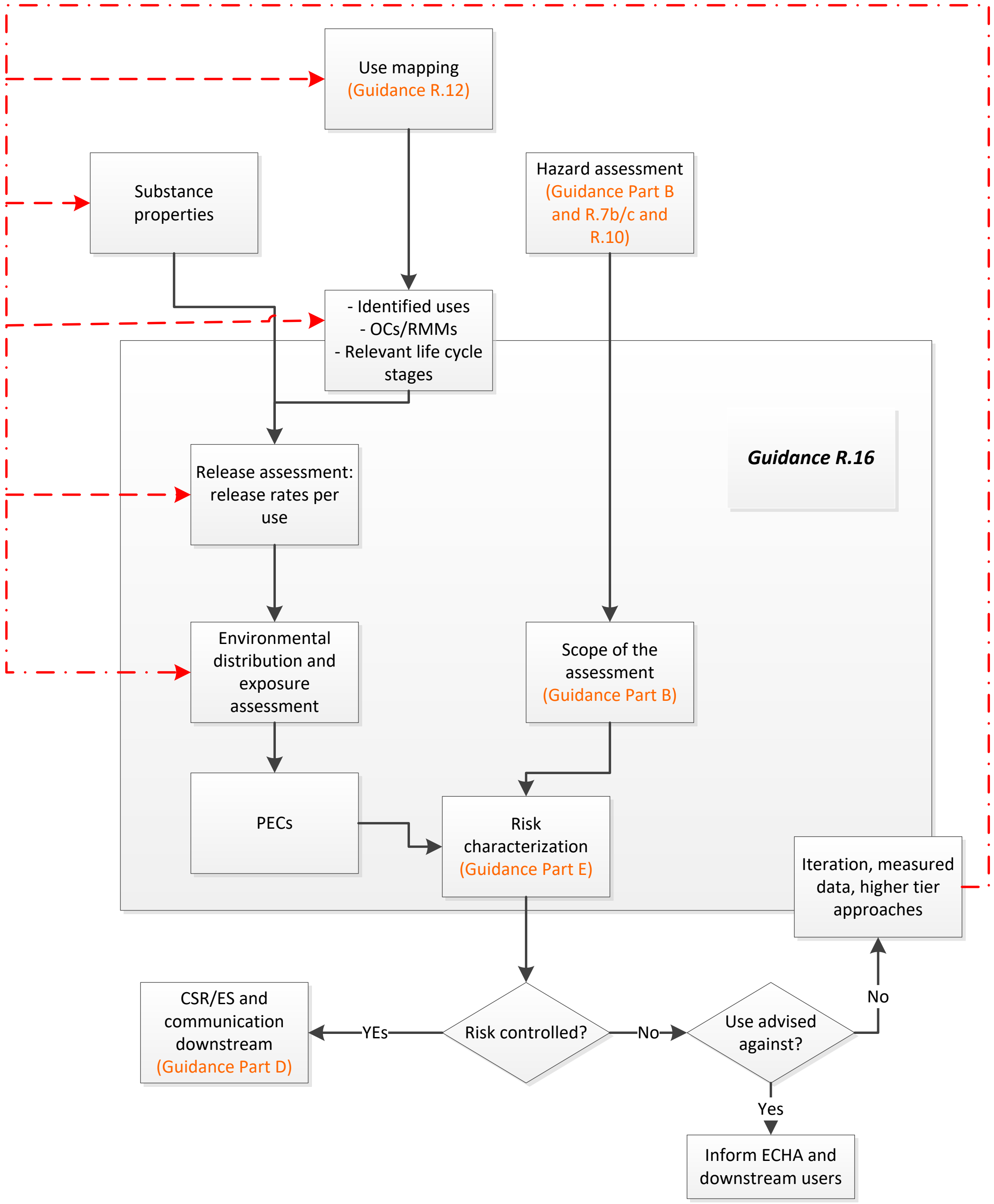

Figure R.16-1 Workflow for environmental exposure assessment

If the risks are not assessed as being controlled after a first assessment, the assessment may be iterated (iteration options are indicated with the red dashed arrows in the Figure R.16-1), either by refining the hazard data (deriving predicted no effect concentrations (PNECs) on the basis of long-term data instead of short-term data for example) or exposure concentrations. The latter may be iterated by:

- Improving the release estimation by:

    - refining or adding more specific **RMMs/OCs** or refining the **tonnage for the use;**
    - refining the parameters in the applied release estimation method based on representative onsite data, such as **release measurement**, which should be linked with the RMMs/OCs.
- Improving the exposure estimation by:
    - using representative **measured data** (e.g. environmental concentrations or measured river flow rates) corresponding to OCs/RMMs in place and assigned to the appropriate spatial scale. More information about the use of measured data can be found in section R.16.4.1.3 and on their selection in Appendix A.16-6;
    - using **higher tier exposure** estimation tools (see Appendix A.16-4.2 for more information);
    - refining the **substance properties** (e.g. degradation rates, partitioning coefficient). The exposure assessment might lead to worst-case results because of limited knowledge of the properties having an impact on fate and distribution of the substance. It might therefore be necessary to refine information related to degradation rates, partitioning coefficients, vapour pressure, water solubility etc.
- Refining the **characterisation of environmental compartments for site-specific assessment** (see section R.16.2.3.3.1). Local and regional environments are not actual sites or regions, but standardised environments based on generic parameters (see Appendix A.16-2.1). When more specific information is available on the location of release sources, this information can be used to deviate from these default parameters and refine the assessment.

R.16.1.3 Scope of the environmental assessment

Companies preparing a registration dossier and carrying out a chemical safety assessment (CSA) will need to decide:

i) whether exposure assessment and risk characterisation are needed, and if yes,

ii) what the required scope of the exposure assessment is.

The starting point in this guidance is that the registrant concluded that exposure assessment is needed because the substance fulfils the criteria of Article 14(4) of REACH. Detailed guidance on establishing whether exposure assessment is required is provided in *Part B.8 of the Guidance on IR&CSA*. This section provides some information on how to define the scope of the environmental exposure assessment more precisely (i.e. whether exposure assessment is expected for an environmental compartment) and the type of risk characterisation required on the basis of the outcome of the hazard assessment. The exposure assessment must cover any exposure that may relate to hazards identified in the hazard assessment. This may include exposure of humans through the environment via ambient air, drinking water and food items.

Substances may chemically transform during use or in the environment, e.g. by hydrolysis, biodegradation or chemical reaction. When such transformation products (or "degradation products" or "metabolites") are stable and/or toxic they should be taken into account in the environmental assessment.

R.16.1.3.1 Environmental protection targets to be addressed

The environmental protection targets to be taken into account for the assessment are listed in Table R.16-1 below. Each of them may be exposed to a certain concentration level of the substance in a related compartment. The hazard for each protection target is to be identified.

It may be possible to derive a PNEC (quantitative threshold for no effect for a given protection target) or it may also be that the hazard is concluded in a qualitative way (see guidance Part B.7). If a PNEC can be derived, the name of the PNEC for each protection target is listed in Table R.16-1.

Table R.16-1 Environmental protection targets

Protection target		Related compartment	PNEC
Biological sewage treatment plant:	Microorganisms	Sewage treatment plant aeration tank	$PNEC_{microorganisms}$
Freshwater ecosystem:	Freshwater organisms	Freshwater	$PNEC_{water}$ (freshwater)
	Sediment organisms	Freshwater sediments	$PNEC_{sed}$ (freshwater)
	(Fish eating) predators[5]	Fish	$PNEC_{oral}$
Marine ecosystem:	Marine water organisms	Marine water	$PNEC_{saltwater}$
	Sediment organisms	Marine sediments	$PNEC_{sed,marine}$
	(Fish eating) predators[5]	Marine fish	$PNEC_{oral}$
	Top predators[5]	Marine predators	$PNEC_{oral}$
Terrestrial ecosystem:	Soil organisms	Soil	$PNEC_{soil}$
	(Worm eating) predators[5]	Earthworms	$PNEC_{oral}$
Air	Atmosphere	Air	$PNEC_{air}$[6]

Knowledge of acute toxicity to freshwater organisms is usually available. For soil and sediment organisms, unless specific test results can demonstrate that no hazard can be identified, a hazard will be systematically assumed if a hazard is identified for aquatic organisms.

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

[6] Usually a $PNEC_{air}$ is not available and a qualitative assessment is to be carried out if some hazard is identified such as ozone depleting. 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.

For substances with low water solubility, the hazard cannot be concluded on the basis of acute aquatic toxicity tests only; a long-term test will usually be needed.

For substances with a high potential for adsorption, even if no hazard can be identified for aquatic organisms, data on soil and sediment organisms may be needed to identify the hazard for soil and sediment organisms.

More details on testing strategies for the environment are provided in *Part B.8* and *Chapters R7b/R.7c/R10 of the Guidance on IR&CSA*.

In addition, **humans exposed via the environment** also need to be protected. This is achieved by assessing:

- Exposure via inhalation; and
- Exposure via the oral route (ingesting drinking water and different food items).

R.16.1.3.2 Identification of the scope of exposure assessment and type of risk characterisation

As mentioned above for each protection target, a conclusion on the hazard has to be reported and can be one of the following:

- A PNEC can be derived (most common situation): quantitative risk characterisation is carried out. This consists of comparing the predicted exposure concentration (PEC) in an environmental compartment with the related PNEC. This is done separately for each of the environmental protection targets (see section R.16.5)
- No PNEC can be derived and:
    - No hazard is identified for that protection target, therefore no exposure assessment is required;
    - A hazard is identified or cannot be excluded and therefore a qualitative risk characterisation will have to be carried out.

Details on PNEC derivation in the different environmental compartments are provided in *Chapter R.10 of the Guidance on IR&CSA*.

For human exposure via the environment, the systemic and local hazard for long term effect when exposed via inhalation and the systemic long term hazard via the oral route serve as basis for the identification of the scope of the exposure assessment together with tonnage considerations (see "Particular considerations (ii)” in this section). Note that even if it can be concluded that the substance is not hazardous for the environmental protection targets, release to the environment and exposure assessment may be needed if a systemic long term hazard is identified for humans. Indeed to estimate the exposure of humans via the environment, concentration of the substance in the various environmental compartments is needed.

For each use, the exposure assessment and risk characterisation must address all the protection targets for which a hazard has been identified. For adapting information requirements based on exposure considerations, an exposure assessment is to be carried out.

For substances fulfilling the PBT or vPvB criteria reliable prediction of long-term exposure is not possible. An emission characterisation and risk characterisation must be conducted. The outcome will be the identification and implementation of RMMs which minimise the emissions to the environment. The approach described in section R.11.3 of *Chapter R.11 of the Guidance on IR&CSA* should be followed.

Figure 16-2 illustrates in a schematic way how the scope of exposure assessment is determined based on the information available for each protection target. The hazard conclusions are illustrated in a similar way to that in which they can be reported in IUCLID section 6 Summary. Not all specific cases are illustrated.

First of all it needs to be clarified whether data is available or testing needs to be carried out for the specific endpoint. This depends on the information requirements (Annex VII to X of REACH) and on the possibilities for their adaptation (Annex XI of REACH). Two situations can occur:

- Although hazard cannot be excluded, it is not possible to get hazard information (testing is technically not feasible) or the assessment can be carried out without hazard information as no exposure is expected.

- Hazard information is not required (e.g. from Annex VII to X column 2 waiver) as other information is sufficient to conclude that no hazard is expected.

More guidance can be found in Part B (sections B1 to B6). Guidance on the testing strategies can be found in *Chapters R.7a/b/c of the Guidance on IR&CSA*.

If data is available the next step is to assess whether a hazard is identified. Hazards are identified according to Sections 1 to 4 of Annex I of REACH. Such identified hazards are of three types:

- hazards for which there are classification criteria and there is information to establish that the substance meets the criteria and is therefore classified;

- hazards for which there are classification criteria, but the severity of the effects seen in the test is lower than the criteria for classification and so the substance is not classified. The registrant should consider whether adverse effects have been observed in studies conducted at the highest practicable & biologically-relevant concentration on environmental toxicity.

- hazards for which currently no classification criteria exist, but there is information to show that the substance has such hazardous properties.

If none of the above is met then it can be concluded that no hazard is identified for the protection target. More guidance can be found in Part B.8.4.

For secondary poisoning specific considerations are made depending on the potential for bioaccumulation of the substance (see the "Particular considerations (i)" below).

For the environment if effects are observed it is usually possible to derive a PNEC for all protection targets (see Table R.16-1 and guidance R.10), with the exception of air. For air other considerations mainly related to the composition of atmosphere are made (e.g. ozone depletion, photochemical ozone creation potential).

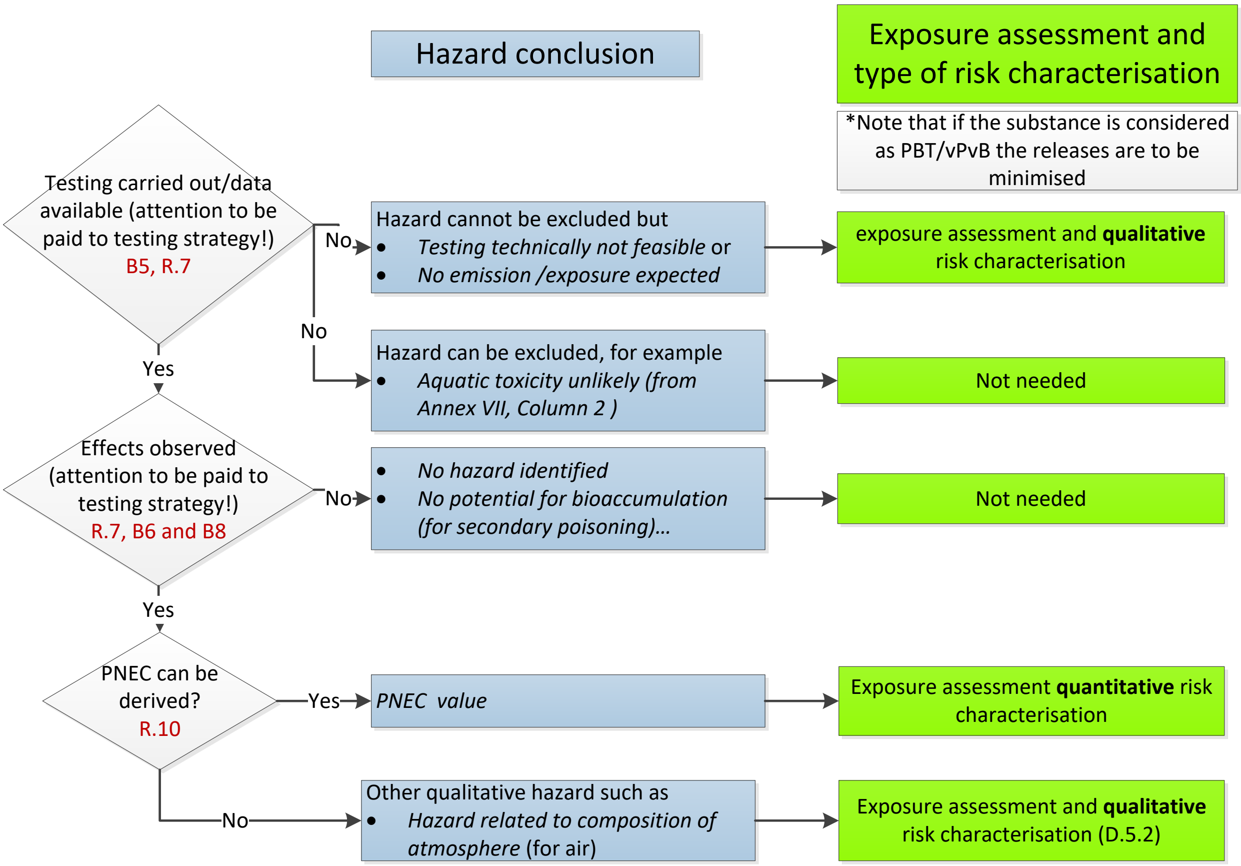

Figure 16-2: Identification of the scope of the assessment and type of risk characterisation for each protection target

Particular considerations (i): scope of exposure assessment for predators and top predators (secondary poisoning)

Secondary poisoning relates to toxic effects to organisms in higher trophic levels 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. If a substance has a bioaccumulation potential and also has a potential to cause toxic effects if accumulated in higher organisms, a detailed assessment of secondary poisoning should be conducted (see also Part B.7.2.7).

Indications of bioaccumulation potential

The first step in the assessment strategy is to consider whether there are indications for bioaccumulation potential.

The most important and widely accepted indication of bioaccumulation potential is a high value of the n-octanol/water partition coefficient (K_{ow}). 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. If a substance:

- has a log $K_{ow} \geq 3$ and a molecular weight below 700 g/mol; 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 of hydrolysis (half-life less than 12 hours) or biodegradability (substance is readily biodegradable)

there is an indication of bioaccumulation potential. See section R.7.10.3 of *Chapter R.7c of the Guidance on IR&CSA* for more information on indicators for bioaccumulation and their interpretation and use.

Potential to cause toxic effects if the substance is accumulated (in higher organisms) via the food chain

It is necessary to consider whether the substance has a potential to cause toxic effects if accumulated in higher organisms (i.e. secondary poisoning). This assessment is based on classifications on the basis of mammalian toxicity data, i.e. the classification includes at least one of the hazard statements H360 "May damage fertility or the unborn child", H361 "Suspected of damaging fertility or the unborn child", H362 "May cause harm to breastfed children", H372 "Causes damage to organs through prolonged or repeated exposure", H373 "May cause damage to organs through prolonged or repeated exposure". When available, avian toxicity may also be considered (more details are available in Guidance R.7.10.14 and R.10.8). Here it is assumed that the available mammalian toxicity data can give an indication on the possible risks of the substance to higher organisms in the environment.

For genotoxic carcinogens there is no need to carry out an assessment for secondary poisoning as the approach followed in the risk assessment for humans indirectly exposed via the environment[7] is expected to also be protective for individual top predators.

If a substance is classified accordingly or if there is any indication of possible effects if the substance is accumulated in higher organisms (e.g. endocrine disruption) then the substance should be considered to have the potential to cause toxic effects.

Particular considerations (ii): scope of exposure assessment for indirect exposure of humans

An assessment of indirect exposure of humans via the environment is generally only conducted if:

- the tonnage >1 000 t/y or
- the tonnage >100 t/Y and the substance is classified
    - as STOT RE[8] 1; or
    - as a carcinogen or mutagen (any category); or
    - as toxic to reproduction (categories 1A or 1B).

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[7] The approach in the human health risk assessment for genotoxic carcinogens is not applicable in the environmental part as the tumour incidence rates and subsequent cancer risks are related to individual risks in humans and it is in most cases difficult to link those effects to populations.

[8] Specific target organ toxicity – repeated exposure.

R.16.1.4 The environmental exposure assessment approach: main principles

The release of a substance and subsequent exposure of the environment are in principle assessed on two spatial scales: **locally** in the vicinity of a representative source of the release to the environment, and **regionally** for a larger area which includes all release sources in that area.

At the local scale, three release scenarios are distinguished to assess the release to the environment:

- for uses taking place at industrial sites; and
- for uses taking place in a widespread manner[9]:
    - uses in a municipality (town) where the releases to water are expected to be collected via a sewer system to be (potentially) treated in a municipal wastewater treatment plant;
    - direct emissions to agricultural soil (such as application of fertilizers and plant protection products in agricultural soil[10]).

It should be noted that in this document the term ‘agricultural soil’ refers to the arable land and grassland together.

This section presents the main elements defining the current approach for an environmental assessment. In the subsequent sections, release estimation and exposure estimation are discussed separately and in more detail.

A clear description of uses is a key pre-requisite for the registrant’s safety assessment (where required) and also for the subsequent communication of the conditions of safe use down the supply chain. Uses may be described by sector associations and be made available to registrants in use maps.

The following life-cycle stages are assumed to take place at “industrial sites”:

- Manufacture;
- Formulation and repacking;
- Use at industrial site;
- Service life at industrial site (use of articles or processing of articles)

The following life-cycle stages are assumed to be “widespread”, i.e. used by consumers or by many users in the public domain, including small, non-industrial companies:

- Widespread use by professional workers;
- Use by consumers;
- Service life by professional workers and consumers.

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[9] Note that for consistency with use description (*Chapter R.12 of the Guidance on IR&CSA*) the term “wide dispersive” previously used is now replaced by the term “widespread”. More information is provided in *Chapter R.12*.

[10] Relevant in case of the assessment of co-formulants of plant protection products and fertilizers (the assessment of the active substances is not covered by REACH)

Chapter R.12 of the guidance on IR&CSA provides details on the various life-cycle stages of a substance and how uses can be described. *Chapter R.18 of the guidance on IR&CSA* provides details on how to determine the activities carried out with waste containing the substances.

For each life-cycle stage, one or more uses can be identified. The release pattern and the estimated release factor are closely related to the life-cycle stages of a substance. The entire life-cycle of a substance, as shown in Figure R.16-3, should be taken into account for the assessment.

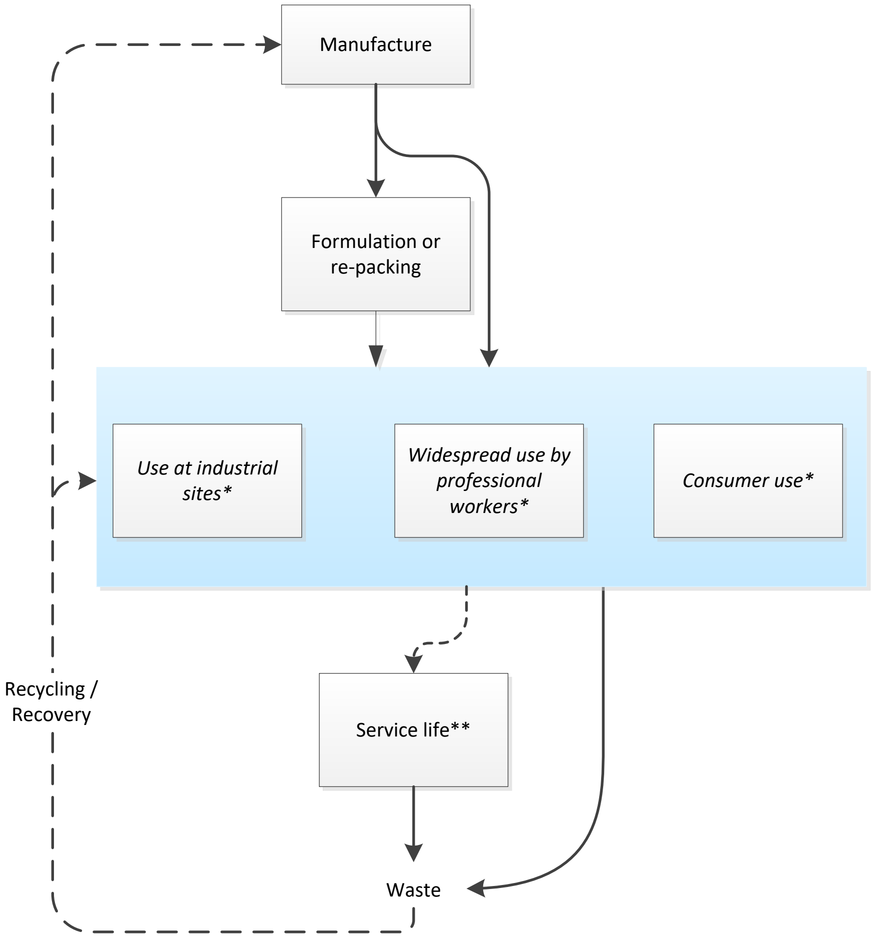

Figure R.16-3: Life-cycle stages of substances (*end uses; **includes processing of articles at industrial sites)

A use may consist of one or more **contributing activities.** Within the use, the contributing activities from the environment perspective and from human health perspective (worker or consumer) are usually described and assessed independently from each other. From the environment perspective usually only one contributing activity per use is defined characterising the process carried out at a site. From the worker or consumer perspective however usually several subsequent/alternative activities are defined for a use.

For each contributing activity, the conditions of safe use need to be described in a contributing scenario. If a use can take place in different conditions then several contributing scenarios may be defined to reflect these differences. For example, more stringent exposure controls may be needed when operating with large amounts of a substance, or different application-techniques may be used for the same purpose but leading to different levels of release. In principle the registrant has the choice to define a use from the environmental perspective as including different contributing activities, or alternatively, the registrant may describe different techniques applied for the same purpose as different uses. For more information on the split between uses and contributing activities, see *Chapter R.12 of the Guidance on IR&CSA*.

Figure R.16-4 below illustrates the relation between use, contributing activities and contributing scenarios.

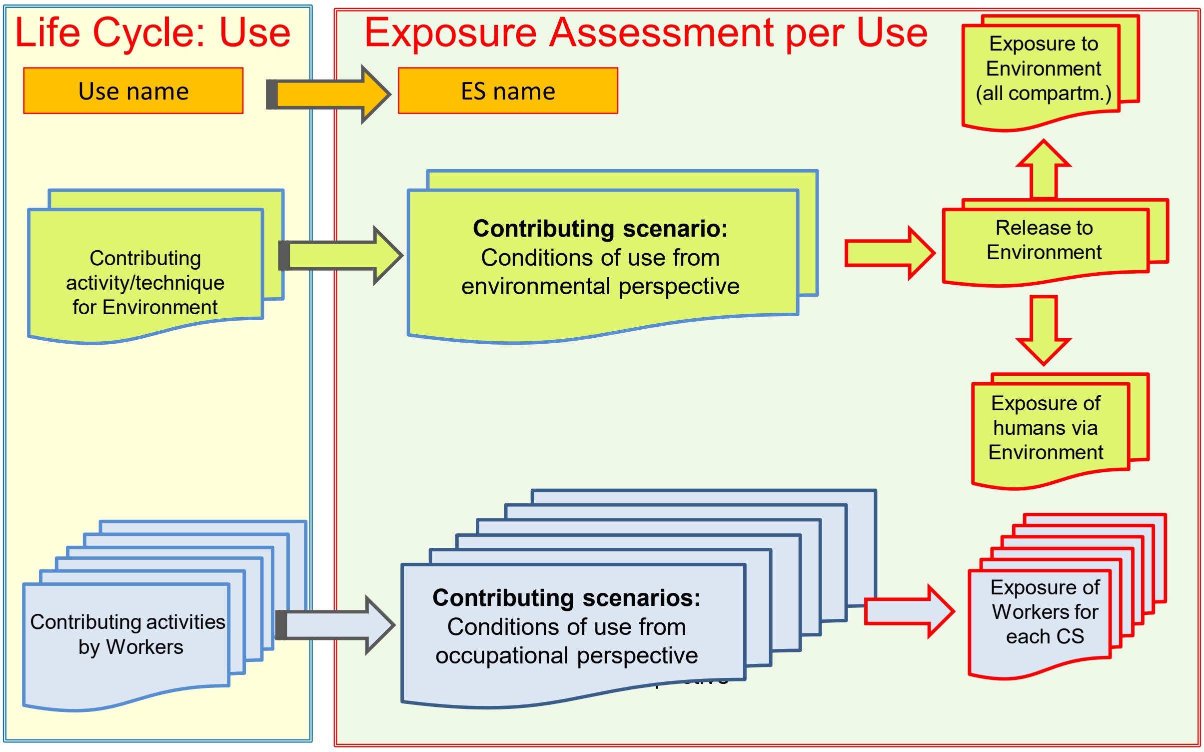

Figure R.16-4: Uses, contributing activities and contributing scenarios: exposure assessment per use

R.16.1.4.1 Local assessment

The concentrations of substances released from a single point source (industrial site or standard municipal biological STP) or from widespread uses that do not pass via STP[11]are to be assessed after release to the environment. The exposure targets are assumed to be exposed at the vicinity of the release point. In general, concentrations are calculated on the basis of a realistic daily release rate or amount (see section R.16.2.1).

Predators, humans and terrestrial organisms are assumed to be exposed to levels averaged over a longer period, and therefore exposure is derived from yearly averaged release rates (instead of daily release rates). This is because exposure is assumed not to be influenced by temporal fluctuation in release rates. In the case of predators and human beings, these fluctuations are also of a rather short-term nature compared to their life span and the time scale on which chronic effects are considered.

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[11] In the present document only the direct application to agricultural soil is considered a widespread use with emissions that do not pass the STP.

In principle, after release to the environment, degradation in the environment and distribution processes should be taken into consideration to estimate the concentrations at the local scale. However, because of the relatively short time between release and exposure, concentrations at local scales are almost entirely controlled by initial mixing (dilution into environmental compartment) and adsorption on suspended matter. Biodegradation may take a role for the soil compartment only. No other process is considered in the calculation of local PECs.

Figure R.16-5 shows the relationship between the local release routes and the subsequent distribution process modelled for the environmental compartments.

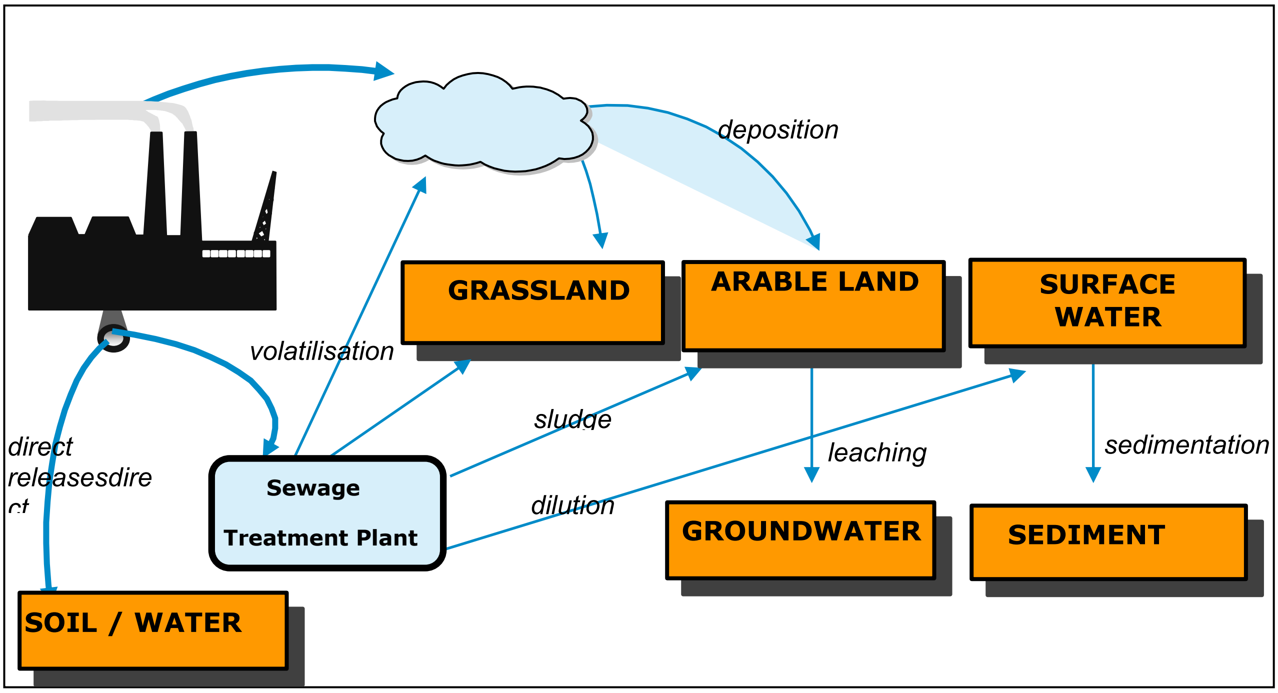

Figure R.16-5: Local distribution processes (for the scenario related to uses at industrial site)

Considerations for uses at industrial sites

Usually, a **generic assessment** is carried out to develop exposure scenarios that can be communicated down the supply chain. These may or may not include alternative contributing scenarios for a given use (e.g. condition of use at large site and conditions of use at small site).

Each use or contributing activity/technique for the environment is usually assessed independently. A combined assessment for several uses (or techniques for a same use) taking place at a same site is usually not covered in the registration dossier, as the variety of combination across the registrants market may be too wide. Each of the site operators downstream will have to ensure that the combination of all their activities carried out at the same site is still safe.

In some cases however, a **site-specific** assessment may be carried out, where more specific data available to the registrants (e.g. corresponding to their own use or to the use of a specific customer or group of customers where the activities are carried out in a similar way) may be used. When information is available to registrants that a combination of several activities (being either several techniques for the same use or various uses taking place at the same site[12]) are often taking place within one site, they are advised to cover the combination of those activities in their assessment. In this case, the registrant would combine those assessments in the "combined risk" section of the CSR.

Considerations for widespread uses

- Uses in a municipality (town)

These widespread uses are assumed to occur in an urban infrastructure. The assumption is that the substance is used by consumers or by many users in the public domain, including small, non-industrial companies. Releases to water are assumed to be collected in a central public sewage system and are then treated by a biological STP. Since the releases to water from all the widespread uses can, by default, be assumed to enter into the same sewage system, combined risk from all the widespread uses should be considered.

- Direct emissions to agricultural soil

This guidance only covers the assessment of uses related to the direct application to agricultural soil such as application of fertilizers or plant protection products. It is to be noted that 'agricultural soil' refers to the combination of arable land and grassland.

R.16.1.4.2 Regional assessment

The concentrations of substances released from all sources in a larger area are assessed for a generic regional environment. The distribution and fate of the substance further than in the vicinity of the release are taken into account. The regional concentrations are used as background concentrations in the calculation of the local PEC. Depending on the case, the contribution of the regional background to the local concentration of the substance can range between insignificant and significant.

For calculating the regional PEC, a multimedia fate-modelling approach can be used (e.g. the SimpleBox model integrated in EUSES, see section R.16.4). All releases to each environmental compartment for each use are taken into account. Regional releases of substances are assumed to occur continuously over the year. Therefore, average exposure levels in space and time are calculated by the steady-state[13] model for the regional scale using annual release rates (see section R.16.2.1). Since releases and fate processes are assumed to take place over an infinite time (many years), regional exposure concentrations can be seen as worst case approximations.

The model for the fate of the substance at the regional scale differs from the model for the fate at the local scale, mainly taking into account that more time is available for transport and transformation processes.

Figure R.16-6 gives a general overview of the distribution processes in the regional model. For details and calculations see Appendix A.16-3.

In EUSES, the regional assessment takes place in a standard region corresponding to 10% of the size of the EU, represented by a typical densely populated EU-area located in Western Europe (~ 20 million inhabitants, 200 · 200 km^2).

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[12] For example, when several life cycle stages such as manufacture and formulation (for the registrant), or formulation and end use (for downstream users) take place at the same site or if several techniques described by different contributing activities take place at the same site.

[13] Corresponding to a situation where releases and fate processes take place over infinite time. In case steady-state is only reached after several decades (e.g. in the case of metals and the soil compartment), it is recommended to calculate both the PEC after a surveyable time period of 100 years and the PEC at steady-state.

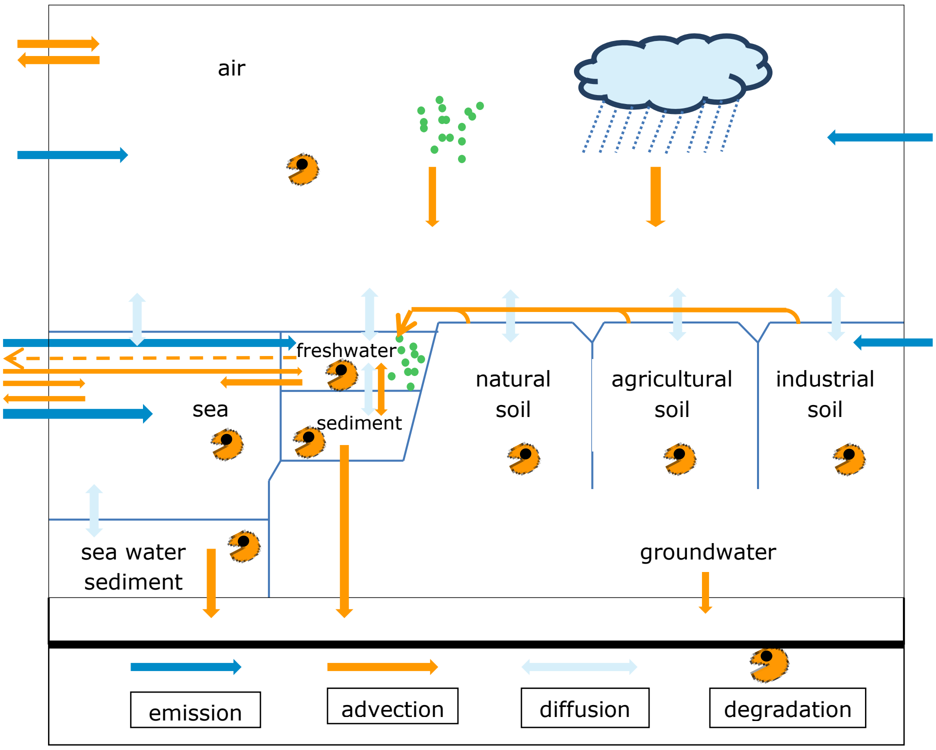

Figure R.16-6: Schematic representation of the model for calculating the regional PECs

In EUSES, a “continental scale” (Europe) is defined to account for the chemical flux - due to passive transport of the substance with air and water - into the regional area. The continental concentrations are not used as endpoints for exposure in the risk characterisation. Figure R.16-7 illustrates the relationships between the continental, regional and local scales.

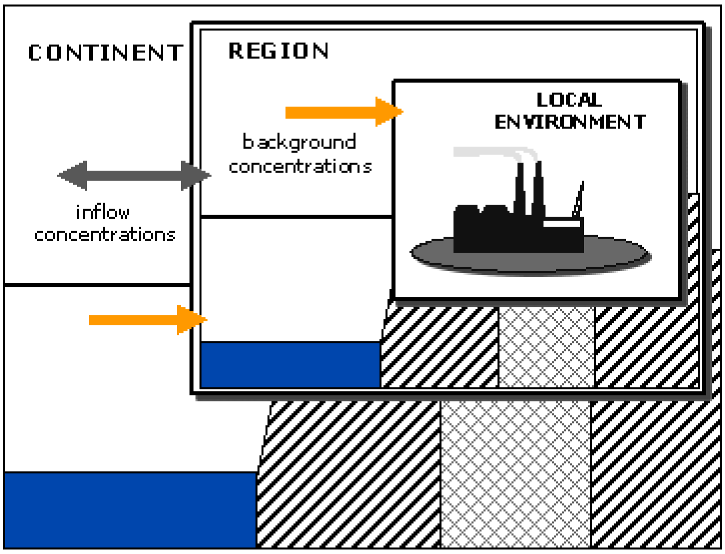

Figure R.16-7: The relationship between the continental, regional, and local scales

R.16.2 Release assessment

R.16.2.1 Key elements of a release assessment

Environmental releases may occur as a result of any process or activity during the life-cycle of a substance. Release estimation is the process whereby releases to the environment are quantified, taking into account the different release pathways and the spatial scale of the releases.

The release of a substance from a certain use depends on the operational conditions (like e.g. temperature, pressure, level of containment of machinery, level of internal regeneration of processing fluids, dry or wet process, dipping or spraying) and risk management practices.

Releases from the use are expected to occur via **different routes**:

- **Water**: the release from industrial sites and widespread use in a municipality is usually to wastewater being (potentially) treated before being ultimately released to fresh or marine water. From the use in agricultural soil releases to water can occur directly, due to drift during spraying application, and/or indirectly via runoff from the soil.
- **Air**: the release to air is mostly related to emission of dust or highly volatile substances or emissions of substances from hot processes. The exhaust air may be cleaned by various techniques before being released to the environment. For widespread uses, emissions to air can occur from the STP or from direct application to agricultural soil in case of spray application[14].
- **Soil**: for all uses taking place at industrial sites or urban areas (also mentioned as municipalities in this guidance) the direct releases to soil are to "non-agricultural soil". For widespread uses, indirect release to agricultural soil may occur when STP sludge is applied or via atmospheric deposition, and direct release occurs when agricultural products such as plant protection products or fertilisers are applied to crops or directly to the agricultural soil are used.
- **Underground**: some substances are directly released to the underground (e.g. when used in fracking).
- **Waste:** releases to waste may occur from the process itself (including the fraction left in packaging when relevant) or as a consequence of the risk management measures (applied to wastewater or exhaust air)[15]. Also, substances incorporated into articles will be "released" to the waste at the end of service life of the article.

The final aim of the release estimation is to calculate the **release rates** as they are the main input parameters to be fed into the exposure estimation (discussed in section R.16.4).

In most cases, the release rates will not be measured but calculated from a release factor applied to the tonnage assumed to be present in a use process:

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[14] The widespread uses mentioned here are local point source. All other widespread uses in professional or consumers activities, are considered to impact the estimation of exposure via the regional contribution (section R.16.4.3)

[15] The fraction of substance released to waste will usually undergo further treatment at a waste treatment site, before being finally disposed of or entering into a new lifecycle after recovery. Waste treatment and final disposal may then lead to releases to water, air or soil.

- The **release factor** expresses the fraction (either kg/kg or %) of the used amount being released to a given release route. A number of methods (see section R.16.2.3) aim to estimate the release factors.
- The **tonnage** systematically refers to three different assessment scenarios, each with its specific reference tonnage:
  - amount used at a typical industrial site (estimation explained in section R.16.2.2.1.1);
  - amount used in a standard town of 10 000 inhabitants which is only relevant for widespread uses (estimation explained in section R.16.2.2.1.2);
  - amount used at regional scale for each use (estimation provided in section R.16.2.2.1.3).

The following release rates are used as input to exposure estimation for uses at sites and widespread uses in a municipality:

- Release rates (expressed in kg/day) to wastewater, surface water, air and soil for each use at the **local scale**:
  - A **local daily release rate** corresponding to the amount of substance released over a day[16].
  - A **local annual release rate** (averaged over the year).
- An **average release rate over the year** (expressed in kg/day) to wastewater, surface water, air and soil **at the regional scale**.

The release rate to a given release route for a use is then calculated using the following equation

$$E_{local,j} = Q_{daily} \cdot RF_j \cdot 1000$$

Explanation of symbols

$E_{local,j}$	Release rate to the release route "j" at the local scale.	[kg/day]
Q_{daily}	Daily use amount at a site or annual use amount in a standard town divided by 365 days)	[tonnes/day]
RF_j	Release factor to release route "j"	[% or kg/kg]

Calculations of release rate at regional scale are discussed in Appendix A.16-4.

Figure R.16-8 illustrates how the various release rates are estimated. More explanations on the tonnage are provided in section R.16.2.2.

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[16] The release rate is given averaged per day (24 hours). This implies that, even when a release takes place only a few hours per day, it will be averaged over 24 hours

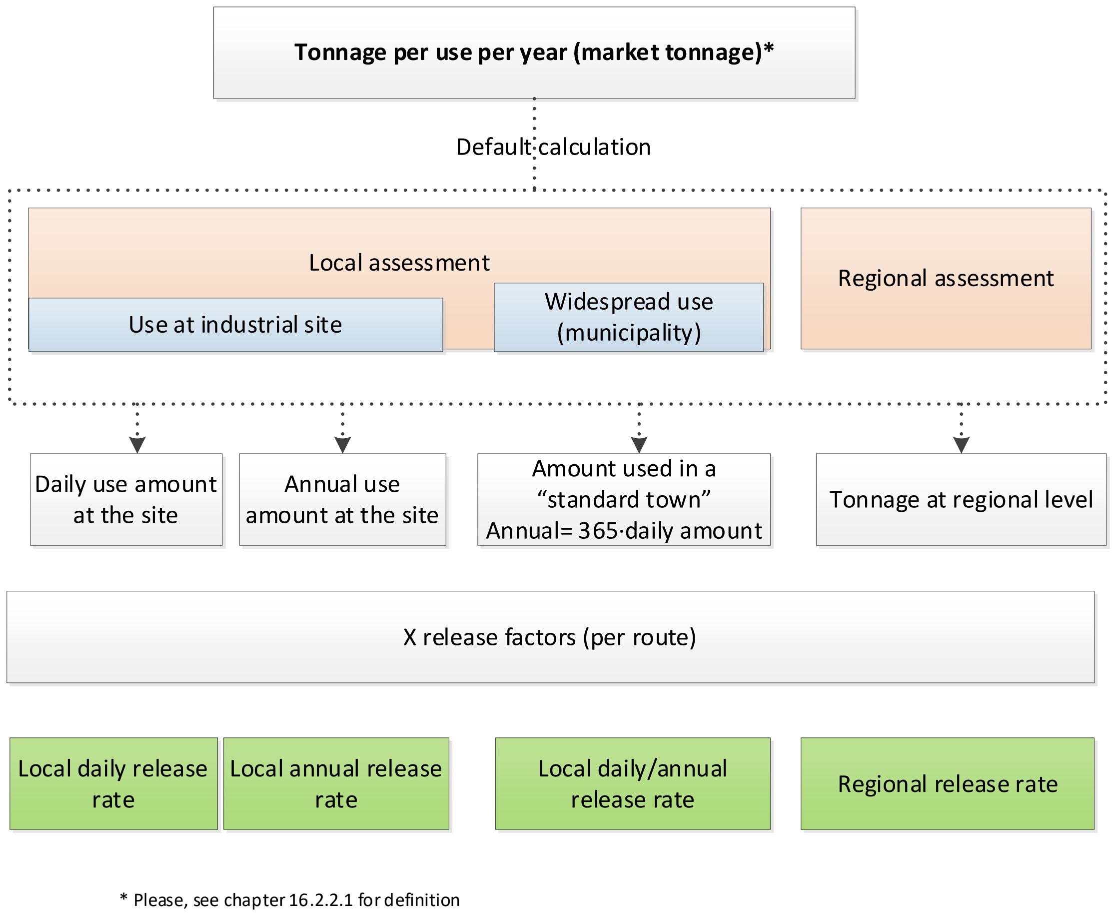

Figure R.16-8: Estimation of the release rates.

The specific release model used in the case of direct application on agricultural soil is described in Appendix A.16-2.4

Specific considerations for uses taking place at industrial site

The scenario for assessing uses at industrial sites considers releases to water, air and soil (see Figure R.16-5).

Releases to water can be treated via various measures (onsite industrial wastewater treatment) and in a biological sewage treatment plant (STP). Indirect releases to air via the biological STP, as a result of water treatment in the STP, are considered in this scenario.

Release to soil at the local scale will occur via the potential application of sludge from a biological STP to agricultural soil, and via atmospheric deposition of substances released to air. Direct releases to soil from the industrial site are not assessed at the local scale, but only at the regional scale.

In the standard case, uses taking place at industrial sites are assessed assuming a **generic, representative site.** Nevertheless, registrants may want to carry out **site-specific assessment**, when they have access to more precise information for example on the setting of the biological treatment plant or on the receiving environment. This may be the case when assessing their own use or when they have received information from specific downstream users. In this case, relevant information about data sources and results has to be provided.

Several release factors from the process to the environment may be considered, depending on the available abatement techniques:

- The initial release factors corresponding to the releases from the process.
- The release factors after onsite risk management, calculated from the initial release factors taking into account the effectiveness of all onsite risk management measures[17]. Due to the fact that a specific model exists for the biological STP in EUSES, these release factors usually exclude the effectiveness of the biological STP calculated by EUSES.
- The releases to the receiving water have to take into account the removal in the biological STP and the potential transfer of the substance from water to air in the STP and to soil via the application of the sludge.

Figure R.16-9 illustrates the relationship between the different releases.

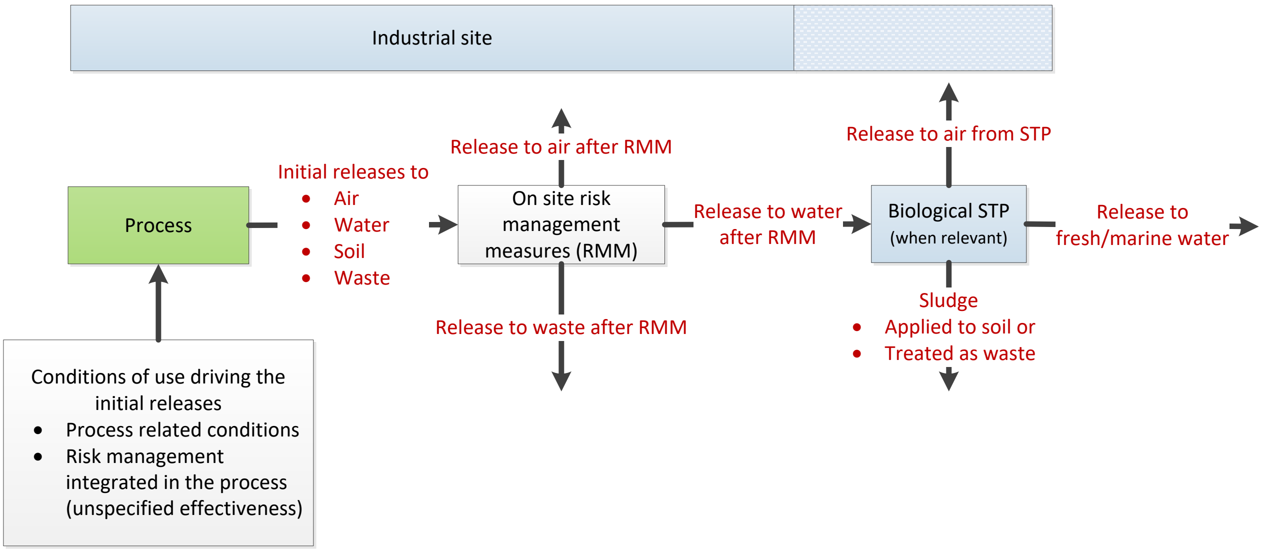

Figure R.16-9: Relationship between the different releases

Specific considerations for widespread uses

- Uses in a municipality (town)

For widespread uses in a municipality (town), it is assumed that the market tonnage is evenly distributed in space and time. The assessment is carried out for a standard town with 10 000 inhabitants.

In the scenario for assessing such widespread uses, the local release to water corresponds to the release from a standard biological STP to which the 10 000 inhabitants are connected. The

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[17] The effectiveness of an RMM is defined as the percentage reduction in release or exposure produced by application of the RMM. The effectiveness of a given measure may depend on the substance properties of the substance.

direct releases to air and soil from widespread uses are not considered at the local scale, but only at the regional one. Nevertheless, indirect releases from the STP to air and to soil via sewage sludge application need to be considered at the local scale, since the STP acts as a point source.

- Agricultural uses

For agricultural uses, it is assumed that the registrant has specific information on the application rate per hectare per year. The release amount to soil (kg/ha) is derived from the tonnage applied per hectare in a year, and the release factor to soil (see also appendix A.16-2.4.2 and A.16-4.2).

When applicable, the direct release amount to water due to drift (kg/ha) is estimated from the amount applied to soil and the release factor to water (see appendix A.16-2.4.3).

Specific considerations for regional releases

All regional releases associated with the different identified uses, both industrial and widespread sources, are cumulated to estimate the total regional release to surface water, wastewater, air and soil.

Specific considerations for releases from waste operations

The amount of substance "released" to waste is one of the criteria for determining to what extent the conditions of waste treatment and the resulting releases to the environment need to be addressed in the CSA. The arguments based on which it may be justified to waive the assessment of the waste life stage are listed in section 18.2.3.1 of *Chapter R.18 of the Guidance on IR&CSA*, and are summarised as follows:

- only a small fraction of the substance ends up in the waste stage, for example due to reaction on end-use, or complete incineration when used in fuels or biologically degraded after being released to wastewater;
- conditions at waste treatment are already covered in the assessment for one of the preceding life-cycle stages and thus no additional risks expected;
- the concentration of the substance in waste is likely to be below the thresholds of Article 14(2).

Where the assessor cannot rule out upfront that waste operations with the substance significantly contribute to the environmental releases, a qualitative or quantitative assessment will be needed. The qualitative assessment may consist of a reference to standard waste treatment/legislation and a justification of why the suggested technique is suitable. When a defined EU standard does not exist, or when the substance is unlikely to be eliminated during the process (e.g. metals by incineration), release estimation and quantitative risk characterisation is necessary. For further details see *Chapter R.18 of the Guidance on IR&CSA*.

For the quantitative assessment it can be assumed that the waste operations take place at an industrial site. *Chapter R.18* explains how to make assumptions on the daily and annual tonnage and suggests default release factors for a number of common waste treatment techniques.

Where the process leading to the recovery of the substance is the same as the substance manufacturing (like e.g. for some metals), this last step in the waste operation (i.e. when recovery follows other waste treatments) may be already covered in the assessment of the manufacturing process. Other operations regularly carried out in the context of recycling/recovery (e.g. dismantling processes, milling and separation processes) may need a particular assessment.

R.16.2.2 Conditions of use

The core part of the exposure assessment (and generation of the exposure scenario) is the definition of the appropriate conditions of use which ensure that the risks are controlled. The term "conditions of use" includes operational conditions (OCs) and risk management measures (RMMs). Risk management may be integrated in the process (thus being part of the operational conditions) or may be applied on top of it.

Changes to the OCs can contribute to the control of risk (like RMMs do), or rather create the need for additional RMMs. Consequently, the manufacturer or importer should always consider the risk management measures and the operational conditions in close relation to each other. This includes particular considerations where emissions are controlled by strategies moving the substance from wastewater or exhaust air to external waste treatment.

Other losses of the substance from the process disposed of as waste (e.g. treatment baths at the end of their residence time) should also be taken into account. In these cases, the registrant should determine a "release factor" to waste, and potentially include special considerations on waste treatment if relevant (more information on exposure estimation from waste life-cycle stage is provided in *Chapter R.18 of the Guidance on IR&CSA*).

The following sections provide information on the various conditions which impact on the release of the substance. As already mentioned the release depends on the amount of substance used (see section R.16.2.2.1) and on the release factor. Section R.16.2.2.2 describes the aspects of the process design and the risk management in place which impact on the release factor. For infrequent uses as described in section R.16.2.2.6 specific rules apply for the risk characterisation.

Finally some environmental conditions (see section R.16.2.2.7), such as the potential for dilution in the environment will have an impact on the exposure levels.

The conditions of use under control of the downstream users are to be communicated downstream in the exposure scenario annexed to the safety data sheet. This holds true regardless of whether or not the RMMs are process-integrated or measures which are "added" to the process. A clear description of all the conditions (including assumed effectiveness of risk management when relevant) is essential, so that downstream users can check whether they operate within those conditions and whether their further downstream uses can be assumed to be safe. More information on the communication to downstream users can be found in guidance Part D.

R.16.2.2.1 Tonnage information

The "tonnage per use"[18] plays a key role in environmental assessment. It serves three purposes (see Figure R.16-8 in R.16.2.1):

- to estimate a default local tonnage for widespread uses;
- to estimate a default local tonnage for uses at a site;
- to estimate the regional tonnage.

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[18] Note: "use" in this context includes manufacturing and service life.

The tonnage per use may correspond to the following, depending on the choices made within a joint submission, in particular whether the CSR is prepared jointly or not:

- the estimated use tonnage for the EU across all registrants' part of the joint submission;
- the registrant's share of the EU tonnage for that use;
- the joint submission's highest share of the EU tonnage (in order to cover all members of the joint submission).

Note that the tonnage per use can be reported in IUCLID and will also serve other purposes such as supporting priority setting by the authorities. More information is provided in *Chapter R.12 of the Guidance on IR&CSA*.

The manufacturer's annual production or the importer's annual import of a substance will be distributed in (or outside) the EU market, and flows down the supply chains. Registrants usually know their own production/import tonnage and have an overview on the markets determining the demand for their product. However a full quantitative breakdown into all end-uses is usually not readily available.

To get information on the annual or daily tonnage used by downstream users (including formulators and industrial users) as well as on the tonnages used by consumers or ending up in service life, the registrants may therefore rely on a combination of:

i) information collected by downstream user sectors (and communicated via use maps); or

ii) information they may collect themselves from their own customers and from analysis of the markets.

Depending on how much information the registrants are able to collect, they may carry out their assessment on the basis of realistic data, or they may have to carry out their assessment on the basis of a worst-case assumption. Please note: The level of detail needed in the tonnage breakdown across uses may depend on the hazard profile of the substance and the variety of uses (range of relevant release factors).

If the assessment is based on a tonnage used by a large site, the evaluation performed using this tonnage ensures control of risk for all smaller customers[19], assuming that conditions of use implemented on large and small sites lead to the same release factors. However this assumption may not always be correct: Large sites may work with dedicated equipment and/or stringent onsite risk management measures, while small sites may carry out the same process with multi-purpose equipment and/or without stringent onsite risk management. Assuming the same emission factor may lead to the definition of unrealistic efficiency (i.e. technical demands) for small sites. Therefore it may be advisable for registrants to consider at least two alternative contributing scenarios for these different situations.

If specific and reliable data are not available to registrants, conservative assumptions (like the use of the total manufactured volume for every identified use or even using the highest possible tonnage on the basis of the higher bound of the registered tonnage) may be made by the registrants. In doing so, the calculated exposure estimates and corresponding RCR will help the registrants to set priorities for collection of more specific information.

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[19] Guidance for downstream users on how to define the relevant tonnage for their own use in the case of multiple suppliers of the same substance or in the case of use of recycled amounts (particularly relevant for the metals industry) is out of the scope of the present R.16 Guidance.

R.16.2.2.1.1 Estimation of tonnage for uses at industrial sites

The following information is needed:

- daily amount used at a site (tonnes/day); and
- annual amount used at a site (tonnes/year).

In the absence of better information, the tonnage for the use can be assumed to be processed at a single site (worst case). Therefore, the **annual use amount at a site** may be set equal, by default, to 100% of the tonnage for the use.

In such cases, the **daily use amount at a site** can be calculated from the annual use amount at the site. The following tables provide default daily tonnage for manufacture, formulation and uses at industrial sites, as a function of the size of the site in terms of annual capacity. 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.

Note: For a given annual use tonnage of a substance, the burden on environment decreases with a higher number of release days.

Table R.16-2: Default estimation of tonnage for site for different life-cycle stages

For manufacture

Tonnage of the substance manufactured per year	No. of release days (days/year)	Substance daily use amount (tonnes/day)
Tonnage < 1 000	20	Tonnage /20
1 000 < Tonnage < 10 000	100	Tonnage /100
Tonnage > 10 000	300	Tonnage /300

For formulation[20]

Tonnage of mixture in which the substance is included for the use (or group of uses) per year	No. of release days (days/year)	Substance daily use amount (tonnes/day)
Tonnage < 100	10 [21]	Tonnage /10
100 < Tonnage < 2 000	100	Tonnage /100
Tonnage > 2 000	300	Tonnage /300

For uses at industrial sites

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[20] 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 registrant has no information on the tonnage of mixture, 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 registrant knows the fraction of the substance in mixture, he can estimate the formulated tonnage (first column) via the equation: tonnage of mixture = tonnage of the substance /percentage of substance in the mixture. In that case this may lead to a change of tonnage band.

[21] The 10 days for formulation compared to 20 days for manufacture and industrial end-uses is based on the consideration that very short production campaigns are more likely in processes of low complexity (like e.g. mixing).

Tonnage of mixture containing substance or substance as such for the use (or group of uses) per year	No. of release days (days/year)	Substance daily use amount (tonnes/day)
Tonnage < 1 000	20	Tonnage /20
1 000 < Tonnage < 5 000	100	Tonnage /100
Tonnage > 5 000	300	Tonnage /300

The registrant may refine the daily and annual use amount, by using suitable and specific data if available, for example on the basis of:

- Site-specific information, such as the actual daily use amount in the manufacturing stage (readily accessible to the registrant);
- Information on the actual amount used by the largest downstream user;
- Information made available by the downstream sector via Specific Environmental Release Categories (SPERCs; see section R.16.2.3) on typical amounts used at a site.

Note that when a use consists of handling the substance in a reservoir (e.g. metal part cleaning, metal cutting), releases may occur when the full content of the reservoir is replaced. The releases during the change of the bath may be:

(i) negligible compared to the daily losses;

(ii) much more important than the daily losses; or

(iii) of the same order of magnitude.

In cases (ii) and (iii) (i.e. when the releases during the replacement of the content of the reservoir play a key role in the estimation of the total release), the standard model for calculating the release rates is not appropriate. This is due to the fact that two reference tonnages are needed to estimate the releases from daily losses and from the change of bath. No standard methodology is yet available to cover such cases.

R.16.2.2.1.2 Estimation of tonnage for widespread uses

- Uses in a municipality (town)

For widespread uses in a municipality (town), a default daily amount used in a standard town is estimated starting from the tonnage for the use, and taking into account:

- the fraction of the "tonnage for the use" used in the region (regional tonnage): 0.1;
- the fraction of the regional tonnage used in the standard town (proportional to the ratio of number of inhabitants in a standard town (10 000) compared to the number of inhabitants in a region (20 000 000)): 0.0005;
- the number of days in a year: 365.

The resulting tonnage is multiplied by an assessment factor of 4[22] to take into account geographical or temporal peaks in the use of a substance, for example, for the use of anti-freeze compounds in window washing fluids for cars.

The daily local widespread use amount (tonnes/day) is therefore by default set equal to the tonnage for the use (tonnes/year) × F (year/day), where:

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[22] To refine this factor, see also refinement options in Table R.16-6.

F (year/day) = $4 \cdot 0.1 \cdot 0.0005 / 365$ day/year = $5.5 \cdot 10^{-7}$ year/day.

- Agricultural use

For widespread agricultural uses of fertilisers or plant protection products applied in the agricultural soil, the amount of assessed substance used per hectare in a year needs to be estimated. This can be calculated using the product application rate and the percentage of substance in the product (as a worst case the latter can be set to 100%).

R.16.2.2.1.3 Tonnage for the regional release estimation

The estimation of the regional tonnage (fraction of "the tonnage for the use" in the region) depends on the geographical distribution of the substance's use. By default, the tonnage at the regional level for the uses at industrial sites is set equal to 100% of the tonnage for the use, while for widespread uses it is set equal to 10% of this tonnage. However, market data could be used to overwrite the default tonnage in the region with a percentage that corresponds to the actual situation. A refined regional tonnage can also be used for the local scale calculation of releases from widespread uses.

When refining the regional tonnage for both use at industrial sites and widespread uses in a municipality (town), the corresponding release to the continental scale is to be adjusted so that the tonnage used for the regional release plus the tonnage used for the continental release is equal to the tonnage for the use.

R.16.2.2.2 Design of technical process

From the environmental perspective, activities can be carried out in predominantly open processes (e.g. use of fertilisers, application of paints outside industrial sites, building and construction works) to rigorously contained processes (e.g. use of hazardous solvents in textile or metal part cleaning) with minimal losses to exhaust air or wastewater. Between an initial release factor to water/air of 100% (fully open system) and an initial release factor of < 0.0001% (largely closed system) various levels of release occur in practice.

For most industrial processes, the initial release factors occurring in practice will depend on the size, technical design, investment cycle and management of the process. For the exposure assessment, registrants may choose a good practice scenario as a basis for their assessment. A number of downstream sectors have published use maps including Specific Environmental Release Categories (SPERCs), describing the conditions of use and the related release factors to be expected in their sector (see section R.16.2.3).

For some substances/uses, rigorous containment (= closed system) may be applied i.e. a dedicated process design aiming to minimise releases into the environment to an extent that the resulting release/exposure is negligible[23]. This includes the onsite treatment of residual initial releases from the process by best available techniques. It also includes rigorous containment for treatment of waste released from the "contained" process. Proper external recovery and/or waste treatment may be a pre-requisite to regard a use as being rigorously contained. Both the technical and non-technical (organisational) means necessary to ensure that the releases can be minimised are to be described in the exposure scenario.

Some processing aids are operated in close loop systems, including internal cleaning steps and recovery. Such reservoirs/baths however need to be exchanged at a certain point in time as a whole. In particular for water-based processing aids, it may be typical practice to treat the exhausted bath onsite and discharge it subsequently as wastewater (see section below). This

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[23] Please note that rigorous containment measures aimed at protecting workers should be examined carefully to assess whether they are also capable of minimising emissions to the environment due to different protection targets.

may result in a single event release rate largely exceeding the initial release from routine operation of the system.

To properly assess such events, a dedicated exposure scenario may be needed, and the daily tonnage needs to be split into “compensation of losses in routine operation” and “renewal of bath”. Often the exhausted/contaminated bath (or parts of it) is disposed of to external waste treatment (including recycling). In such cases, the environmental releases can be set to 0 but the exposure scenario should clearly state that the exhausted bath should be eliminated as a waste and relevant assessment of the waste life cycle stage should be carried out.

R.16.2.2.3 Onsite risk management measures

The initial releases from the technical process may need onsite treatment before being released with the exhaust air or wastewater. Examples of RMMs intended to reduce release are filters, scrubbers, biological or physico-chemical wastewater treatment plants. RMMs reducing releases to one environmental compartment may increase the releases to other compartments (e.g. wet scrubber collects release to air but may redirect them to water) or to waste.

It is important to assess and communicate how the conditions of use will impact on release in quantitative terms. Thus, the exposure reducing effect (i.e. the effectiveness of each measure) needs to be expressed in quantitative terms (to the extent possible) that can be fed into the release estimation. Technically achievable efficiencies for environment protection techniques in various industry sectors are described in BREF documents[24] under the Industrial Emissions Directive and the Emission Scenario Documents of the OECD[25]. Please note that substance-specific emission factors or treatment efficiencies are usually not readily available in BREFs, and thus BREFs can rarely be used as the only source of information.

Where such information is not available, experience from downstream sectors may be used to make realistic assumptions. In this case, examples of techniques which allow the claimed efficiency of control/reduction of exposure to be achieved should be provided in the exposure scenario attached to the chemical safety report (CSR) and the safety data sheet (SDS).

Industry sectors will usually describe the relevant measures for their uses within SPERCs (see section R.16.2.3.2).

Among all the types of onsite risk management measures, a model exists in EUSES only for biological treatment. Therefore, onsite measures by biological treatment are addressed in a specific sub-section.

R.16.2.2.4 Biological sewage treatment plant (STP)

Biological sewage treatment plants (STPs) are a standard practice in Europe. It is therefore a common measure for many uses at a site and can be assumed as a standard RMM for widespread uses in a municipality (town).

A model for the biological STP is incorporated in EUSES and further details are provided in section R.16.3. The key transfers of substance from a biological treatment plant are the following:

- releases to the environment by water are reduced by degradation, volatilisation and adsorption on sludge;
- releases to air may occur;

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[24] Available at: http://eippcb.jrc.ec.europa.eu/reference/.

[25] Available at: http://www.oecd.org/env/ehs/risk-assessment/emissionscenariodocuments.htm.

- releases to agricultural soil will occur if the sludge is applied as fertiliser (leading to a transfer of substance from water to soil and by further transport to crops etc.).

By default, it may be assumed that the releases to water are treated in a standard biological sewage treatment plant (STP) before being released to the environment and the STP-sludge is applied to agricultural soil. Nevertheless, for uses taking place at industrial sites, the assumptions for the biological STP may be modified (see section R.16.3). In such cases they need to be communicated downstream.

R.16.2.2.5 Waste treatment operations

Waste incineration (municipal waste incineration, hazardous waste incineration, sewage sludge incineration) and landfilling are standard practice in Europe with operating standards and emission standards set by harmonised waste legislation. For other waste treatment operations, the best available technique may be defined under the Industrial Emissions Directive. An assessor under REACH can make reference to these harmonised standards if applicable to his substance and the waste it is contained in. A registrant can also determine and communicate which types of waste treatment technique are not suitable for his substance[26].

R.16.2.2.6 Frequency of release

For uses taking place at industrial sites, the releases of substances can either be **continuous** or **intermittent**. Intermittent releases are for example the result of batch processes. Intermittent releases are defined as occurring infrequently, i.e. less than once per month and for no more than 24 hours. For infrequent uses, specific rules can then be applied for the risk characterisation as described in section R.16.5.

When registrants want to assess a use assumed to be intermittent (for example, their own use or based on their knowledge of their customers' conditions), they will have to clearly indicate in their exposure scenarios that releases should take place less than once per month and for no more than 24 hours.

Note that for widespread uses in a municipality (town), intermittent releases cannot be assumed.

For agricultural uses a single application (i.e. release) per year to soil (arable land or grassland) is assumed by default, during 10 years of consecutive application. However, multiple applications in a year can be considered as described in Appendix A.16-2.4. For these uses any direct releases to surface water take place on the day of application (i.e. single release once or multiple times in a year).

R.16.2.2.7 Environmental conditions impacting on exposure

The releases are diluted in the receiving environment and this will be taken into account in the local assessment. For widespread uses in a municipality (town) as well as for the generic assessment of uses at industrial sites, standard settings have been defined which are implemented in EUSES.

- A standard dilution of 10 is used when releasing to a freshwater environment (corresponding to an effluent flow rate of 2 000 m^3/day discharging into a river of 18 000 m^3/day)
- A standard dilution of 100 is used when releasing to a marine environment.

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[26] For more detailed information on the waste life-cycle stage, please consult Chapter R.18.

When carrying out a site-specific assessment (for own use or specific customers), specific data on the receiving water or dilution into marine water may be used with regard to the dilution capacity of the environment (site-specific data should be justified and explained). However, it should be noted that a dilution factor higher than 1 000 should not be used in any case, since the concentration in the mixing zone can be higher than the concentration estimated by a complete mixing of the effluent and the mixing zone can be very large for high dilution factors (see Appendix A.16-2.3.3). The dilution into the receiving environment assumed for the assessment of a use at industrial sites is to be communicated to the downstream user, in particular when a higher dilution is expected than the default one.

For widespread agricultural use the surface water compartment is represented by a ditch (from FOCUS Tier 1 and 2[27]) in contact with agricultural soil and receiving direct and indirect emissions. The ditch is assumed to be 0.3 m deep, and the ratio field/waterbody is 10. A residence time in the water of 40 d is assumed (Table R.16-21).

Other environmental conditions may impact on the fate of the substance and therefore on its exposure level. For example, some substances' behaviour may depend on the salinity, pH or hardness of the environment. Such information can usually not be taken into account into the assessment and worst-case situations are to be assumed. As this may not always be easy to determine (as what may be worst for the water is usually not for sediment for example), considerations on variability and uncertainty may have to be made.

Nevertheless, there may be some situations where for their own site or for specific customers' sites those specific environmental conditions may be known and taken into account to decide on the values taken for some physico-chemical and fate properties which impact on the exposure levels (see section R.16.4.2).

R.16.2.3 Release estimation methods

There are several sources of information to support registrants for their estimation of the releases.

- Default release factors have been associated to the **Environmental Release Categories (ERCs)**, assuming no onsite risk management is in place (see section R.16.2.3.1).
- Some sectors have developed **SPERCs** which may be available as such or via sector use maps see section R.16.2.3.2).
- **Other published information** may be available (e.g. OECD, National Authorities; see section R.16.2.3.3).
- Specific data may be available to the registrant for the **assessment of well-defined sites** (registrant's own site or customer's site on which specific knowledge is available to the registrant; see section R.16.2.3.4).

R.16.2.3.1 Environmental Release Categories (ERCs)

ERCs are use descriptors defined from an environmental perspective. They are defined in *Chapter R.12*.

A set of default (initial) release factors associated to each ERC has been defined during the process of REACH guidance development. Those release factors are assumed to be conservative default values, assuming no specific risk management measures are in place. The

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[27] https://esdac.jrc.ec.europa.eu/public_path/projects_data/focus/sw/docs/Generic%20FOCUS_SWS_vc1.4.pdf

values of the release factors for each ERC and their source are documented in Appendix A.16-1.

In a first instance, or in the absence of more specific information, assessors may use the release factors associated to the ERC to carry out their release estimation.

If a specific RMM is applied in current practice (for example, according to the best available techniques) and the effectiveness of such a technique for the respective substance is known, release factors can be reduced accordingly and taken into account in the development of the ES.

Note that in a few situations the assessment carried out on the basis of one ERC also covers the assessment if another ERC would have been selected. This is true for the following cases:

- For some widespread uses in a municipality (town) which may take place indoor and outdoor under the same conditions, the release factors to water and air are similar but an additional release to soil is assumed in the ERC for the use outdoors. Therefore, the assessment on the basis of the "outdoor ERC" may cover the assessment of the equivalent use indoor.
- For the processing of articles at industrial sites, a process with high releases may cover a process with low releases. Nevertheless, note that usually the two types of processing are of a very different nature with very different conditions of use. Therefore, it may not be relevant to try to cover the two cases within the same contributing activity/use.

The practical implication of these assumptions is described in Table R.16-3 below.

Table R.16-3: Situations in which the assessment based on a specific ERC would also cover an assessment based on another ERC

When an assessment is based on….		It may cover an assessment based on	
ERC 8d	Widespread use of non-reactive processing aid (no inclusion into or onto article; outdoor)	ERC 8a	Widespread use of non-reactive processing aid (no inclusion into or onto article; indoor)
ERC 8e	Widespread use of reactive processing aid (no inclusion into or onto article; outdoor)	ERC 8b	Widespread use of reactive processing aid (no inclusion into or onto article; indoor)
ERC 9b	Widespread use of functional fluid (outdoor)	ERC 9a	Widespread use of functional fluid (indoor)
ERC 10a	Widespread use of articles with low release (outdoor)	ERC 11a	Widespread use of articles with low release (indoor)
ERC 10b	Widespread use of articles with high or intended release (outdoor)	ERC 10a	Widespread use of articles with low release (outdoor)
		ERC 11a	Widespread use of articles with low release (indoor)
		ERC 11b	Widespread use of articles with high or intended release (indoor)
ERC 12b	Processing of articles at industrial sites with high release	ERC 12a	Processing of articles at industrial sites with low release
		ERC 12c	Use of articles at industrial sites with low release

R.16.2.3.2 Specific Environmental Release Categories (SPERCs)

Specific Environmental Release Categories (SPERCs) correspond to sets of information describing specific good practice conditions of use and the corresponding release estimates (to water, air, soil and waste). They are developed by sector groups of chemical industry and their downstream customer industries to refine the emission estimates obtained by using the ERCs' release factors, taking into account specific operational conditions and RMMs applied for the use in the sector.

SPERCs are normally defined for one type of mixture applied in a specific process/technique/contributing activity. It consists of quantitative release factors for calculation of the environmental release and descriptive information on the conditions under which the release factors apply. A SPERC may contain one or more sets of release factor applying to substances with specific properties (e.g. ranges of vapour pressure or water solubility)[28].

SPERCs are documented in SPERC factsheets and they should be referred to in use maps developed by the sectors. Detailed explanatory information beyond what an assessor may need when preparing a registration may be provided in a background document to the SPERC factsheet. Such background documents may be crucial in particular to provide complementary/additional source information and justification for the release factors provided in the SPERC. SPERCs are made available via sector websites. An overview table of association activities related to SPERCs (such as the development of SPERCS or use maps) can be found on the Cefic website at www.cefic.org/Industry-support/Implementing-reach/Guidances-and-Tools1 and on the ECHA website at https://echa.europa.eu/csr-es-roadmap/use-maps/concept. SPERCs can be used in exposure assessment tools like Chesar (Platform).

The descriptions of the conditions of use in the SPERC factsheet should be detailed for the CSR but should also be described in a standardised manner for communication in the supply chain. Cleaning and maintenance processes as well as loading/unloading may be described separately from the main process to ensure that significant and emission relevant aspects are described (and transferred to the CSR and ES for communication).

The effectiveness of RMMs is already included in the release factors provided in the SPERCs. When available it should be provided in the SPERCs factsheets together with an indication of how this effectiveness was derived (e.g. information sources). This aspect of RMM effectiveness is to be developed further as soon as more information is available.

R.16.2.3.3 Other published sources

Other sources of information for the refinement of release factors or release rates exist as well. One of them is the Emission Scenario Documents (ESDs). An ESD is a document that describes the sources, production processes, pathways and use patterns with the aim of quantifying the releases of a substance into water, air, soil and/or solid waste. ESDs have been developed and agreed within the OECD or Member States.

Some of the ESDs above refer to substances used in biocidal products. For a more comprehensive list of ESDs for such substances consult the ECHA website at: http://echa.europa.eu/guidance-documents/guidance-on-biocides-legislation/emission-scenario-documents;jsessionid=E6EFCEC70A6CAA6A6992F45BD81B665C.live1.

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[28] Such differentiation of release factors for one set of conditions of use is introduced as "sub-SPERCs" in tools such as Chesar.

The "Technical guidance document on risk assessment" – Part IV (EC 2003) also presents a list of ESDs for the different industrial categories (ICs) and biocidal product-types (BPTs). The document can be downloaded from here: https://echa.europa.eu/documents/10162/16960216/tgdpart4_2ed_en.pdf.

Other sources of information that can be considered when refining release factors are permits set by authorities, determining maximum release rates into environmental compartments (surface water and air).

Care needs to be taken to provide an appropriate description of the link between the release factors derived from ESDs or other documents and the corresponding OCs/RMMs to be described in the exposure scenario. In this respect A and B tables of the TGD (2003) for example are not acceptable, unless they clearly provide more specific information on RMMs/OCs and link them to the release factors proposed. Otherwise, they are considered insufficient to meet the REACH requirements.

As for SPERCs, when using another source of information in an assessment it is essential that the release factors are well connected to their related set of conditions of use. Detailed explanations on the origin of the release factors are to be provided in the CSR and the conditions of use are to be communicated via the exposure scenarios annexed to the safety data sheet (SDS).

R.16.2.3.3.1 Site-specific information

Specific information may be available to registrants for assessing the releases at their own site or at specific customers' sites.

For example, measured releases may be available[29] when licences and permits set by authorities require frequent and regular monitoring of releases to environmental compartments. In general, release data may be collected at different points of the flow: release from process, after onsite abatement or after onsite STP, before discharge to air or receiving river. Typically, concentrations in the released air or water stream and the air/water flow-rate can be used to calculate a release rate (e.g. in kg/day). Release may also be estimated from site mass balance information.

The quality and representativeness of the measured data is to be carefully analysed (see Appendix A.16-6 for more details). The data should be representative for the conditions of use described in the exposure scenario, which may be a particular challenge when the representativeness is to be ensured across various sites. Measured data required for site licences and permits (with documented number/frequency of sampling, analytical methods, basic statistics) can be a good source of information for REACH. Depending on the exposure assessment model, the measured release rates can be directly entered into the model, or a corresponding release factor (% or dimensionless) can be re-calculated from measured release rates and the local daily use amount, e.g. in kg/day).

In all cases, it is essential that documentation is available and referred to in the CSR. In particular a description of the methodology applied (for measurements/data collection) should be available as well as a reasoning why the data are considered relevant for the release estimation from the specific use/contributing scenario. This is particularly important where monitoring data are replacing modelled emission estimates for generic sites. For further details on the factors potentially impacting on the relevance and representativeness of measured datasets refer to Appendix A.16-6.

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[29] Measured release may be available for water, rarely for air.

R.16.2.3.4 Specific considerations for article service life

For substances incorporated into/onto articles, the service life in the article needs to be covered in the use description and in the exposure assessment. When assessing the article service life, particular considerations on the time pattern of release need to be made. For substances as such and in mixtures, it is assumed that the releases take place in the year of manufacture. However, for the article service life and the subsequent waste life stage this assumption is often not applicable since the release occurs over a longer period after manufacture.

In particular, it is assumed that the release to the environment takes place continuously over the total service lifetime and homogeneously disperses in the environment. It is therefore treated as widespread use. How long an article type and the substances in it has been on the market (and potentially stocked up leading to simultaneous release from all articles in stock) needs to be taken into account. Assuming a relatively constant consumption (with regard to volumes and areas of use), registrants should make themselves aware on whether the product-cycle of their substance has reached a steady state. This means that the annual quantity removed (by waste incineration, degradation etc.) is equal to the quantity of substance supplied annually.

The release factor corresponding to the steady state situation can be expressed as the (measured or modelled) release from the article over one year multiplied by the service lifetime of the article (the expected use time of the article before going to the waste stage). This release factor is called "release factor over service lifetime". In such a way the release factor account for the stock of the article in the market.

Release into the environment (via air, water, soil) is then calculated from the release factor over the service lifetime of the article and the yearly amount of the substance used for the production of the article.

For example, the calculation of the release factor for an additive in a plastic article with low release is done according to the OECD Emission Scenario Document on plastic additives (OECD 2004b). In this case, the release factor is 0,16% expressed on a yearly basis. The service lifetime of the article is assumed to be 20 years. The release factor should then be multiplied by the service lifetime, determining a (cumulative) release factor over the service lifetime (of all articles of this type simultaneously in use) of 3.2% per year (this concept is also reflected for calculation of the ERC 10A release factor, see Appendix A.16-1). The release rate to the environment is then calculated multiplying the release factor over the service life by the yearly amount of the substance used for the production of the article.

Both the release factor from a single article and the service lifetime can be refined. The default service lifetime can be refined based on market data. The release factor from the single article can be refined based on measured data or other models.

As the manufacturers or importers of the substance will in many cases not have detailed knowledge about the characteristics of the articles produced and use conditions during the service life of these articles, they may need to collect information from their downstream users on issues which are relevant for the release and exposure estimation and may consequently need to be defined in the ES, in particular the following:

- Article types in which the substance is used.
- Total quantity of the substance incorporated into the article.
- Indication of which fraction of this total substance is released to the environment; this depends on different factors such as:
    - duration of article use (i.e. the service lifetime of the article).

- Surface area/volume ratio, influencing the evaporation/migration potential of substances from the article surface: articles with high surface area/volume ratio (e.g. plastic sheets) may have higher emissions for the same substance than those with a low surface area/volume (depends on substance properties and interaction with matrix).
- Interaction between substance and article matrix type, often being an important driver for the release from articles.
- Accelerated wear and tear or factors enhancing emissions: exposure to light, temperature, weathering or erosion, intense use (e.g. brake pads).

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 estimation. 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; Examples: Second-hand computers, cars, textiles;
- 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 in another ES; Examples: Tyres at the end of their first service life can enter into various kinds of utilisation; waste paper may be converted into isolation material;
- 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; Examples: Plastic, rubber and paper material.

The assessor will ultimately need an emission factor (release rate) per year. In a Tier 1 assessment, a default emission factor can be used based on the ERCs (see section R.16.2.3.1). Specific information can be used to substitute the defaults, e.g. based on models or based on testing.

Note: The waste operations carried out with the article at the end of its service life need to be considered in the CSA/CSR. As outlined in section, such considerations may consist in a few arguments only justifying why particular risks from waste operations are not expected (and thus no need for exposure estimates or particular advice regarding waste treatment). However in certain cases there may be the need to carry out an exposure assessment (including exposure estimates) for one or more waste operations relevant for that substance. Typical examples are dismantling, milling or separation processes bringing metals into a form suitable for recovery.

R.16.3 Biological sewage treatment plant

R.16.3.1 Introduction

Wastewater effluents may be treated in a biological treatment plant before being released to the environment. The biological STP model described in this guidance is based on the version 4 of SimpleTreat (SimpleTreat 4.0, Struijs, 2014[30]), which is currently implemented in EUSES (version 2.2.0) and integrated in Chesar Platform (see R.16.1.1 and R.16.4.1.2).

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[30] The new features in the updated version of SimpleTreat are described here: https://www.rivm.nl/bibliotheek/rapporten/601353005.pdf; a comparison of with previous SimpleTreat 3.1 is provided

If the registrant wants to use another version of the SimpleTreat or other biological STP models he needs to:

- Provide clear explanations for his choice;
- Report the outcome of his assessment in terms of fractions directed to air, sludge and the effluent (water stream) from the biological STP (see R.16.3.2) directly into EUSES to correctly estimate different PECs.

For widespread uses in a municipality (town), it can be assumed that the effluents are treated in a "standard STP". A standard STP is defined by:

- an effluent discharge rate of 2 000 m^3/day[31]; and
- the assumption that the sludge is applied to agricultural soil.

For uses at industrial sites, the situation with respect to wastewater treatment at industrial installations can vary. Many of the larger industrial installations are usually connected to a municipal wastewater treatment plant or have treatment facilities onsite.

Registrants may decide to develop generic exposure scenarios also assuming a "standard STP". They may also develop more specific exposure scenarios on the basis of their knowledge of their customers (or customer groups). For example, if they are aware[32] that a part of the industry downstream is composed of big sites with large biological STPs where the sludge are treated as waste and not applied to agricultural soil, they may develop specific exposure scenarios taking those assumptions into account.

For the estimation of the release at the regional scale (see Appendix A.16-3), it is necessary to know 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. It is assumed at EU scale that 80% of the wastewater is treated in a biological STP and the remaining 20% released directly into surface waters. These values were considered to be representative of the situation in large urban areas at the time of the revision of the TGD, and are implemented in EUSES.

Those values have not been updated since then although the proportion of the population connected to at least secondary wastewater treatment plants has been gradually increasing and is above 80 % in eleven EU Member States for which data are available, and is exceeding 90 % in some countries (i.e. highest rates in Malta, the Netherlands, the United Kingdom, Germany, Spain and Luxembourg) (source: Eurostat[33]).

In some situations, **removal of the substance in the sewer** before it reaches the municipal wastewater treatment plant, can be taken into account, e.g. for rapidly reacting substances, when the release takes place to a municipal STP (see Appendix A.16-2.3.1).

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here: https://www.umweltbundesamt.de/sites/default/files/medien/378/publikationen/texte_13_2015_application_of_simple_treat_4.0.pdf

[31] This has been set on the basis of 200 l of wastewater per capita per day for a population of 10 000 inhabitants.

[32] Such information may be available in the sectors and conveyed to registrants via use maps and SPERCs.

[33] Eurostat – Water statistics: http://ec.europa.eu/eurostat/statistics-explained/index.php/Water_statistics#Wastewater_treatment

R.16.3.2. Biological STP model

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.

The sewage treatment plant model SimpleTreat (Struijs,2014) 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 nine compartments (see Figure R.16-10). The model allows the "primary settler" section to be omitted, as could it be the case for certain biological industrial wastewater treatment plants.

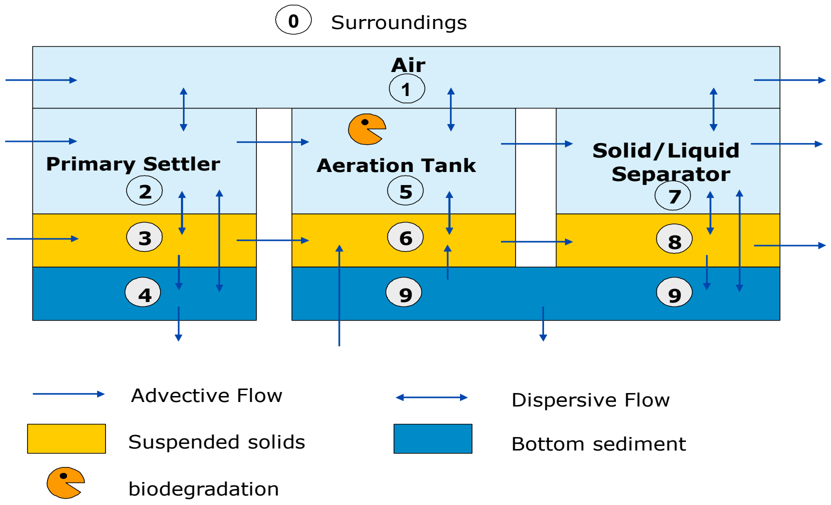

Figure R.16-10: Schematic design of the sewage treatment plant model SimpleTreat

R.16.3.2.1 Default fate in a biological STP

The concentration in the influent of the STP, i.e. the untreated wastewater, can be calculated from the local release to wastewater, potential degradation of the substance in the sewer, and the influent flow to the biological STP. The latter equals the effluent discharge (assumed to be 2 000 m^3/day in a standard STP).

Based on the amount of substance in the influent and *fractions directed to air, sludge and the effluent* (water stream) from the biological STP, the amount released to those three compartments can be estimated.

More details and calculations are provided in Appendix A.16-2.3.1.

SimpleTreat provides release fractions to air, water and sludge as a function of Henry's Law constant and adsorption properties (log Kow or, if available, log Koc) for different biodegradation categories. Those biodegradation categories have been derived from the biodegradation screening tests. Nevertheless, the use of SimpleTreat gives more accurate values. When measured degradation rates or removal data from sewage treatment plant (STP) simulation test (see section R.16.3.2.2 below) are available, this information can also be used to predict release fractions in SimpleTreat.

The SimpleTreat model may predict concentrations in effluent that significantly exceed the solubility in pure water. In such cases the effluent concentration may be re-set to a value closer to the water solubility; however the registrant should consider that:

- The fraction of substance in suspended matter might be considered to calculate the concentration in the STP effluent.
- There should be compensation in the fraction going to the sludge and potentially applied to agricultural soil. This will be reflected in a higher *fraction directed to sludge* from biological STP.

The approach described in the previous points might not be valid for substances dispersed in suspension or emulsion, substances with density lighter than water (therefore floating on the surface) or when the substance forms a film on the water phase. In these cases, the effluent concentration from the STP might actually be higher than the solubility of the substance itself and the compensation towards the fraction going to the sludge is not applicable anymore.

R.16.3.2.2 Refinement of behaviour in biological STP based on further substance properties

Refined information on the behaviour of a substance may be available enabling refinement of the estimations of the fractions released to air, sludge and effluent.

<u>Simulation test data</u>

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 wastewater treatment plant or other environmental situations, for example, a river. For information on simulation testing, see section R.7.9 of *Chapter R.7b of the Guidance on IR&CSA*.

<u>Measured data in full scale STP</u>

The percentage removal may be based upon measured influent and effluent concentrations. Nevertheless, in such cases, caution is needed to avoid underestimating the release to agricultural soil via the application of sludge, when adjusting the overall removal rates based on monitoring data. As with measured data from the environment, the measured data from STPs should be assessed with respect to their adequacy and representativeness (see Appendix A.16-6). Furthermore, for generic assessment, data from dedicated STPs should be used with caution. For example, when measured data are available for highly adapted STPs, these data should only be used for the assessment of the specific site.

R.16.4 Exposure estimation

R.16.4.1 Introduction

R.16.4.1.1 Principles

As explained in section R.16.1.4.1, exposure is to be estimated in all the compartments for which a hazard has been identified for the related protection target.

Exposure of the environment is the result of the release of a substance (section R.16.2), which may partly be degraded/removed by risk management measures (section R.16.2.2) and the subsequent distribution and degradation within the environment (section R.16.4.2).

Exposure estimates are called predicted environmental concentrations (PECs). They may be obtained:

- By modelling. EUSES is the most commonly used model, but other models may be used as well (see Appendix A.16-4). Input into the exposure estimation calculations are:
    - release rates as described in section R.16.2;
    - removals and distribution in biological sewage treatment plants (section R.16.3);
    - substance physico-chemical and fate properties (including partition coefficient and degradation rates) as described in section R.16.4.2.
- Using measured exposure (see Appendix A.16-6).

Two types of PEC values are derived to be used in further risk characterisation: the regional concentration (PECregional) and the local concentration (PEClocal). These two types of concentrations differ in temporal and spatial scale.

The local concentration (PEClocal) close to a point source emission is usually calculated as the sum of the concentration from the point source and the background concentration (the regional concentration (PECregional)). The background concentration is obtained from a so-called regional distribution calculation. Representative monitoring data may be used for the derivation of the regional and/or local concentrations as well.

Local environmental distribution

A generic standard environment is defined to allow for a chemical safety assessment at the European level. As it is impossible to characterise an 'average European environment', default parameter values are chosen which reflect typical or reasonable worst-case settings. Dedicated modelling approaches are used to calculate the concentrations in air, surface water and soil. The sediment and groundwater concentrations are estimated from the surface water and soil concentration respectively.

In defining the standard environments, a number of assumptions have been made with respect to the spatial and time scales, which are described in Appendix A.16-2.1.

Regional distribution

For calculating the regional PEC, the multi-media fate-model SimpleBox may be used. The basic characteristics of this model are shown in Figure R.16-6. A description of the assumptions made is given in Appendix A.16-3.

In the multi-media model used, the environmental media are represented by the following homogeneous and well-mixed compartment 'boxes':

- Atmosphere;
- Surface water (freshwater and marine environment);
- Sediment (freshwater and marine environment);
- Soil.

R.16.4.1.2 Existing tools for exposure estimation

EUSES (embedded in Chesar Platform) uses models for exposure estimation[34].

Besides the release estimation, only a few data on substance properties are needed to calculate PECs using EUSES.

The output data from the tool (to be used in the CSA) are:

- Local and regional PEC values specified in mg/L (water) or mg/kg (soil and sediment).
- Concentration in food (for the assessment of secondary poisoning) (mg/kg food).
- Regional and local total human doses taken up via the environment of the substance.

At the time of writing, the most updated version of EUSES is incorporated in Chesar Platform with scientific improvements compared to its standalone version[35] and therefore the explanation of the fate and transport mechanism in this guidance reflects what is implemented in that version.

More information on EUSES and other exposure estimation tools that are currently available is provided in Appendix A.16-4.

R.16.4.1.3 Use of environmental measured data

Actual measured concentrations of the substance in a particular environmental compartment can be used to facilitate the interpretation of model output and, when appropriate, can be used as predicted environmental concentrations (PECs)[36]. As many more factors may impact on these measured data, they have to be carefully evaluated for their quality and representativeness. Measured data at the local scale, representative for a specific use situation have to be clearly linked to the operational conditions and risk management measures described in the exposure scenario.

For some substances measured data will be available for air, fresh or marine water, sediment, biota and/or soil. These data have to be carefully evaluated for their quality and representativeness according to the criteria below. They are used together with calculated environmental concentrations when deciding on the environmental concentration to be used for exposure estimation. 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 shall overwrite the calculated values.

The evaluation should follow a stepwise procedure:

- adequate measured data should be selected by evaluation of the sampling and analytical methods employed and the geographic and time scales of the measurement campaigns (see Appendix A.16-6 for more details);
- the data should be assigned to local or regional scenarios by taking into account the sources of release and the environmental fate of the substance. If there is no spatial

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[34] EUSES is currently owned and updated by ECHA, and the most updated version of it is available in Chesar Platform.

[35] EUSES 2.2.0 standalone

[36] The modelling in EUSES assumes full mixing between the wastewater and the river water and potential high concentration close to the point of discharge can be disregarded for the purpose of environmental assessment under REACH. Therefore, calculated PECs correspond to an equally distributed concentration reached somewhere downstream from the point of discharge. In contrast, measured concentrations can be influenced by plumes. Depending on the point of sampling this could lead to an under/overestimation of the PEC. The modelled PEC might be preferable, even if a large amount of 'reliable' sampling has taken place near the point of discharge.

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; the regional concentration (i.e. PECregional) is by definition already included.

- 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 comparison of measured data and a calculated PEC (section R.16.4.1.4).

If measured data related to environmental concentrations are available and are:

(i) of a suitable quality;

(ii) supported by sufficient contextual information; and

(iii) assigned to the appropriate spatial scale, and

   a. representative of the OCs/RMMs that are expected to be in place (for data for the local scale);

   b. representative of a stable market (for data for the regional scale),

it can be used for the exposure estimate.

Sometimes, it may also be possible to estimate exposure based on measured data for another substance which however possesses similar physico-chemical characteristics or similar properties regarding its environmental fate and has a similar use pattern.

R.16.4.1.4 Decision on the environmental concentrations used for exposure estimation

When PECs have been derived from both measured data and calculation, they need to be 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 of substances. The following cases can be distinguished:

- 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. If the PEC based on measured data has been derived from a sufficient number of representative samples, then they should override the model predictions. On the other hand, if used for estimation of a local PEC, measured data may not be appropriate if they represent only the background concentration (PECregional) in the regarded environmental compartment.

- Calculated PEC << PEC based on measured concentrations

  This result might indicate that relevant sources of release were not taken into account when calculating the PEC. It should nevertheless be highlighted that registrants have the option to assess their own tonnage: therefore, the discrepancy can be explained by releases from other registrants of the same substance. Also, measured data can represent multiple sources (including those outside the scope of REACH) and possibly natural sources and/or historical contamination. Alternative causes may be spillage, a recent change in use pattern or release reducing risk management_measures that are not yet reflected in the samples. On the other hand use of unsuitable models for the assessment or an overestimation of degradation of the compound may also be the explanation.

In any case, for risk characterisation purposes, the exposure value with the highest confidence should be used. If it is confirmed that the PEC based on measured concentrations is representative for the exposure situation of the substance and 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 shall overwrite the calculated PECs. When deciding on exposure values to be used for risk characterisation it is necessary to consider all environmental compartments, to account for the possibilities of transfer and equilibrium between compartments.

R.16.4.2 Distribution and fate of the released substance in the environment

R.16.4.2.1 Principle

After entering the environment, substances are transported within a compartment, such as in air or in soil, or between several compartments (between air and water, air and soil or water and soil). The final distribution of the substance between compartments is mainly driven by the partitioning of the substance between the different media as well as by its abiotic or biotic degradation.
To estimate exposure of higher tier organisms via their food (secondary poisoning, see section R.16.4.3.8; or exposure of humans via the environment, see section R.16.4.3.9) bioaccumulation is to be taken into account. Indeed, some xenobiotics are taken up by organisms and bioaccumulation leads to higher concentrations of a substance in an organism than in its immediate environment, including food.

To assess the environmental exposure, the following processes should be considered:
- Partitioning between air and water (volatilisation);
- Adsorption to aerosol particles (gas-aerosol partitioning);
- Partitioning between solids and water in soil, sediment and suspended matter (adsorption and desorption);
- Partitioning between water/solids and biota (bioconcentration and biomagnification);
- Transformation processes in the environment, including biological (biotic) and abiotic (e.g. hydrolysis). Where stable and/or toxic transformation products occur these should be considered into the assessment.

In this section, the main concepts related to the substance fate and distribution characteristics relevant for exposure estimation are presented.

The models implemented in EUSES and illustrated in Figure R.16-5 and Figure R.16-6 are based on:
- Assumptions on a “standard environment”, i.e. size of the different compartments, characteristics (such as how much suspended matter is expected in freshwater, how much organic carbon is assumed in sediments, …). This standard environment is described in Appendix A.16-2.1; and
- Fate properties of the substance, i.e. partitioning, degradation, accumulation properties.

Depending on the complexity of the fate model used, a lower or higher number of parameters characterising the substance properties may play a role for the estimation of the behaviour of the substance. The following minimum information on substance properties is required for an assessment based on EUSES: molecular weight, water solubility, vapour pressure, melting point, octanol-water partition coefficient, information on ready biodegradability, Koc and, if relevant, BCF. For the estimation of the following parameters, QSARs are available within EUSES:

- Various partition coefficients (Kps) (for the calculation see Appendix A.16-2.2);
- Degradation rates (see section R.16.4.2.3 and Appendix A.16-2.2.2);
- Bioaccumulation factors (BCF earthworm, BMF…) (see Appendix A.16-2.2 for more information).

Depending on the case, more or less information on the substance fate properties additional to the minimum required may be available. When available reliable test data should be used as input instead of the QSARs outputs. Registrants will have to decide when to rely on the QSARs included into EUSES and when more specific information needs to be generated.

Most of the models enabling such estimation have been developed mainly from the experience gained on organic substances. This means that the used methodology cannot always be applied directly to metals without modifications. Specific guidance on how to model fate and distribution characteristics for metals can be found in Appendix A.7.13-2[37]. In particular for an inorganic substance, it is also advised to provide information on the abiotic transformations, and solid-water partition coefficients and the water-biota partition coefficients.

There are also limitations in the applicability of the environmental fate models which depend on LogKow and Henry's law for use with insoluble nanomaterials (and other insoluble particles or substances). As models are emerging for estimating the environmental fate of nanomaterials, manufacturers or importers may use them with scientific justifications or collect measurement information on environmental release, fate (including (dis)aggregation and (dis)agglomeration) and levels in the environment where appropriate. Proposals on updates for EUSES for nanomaterials are mentioned in the document published by RIVM mentioned above.

R.16.4.2.2 Partitioning in the environment – specific cases

Specific considerations for estimating partition coefficients in the marine environment

The ionic strength, composition, and pH of seawater, compared with freshwater, have potential effects on the partitioning of a substance with other compartments. To a large extent, these effects are associated with differences in water solubility and/or speciation of the substance, compared to freshwater.

Measured partition coefficients between water and a second compartment, if available, are however 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, but the techniques that allow such an extrapolation are also largely based on freshwater data sets. Therefore, to assess the distribution of substance in the marine environment, it is necessary to consider the extent to which partition coefficients may differ between seawater and freshwater:

- For non-ionisable organic substances unless measured seawater data of equal reliability are available, freshwater data can be used without adjustment for the marine environment.

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[37] https://echa.europa.eu/documents/10162/17224/information_requirements_r7_13_2_en.pdf/0497e68d-4bb5-4b12-a4db-52ce0c1bc237?t=1322594777855

- For ionisable organic compounds, mostly the procedure to correct partition coefficients for ionisable substances, as described in section R.7.1.20 *of Chapter R.7a of the Guidance on IR&CSA*, may be considered sufficiently reliable for marine conditions.
- For inorganic substances such as metals, usually measurements under marine conditions may be necessary; exceptionally, extrapolation from freshwater data may be possible.

Ionising substances

The degree of ionisation of an organic acid or base greatly affects both the fate (solubility, adsorption, bioconcentration) and the toxicity of the compound. Further guidance on how to take this into account in the assessment is provided in sections R.7.1.17 and R.7.1.20 *of Chapter R.7a of the Guidance on IR&CSA*

Particles

Estimates based on "partitioning" are limited to distribution of a substance in molecular form. However, substances may also 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, air distribution may also 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.

R.16.4.2.3 Degradation in the environment

After release into the environment, a substance may undergo various degradation processes in the various compartments. Degradation may be triggered by water contact (hydrolysis), light (photolysis) and microorganisms. These processes can be quick or slow, complete (resulting in small inorganic molecules) or incomplete (transformation products may be considered for assessment). For quickly hydrolysing substances, there is usually the need to investigate the potential occurrence of hazardous hydrolysis products.

For biodegradation, various types of screening tests are available. If a substance passes or fails the test, a conservative degradation rate can be estimated (see Table R.16-12 and Table R.16-14). If screening tests show that the biodegradation is incomplete and/or slow, simulation tests can be used to establish more realistic degradation rates and an analysis of potentially relevant stable transformation products.

Appendix A.16-2.2.2 shows how EUSES calculates the degradation rates from the screening readily biodegradability tests.

In general, the assessment of degradation processes should be based on data, which reflect the environmental conditions as realistically as possible. For an in-depth discussion on the information requirements on degradation, see section R.7.9 *of Chapter R.7b of the Guidance on IR&CSA*.

The rate constants and half-lives to be estimated for the various degradation processes are listed in Appendix A.16-2.2.2, together with the equation for calculation.

Further guidance on how to deal with information on degradation is given in Appendix A.16-2.2.2.

R.16.4.3 Exposure estimation

In the following sections, the principles which are at the basis of the calculation of the predicted exposure concentration (PEClocal) for each compartment are presented.

For most of the compartments (except for the biological STP) a PEC regional, which is also to be estimated, is integrated in the calculation of the PEClocal. For naturally occurring substances like inorganics, the natural background concentration in relevant compartments also needs to be taken into account.

Table R.16-4: Derivation of PEC-values in EUSES

Target	Medium of exposure	Section/Appendix
Aquatic compartment (incl. marine environment)	Surface water	R.16.4.3.2and R.16.4.3.4 Appendix A.16-2.3.3and A.16-2.3.5
	Sediment	R.16.4.3.3 Appendix A.16-2.3.4
	Predators (fish eating)	R.16.4.3.8 Appendix A.16-2.3.8
Terrestrial compartment	Arable land[38]	R.16.4.3.5 Appendix A.16-2.3.6
	Grassland[39]	R.16.4.3.5 Appendix A.16-2.3.6
	Groundwater	R.16.4.3.6 Appendix A.16-2.3.7
	Predators (worm eating)	R.16.4.3.8 Appendix A.16-2.3.8
Air compartment	Air	R.16.4.3.7 Appendix A.16-2.3.2
Microorganisms	STP aeration tank	R.16.4.3.1 Appendix A.16-2.3.1

For the biological STP, a concentration in the STP (PEC_{stp}) is estimated.

For **fresh and marine water**, the $PEClocal_{water}$ is the sum of the local concentration during the release episode from an STP or during the release period from agriculture use, the regional PEC (see section R.16.1.4.2) and, where relevant, a natural background concentration (relevant for naturally occurring substances).

For **fresh and marine sediments**, the PEC is usually estimated from the PEC in water assuming a thermodynamic partitioning equilibrium with water; in case measured data for $PECregional_{sediment}$ are available these can be used to overwrite the regional contribution to $PEClocal_{sediment}$.

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[38] Arable land and grassland are together referred to as 'agricultural soil'. For exposure of the terrestrial ecosystem PECsoil is calculated for the arable land; PECsoil calculated for the grassland is used for human exposure via the environment.

For **air**, the PEClocal$_{air}$ is the sum of the local concentration (at 100m from the point source[39]) averaged over the year and the regional PEC.

For **soil**, the PEClocal$_{soil}$ is the sum of the local concentration in agricultural soil averaged over 30 days[40], the regional PEC and, where relevant, the natural background concentration (relevant for naturally occurring substances). Arable land and grassland are together referred to as 'agricultural soil'. For exposure of the terrestrial ecosystem PEClocalsoil is calculated for the arable land. Concentrations in other soil compartments and groundwater or at other scales are also calculated as they are needed for the estimation of exposure for secondary poisoning or humans via the environment. They are not used as such in the risk characterisation.

For **secondary poisoning**, the concentrations in the food of predators are estimated from the concentrations in the environment and the bioaccumulation. Two concentrations are estimated; one on the basis of the PEC local (in water or soil) and one on the basis of the PEC regional. The model (supported by EUSES) agreed considers that the PEC for secondary poisoning is the mean of those two concentrations.

For **humans via the environment**, a local and a regional exposure are estimated independently. The local scenario is a worst-case scenario.

Details about calculations are given in Appendix A.16-2.3. The calculations of regional steady-state concentrations (PECregional) are presented in Appendix A.16-3.

In defining the standard environments, a number of assumptions have to be made with respect to scale and time. These are summarised briefly in the following subsections. More details are given in the relevant sections in Appendix A.16-2.

R.16.4.3.1 STP concentration for evaluation of inhibition to microorganisms

For the modelling of the STP, it is considered that the microorganisms are exposed to a total concentration of the substance equal to the one in the STP effluent, i.e. that PEC$_{stp}$ is equal to Clocal$_{eff}$.

As explained in Appendix A.16-2.3.1, assuming steady state and complete mixing in all the tanks of the STP, the concentration dissolved in the activated sludge in the aeration tank, to which the microorganisms are exposed, is assumed to be equal to the concentration in the effluent. This concentration is the result of a simple mass balance: there is an inflow of sewage in one hand, and in the other hand removal via degradation, volatilisation and the outflow of activated sludge into the secondary settler.

In the case of intermittent releases (releases taking place less than once per month), it is considered that the microorganisms are exposed to a total concentration of the substance equal to the one in the STP influent, i.e. that PEC$_{stp}$ is equal to Clocal$_{inf}$. This intends to account for the fact that the microorganisms capable of biodegrading the substance may be completely lost in between the intermittent influent discharges. As a consequence, the concentration in the aeration tank may increase and therefore the concentration in the influent of the STP is more representative for the PEC for microorganisms.

In some situations, removal in the sewer before entering the STP can be taken into account. This is the case for rapidly reacting substances, substances following fast abiotic degradation as well as for substances for which biodegradation in the sewer is proven by OECD 314 A or

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[39] For widespread uses, the point source is the biological STP.

[40] In some cases the initial local concentration (calculated after the last application, not averaged) may need to be used instead of the concentration averaged over 30 days, see section R.16.4.3.5)

similar literature or monitoring data, when the release takes place to a municipal STP. Sewer degradation should not be taken into account for releases to an industrial (on site) STP (due to the plausible short distance from site to STP and the high variability in wastewater, e.g. in terms of organic content) and releases into rainwater sewers (due to the expected high flow rate and low organic load). In case sewer degradation is relevant, it will reduce $Clocal_{inf}$ and therefore the concentration to which microorganisms in the STP are exposed.

R.16.4.3.2 Concentration in freshwater

- Uses at industrial sites and in a municipality (town)

The effluent of the sewage treatment plant is diluted into the surface water. Figure R.16-11 shows the most important fate processes of the aquatic compartment.

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

The concentration in surface water ($PEClocal_{water}$) is in principle calculated after complete mixing of the effluent outfall. Because of the short time between effluent discharge and exposure location, dilution will usually be the dominant "removal" process. Therefore, degradation in surface waters, volatilisation from the water body, and sedimentation are not normally taken into account as removal processes. To allow for sorption, a correction is made to take account of the fraction of substance that is adsorbed to suspended matter. For the dilution factor, a default value of 10 is usually used, corresponding to an effluent rate of 2 000 m^3/day being released into a river having a flow rate of 18 000m^3/day. For site-specific assessment, such parameters may be modified (see also section R.16.2.2.7). It should be reminded that the dilution factor should not be set to a value higher than 1 000 in any case (see R.16.2.2.7 and Appendix A.16-2.3).

The resulting dissolved concentration is used for comparison with $PNEC_{water}$.

More details on how the concentration is calculated are provided in Appendix A.16-2.3.3.

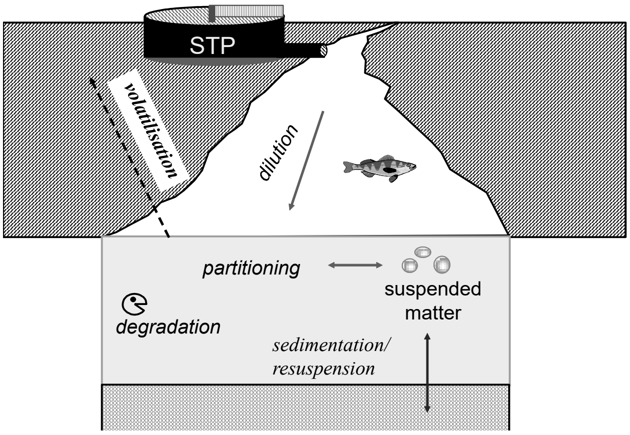

Figure R.16-11: Fate processes in the surface water

- Agricultural use

The releases to surface water due to agricultural use can have two sources:

- Direct release via drift when the application method is spraying
- Indirect release via runoff from the soil

The scenario assumes that releases from drift occur in each application day whereas the runoff is only accounted for after the last application.

The concentration in surface water is calculated for each day during 365 days (not an average) taking into account the releases from drift (when applicable, as indicated above) and runoff, dilution in the water body and removal processes from the water (biodegradation and sorption to suspended matter).

The resulting maximum concentration over the year is used for comparison with $PNEC_{water}$. In addition, the annual average concentration is also calculated and used to estimate fish concentration which is taken into account for freshwater secondary poisoning and human's consumption of fish (R.16.4.3.8).

More details on how the concentration is calculated are provided in Appendix A.16-2.4.

R.16.4.3.3 Concentration in 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 thermodynamic partitioning equilibrium between water and suspended matter.

PEClocal for sediment can be compared to the PNEC for sediment dwelling organisms.

More details on the calculation method are provided in Appendix A.16-2.3.4.

R.16.4.3.4 Concentration in marine aquatic compartment

The use of local marine exposure scenarios can be necessary for specific sites releasing directly into the sea. In such cases, potential local releases to the marine environment can occur and, hence, it is necessary to perform a local exposure estimation for the local marine environment.

Normally, only dilution and adsorption to suspended sediment need to be considered. Therefore, the same estimation model as for inland exposure estimation can be used to obtain the local concentration in seawater, using a realistic worst-case dilution factor for discharges to a coastal zone of 100. For site-specific assessment, a specific dilution factor may be used. A valid local distribution model may be used if available.

More details on the calculation method are provided in Appendix A.16-2.3.5.

R.16.4.3.5 Concentration in soil

- Uses at industrial sites and in a municipality (town)

The concentration in soil ($PEClocal_{soil}$) is calculated as an average concentration over a certain time-period in arable land, fertilised with sludge from an STP[41] and receiving continuous aerial deposition from a nearby point source (see section R.16.4.3.7) (production/processing site and STP aeration tank). The processes by which the substance is removed from the soil compartment also need to be considered (degradation, volatilisation and leaching).

Figure R.16-12 shows the most important fate processes in the soil compartment. Input and output fluxes for the soil compartment are described in Figure R.16-5 where the general distribution in the environment is depicted.

Two different soil types are distinguished: arable land and grassland, which differ in the amount of sludge applied and the mixing depth.

For exposure of the terrestrial ecosystem, the concentration in arable land is generally averaged over 30 days. However, the concentration calculated directly after the last application is used when the PNEC for the terrestrial compartment has been derived based on terrestrial ecotoxicity tests in which the results are expressed based on initial, nominal concentrations in a test with a single application (and therefore do not account for degradation).

For human indirect exposure (exposure of humans via the environment), the concentration is averaged over 180 days. The concentration in groundwater is calculated below this arable land area. Furthermore, crops are grown on arable land for human consumption, and cattle, producing meat and milk, are grazing on grasslands.

- Agricultural use

In addition to what is described above for sludge application in soil, there are some specific aspects which need to be considered for the direct application of a substance to agricultural soil, as co-formulant of a fertilizer or plant protection product:

- The mixing depth for arable land depends on the use of ploughing in the application (i.e. ploughing is different for fertilizers or plant protection products), and
- The concentration in groundwater is calculated for both the arable land area and the grassland, and the higher value used in the assessment.

More details on the calculation methods are provided in Appendices A.16-2.3.6 and A.16-2.4.

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[41] In the exposure estimation, it is assumed that sludge from a biological STP is spread on agricultural soil for 10 consecutive years.

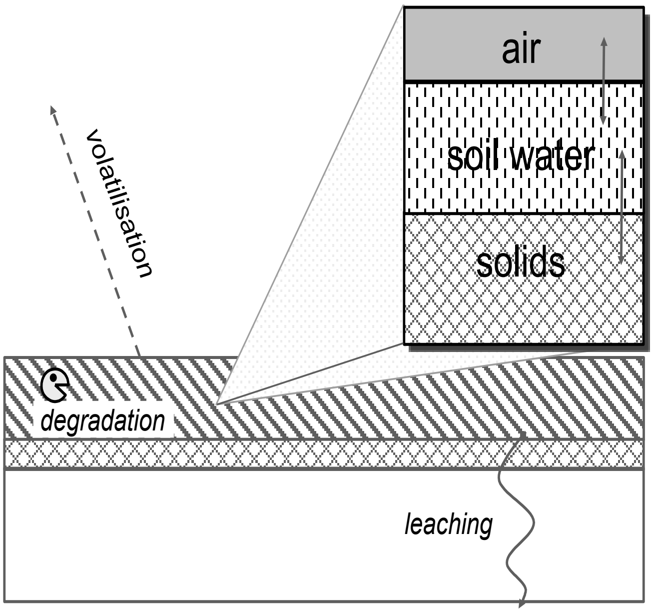

Figure R.16-12: Calculation of PECsoil

R.16.4.3.6 Concentration in groundwater

The concentration in groundwater is calculated only for indirect exposure of humans through drinking water. For the calculation of groundwater levels, several numerical models are available (mainly for pesticides). These models, however, require a characterisation of the soil on a high level of detail. This makes these models less appropriate for the initial standard assessment. Therefore, as an indication for potential groundwater levels, the concentration in porewater of arable land (and also in grassland, in case of agricultural use) is taken. It should be noted that this is a worst-case assumption, neglecting transformation and dilution in deeper soil layers.

More details on the calculation method are provided in Appendix A.16-2.3.7.

R.16.4.3.7 Concentration in atmosphere

- Uses at industrial sites and in a municipality (town)

The air compartment receives its input from direct release to air, and volatilisation from the sewage treatment plant. A certain amount of substance is transferred from the air compartment to the soil compartment via deposition. Deposition is calculated as an average for a circle around the source with a radius of 1 000 m, which is supposed to represent the local agricultural area. Deposition is used as input for the soil assessment, annual average deposition fluxes are used.

The most important fate processes in air, are schematically drawn in Figure R.16-13.

An annual average concentration in air at 100 metres from the source (this distance is assumed to be representative for the average size of an industrial site) is calculated. For uses at industrial sites, both releases from point source and from STP (if any) are considered while for widespread uses only the release from STP is considered. For the calculation of $PEClocal_{air}$, the PECregional is added to the average annual concentration in air.

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 calculation of the intake of substances through inhalation in the indirect exposure of humans.

Many air models are available that are highly flexible and can be adjusted to take specific information on scale, release sources, weather conditions etc. into account. For many substances, this type of information is normally not available. Hence, a standardised exposure estimation is carried out making a number of explicit assumptions and using a number of fixed default parameters. More detailed information on the model is provided in Appendix A.16-2.3.2.

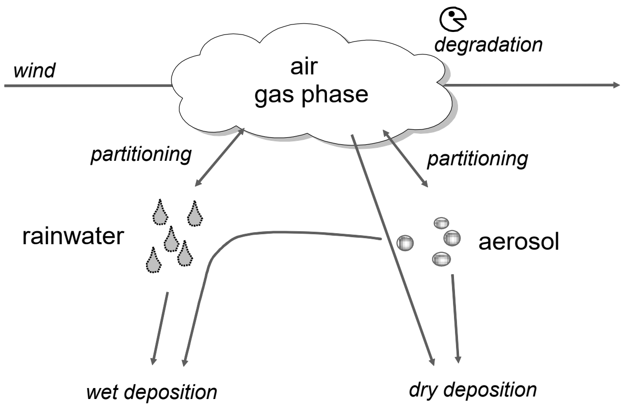

Figure R.16-13: Fate processes in the air compartment

- Agricultural use

In the agricultural use scenario the air compartment receives its input from volatilisation during spray application (when spray application takes place).

For consistency with the current EUSES implementation, the emission to air is considered as a point source release. In particular, air concentration at the receptor is calculated 100 m away from the source.

Compared with EUSES implementation a difference is that the air concentration during episode (i.e. spraying task) is not averaged over a year but over a 30 days period to get $Clocal_{air}$ due to the reduced emission days in a year. This is then added to the PECregional for the calculation of $PEClocal_{air}$, which is used for the calculation of the intake of substances through inhalation in the indirect exposure of humans.

More detailed information on the model is provided in Appendix A.16-2.4.

R.16.4.3.8 Predators (secondary poisoning)

The predicted concentration in the food for predators, i.e. the concentration in worms and fish, are estimated on the basis of:

- For fish-eating predators: the local and regional PECs for surface water, the bioconcentration factor (BCF) for fish and biomagnification factors (BMF). The PEC is calculated as the mean of the concentration in the (top) predator food obtained from the PEC local and from the PEC regional. Top predators are considered for marine water assessment only. (see Appendix A.16-2.2 for more information on BCF and BMF and their roles in the calculations). To be noted that when assessing an agricultural use (i.e. a direct release, not via STP sludge), fish-eating predators and top predators are not considered, as it is assumed that the ditch is not connected to other surface water bodies (therefore, not connected to the marine environment).
- For worm-eating predators: the local and regional PEC for soil and BCF for worms. The PEC is calculated as the mean of the concentration in the predator food obtained from the PEC local and from the PEC regional.

In this section, the general principles are outlined. The details of the individual assessment steps and PEC calculations are described in Appendix A.16-2.3.8.

A) Fish-eating predators and top-predators (marine food chain):

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 or freshwater aqueous phase and receive the substances from this source. A relatively simple food chain is modelled which consists of the marine/freshwater phase, marine/freshwater food, marine/freshwater fish and two separate levels of predators (top predators relevant for marine water only). This food chain is visualised in Figure R.16-14 below. As can be seen from this scheme, risks for three different trophic levels need to be assessed:

1. *Risks to marine/freshwater fish:* No specific calculation needs to be performed for estimating the risk to fish as this is covered by the risk assessment for aquatic organisms.
2. *Risks to marine/freshwater predators:* The risks to marine/freshwater predators is calculated as the ratio between the concentration in their food (marine/freshwater fish) and the no-effect concentration for oral intake ($PNEC_{oral}$). The concentration in the marine/freshwater 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} information for other organisms such as mussels may also 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 ($PNEC_{oral}$). 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.

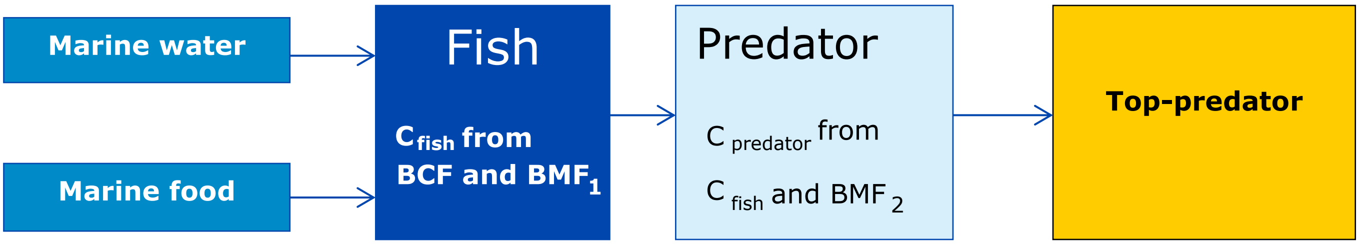

Figure R.16-14: Secondary poisoning: aquatic food chain for marine water

B) Secondary poisoning via 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).

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.

R.16.4.3.9 Humans exposed indirectly via the environment

Indirect exposure of humans via the environment may occur both through the consumption of food (e.g. fish, crops, meat and milk) and drinking water (oral route), and via the inhalation of air (inhalation route). Exposure via the oral route can be estimated based on the concentration in food products (and drinking water) and the amount of each food consumed (and water drunk). In EUSES, a generic "food basket" is defined that describes the quantities and types of different food types that are consumed and their consumption rates. The concentration of a substance in food is related to its concentration in water, soil and air and to its potential for bioaccumulation or biotransfer between compartments.

The different routes of exposure are illustrated in Figure R.16-15.

It should be noted that for assessment of agricultural uses, only groundwater is considered as drinking water. In this case surface water (from the ditch) is not considered.

Human behaviour related to food consumption shows appreciable variation between different EU countries but also within countries. Equally, large variations can occur between individuals. The distribution and intensity of local sources of exposure will also be different between EU countries. As a consequence, indirect exposure is likely to vary greatly within a given population. Therefore, the exposure model (with its underlying assumptions) will have a major influence on the result of the assessment. This choice of exposure model will always be a compromise between realism and effort, as a realistic solution is difficult to obtain (this would involve elaborate statistical evaluation of human sourcing and mobility behaviour, as well as of the distribution and intensity of all local sources of exposure).

The EUSES "Food basket" consumption rates for individual food types are derived from the highest country-average consumption rate observed across Member States. This leads to a worst-case food basket. However, in practice, usually only one or two food groups dominate the total exposure.

In EUSES, indirect exposure to humans is assessed on two spatial scales: locally near a point source of the substance, and regionally using averaged concentrations over a larger area. In the local assessment, all food products are assumed to be derived from the vicinity of one point source. In the regional assessment, all food products are assumed to be taken from within the region (i.e. no imports or exports of food products). It should be noted that the local and regional environments are not actual sites or regions, but standardised environments as defined in Appendix A.16-2.1 and Appendix A.16-3. Clearly, the local scale represents a worst-case situation as people do not consume 100% of their food obtained from the immediate vicinity of a point source. Equally, the regional assessment represents a highly averaged exposure situation, which does not describe individuals who consume food products from the vicinity of point sources.

In light of these limitations, it is clear that a generic indirect exposure estimation, as described by the calculations detailed in Appendix A.16-2.3.9, can only be used for screening purposes to indicate potential problems. The assessment should be seen as a helpful tool for decision making but not as a prediction of the human exposure actually occurring at some place or time.

It should be noted that extreme consumers of certain food products are not accounted for using this approach. Taking extreme consumption into account would lead to even more severe worst-case assessments.

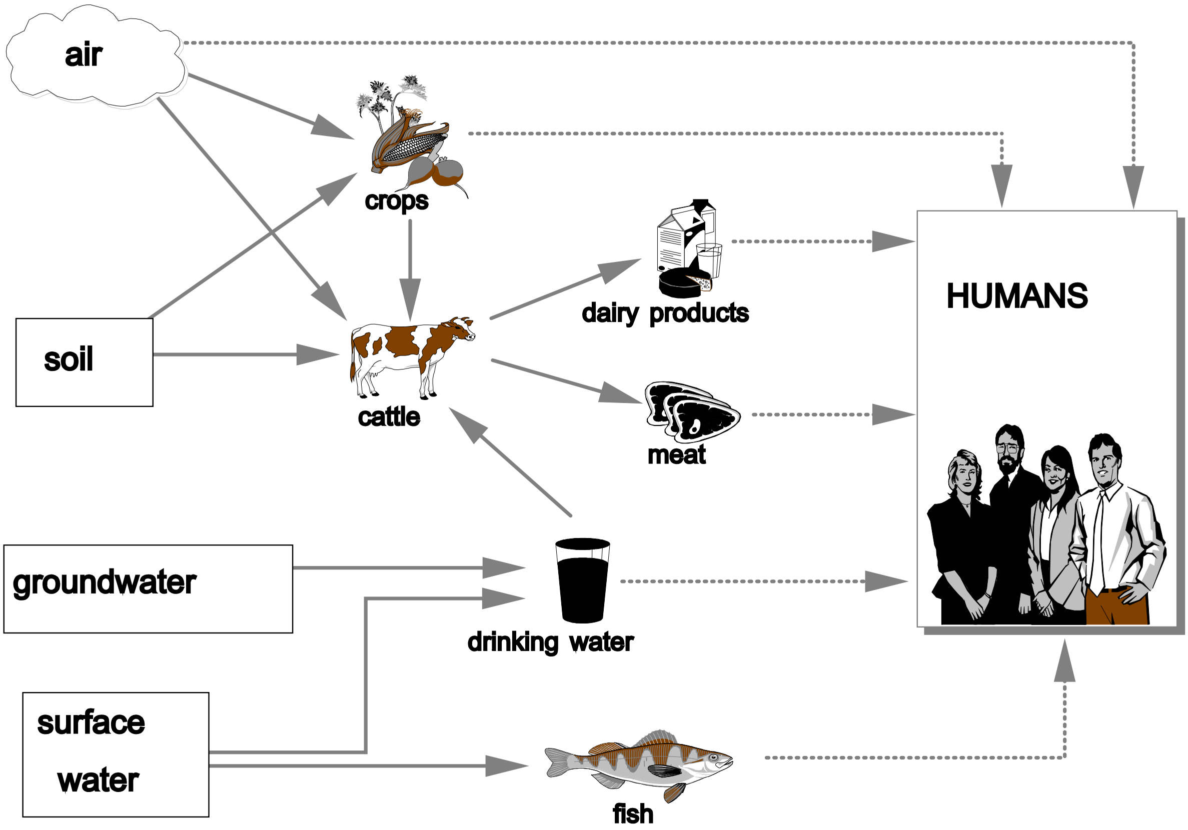

Figure R.16-15: Schematic representation of the exposure routes considered in indirect exposure to humans via the environment

As the modelling approach can be considered conservative, if both local and regional-scale assessments do not indicate a potential risk (or high exposures), there is generally no reason for further assessment, unless there is some other indication that the modelling approach is not appropriate (e.g. for substances with physico-chemical properties that are not compatible with EUSES, see section R.16.4.2.1). However, if either local or regional-scale assessments indicate a risk, there is usually a need for refinement of the assessment before any decisions are taken to reduce risks (e.g. recommendations for more stringent risk management measures).

When refinement of the assessment is necessary, it should initially be considered if the release estimates are realistic. Subsequent refinements, if needed, should focus on the concentrations in relevant environmental compartments (which might involve better estimates of degradation half-lives), concentrations in the food items present in the "food basket" or on the consumption rates of the food items. Refined data could be derived on the basis of monitoring data (e.g. food basket surveys) and/or alternative modelling approaches (e.g. for the plant uptake model). It may also be considered whether additional risk management may be needed for some uses leading to high releases to the environment.

It should be noted that there is no testing strategy triggered by the indirect exposure estimation.

R.16.5 Risk characterisation

Once the expected exposure under actual or anticipated conditions of use is estimated, these exposure levels are used to characterise the risks by comparing them with the outcome of the hazard assessment.

Exposure levels are compared to either quantitative or qualitative hazard information.

As explained in section R.16.1.3.2, when suitable predicted no-effect concentrations (PNECs) are available, a quantitative risk characterisation can take place for each use by comparing the exposure concentration in each compartment with the relevant PNEC (so-called Risk Characterisation Ratios (RCRs) can be derived[42]). If there are continuous releases, organisms with a relatively short lifespan, like aquatic organisms, are exposed locally to toxic concentrations of the substance for a considerable proportion of their lifetime. Therefore, for these organisms, the average exposure levels during release episodes are assumed to be continuous. It follows from this assumption that the estimated environmental concentrations can be considered as estimates of long-term exposure levels for these organisms, which can be compared to no effect concentrations derived from long-term toxicity data.

If the RCRs for each protection target are below 1, the risks may be considered to be adequately controlled.

When no-effect levels cannot be established for certain effects, a qualitative assessment of the likelihood that these effects are avoided when exposure scenarios are implemented shall be carried out.

If the risk characterisation shows that risks are not controlled, registrants have different options. They can either refine the assessment on the basis of further hazard and/or release/exposure information until control of the risk can be demonstrated or conclude that some uses may not be safe and thus advise against these. To produce a meaningful risk characterisation, it is important that the assessor understands and takes the uncertainties associated with the information/data that is provided into account (related to both hazard assessment and exposure assessment). *Chapter R.19 of the Guidance on IR&CSA* contains

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[42] RCR= PEC/PNEC.

more information on using uncertainty analysis to assist the registrant in interpreting the risk characterisation and refining the iterations in the CSA process.

Table R.**16-5** provides an overview of the risk characterisation for the various protection targets.

Further guidance on risk characterisation is provided in Part E of the Guidance on IR&CSA.

Table R.16-5: Summary of the protection targets and relevant considerations on risk characterisations

Protection target		Risk characterisation ratio	Remarks
Biological sewage treatment plant:	Microorganisms	$PEC_{stp}/PNEC_{microorganisms}$	
Freshwater ecosystem:	Freshwater organisms	$PEClocal_{water}/PNEC_{water(freshwater)}$ $PECregional_{freshwater}/PNEC_{water(freshwater)}$	Specific considerations in case of intermittent release The comparison of the local RCR and of the regional RCR provides an idea of the contribution of the specific use to the risk
	Sediments organisms	$PEClocal_{sed}/PNEC_{sed(freshwater)}$ $PECreg_{sed}/PNEC_{sed(freshwater)}$	Specific considerations in case equilibrium partitioning applied for adsorptive substances (see below) The concentration is to be expressed in dry sediment as the PNEC is expressed in dry weight.[43]
	(Fish eating) predators[44]	$PEC_{oral,predators}/PNEC_{oral}$	

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[43] The conversion factor for suspended matter from wet weight to dry weight can be calculated with Equation R.16-2

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

Marine ecosystem:	Marine water organisms	$\text{PEClocal}_{\text{seawater}}/\text{PNEC}_{\text{saltwater}}$ $\text{PECregional}_{\text{seawater}}/\text{PNEC}_{\text{saltewater}}$	Specific considerations in case of intermittent release
	Sediment organisms	$\text{PEClocal}_{\text{sed,marine}}/\text{PNEC}_{\text{sed,marine}}$ $\text{PECregional}_{\text{sed,marine}}/\text{PNEC}_{\text{sed,marine}}$	Specific considerations in case equilibrium partitioning applied for adsorptive substances (see below)
	(Fish eating) predators Top predators	$\text{PEC}_{\text{oral,predator,marine}}/\text{PNEC}_{\text{oral}}$ $\text{PEC}_{\text{oral,top predator,marine}}/\text{PNEC}_{\text{oral}}$	
Terrestrial ecosystem:	Soil organisms	$\text{PEClocal}_{\text{soil}}/\text{PNEC}_{\text{soil}}$ $\text{PECregional}_{\text{natural soil}}/\text{PNEC}_{\text{soil}}$	Specific considerations in case equilibrium partitioning applied for adsorptive substances (see below) The concentration is to be expressed in dry soil as the PNEC is expressed in dry weight.[45]
	(Worm eating) predators	$\text{PEC}_{\text{oral,predators}}/\text{PNEC}_{\text{oral}}$	
Air	Atmosphere	$\text{PEC}_{\text{air}}/\text{PNEC}_{\text{air}}$	An RCR based on a PNEC_{air} will be extremely rarely available. Note that this usually refers to exposure of plants via air. Qualitative considerations for e.g. ozone depletion, photochemical ozone creation potential
Humans via the	Exposure via inhalation	PEC_{air}/DNELinhalation long term systemic	

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[45] The conversion factor for soil concentration from wet weight to dry weight can be calculated with Equation R.16-2

environment	Exposure by ingestion	Total dose/$PNEC_{oral}$ long term systemic	

Specific considerations for adsorptive substances

For substances with (i) a log Kow greater than 5 or (ii) when log Kow is not available and log Koc>3 or (iii) with an adsorption or binding behaviour not triggered by the lipophilicity (i.e. log Kow) but by other mechanisms (e.g. ionising substances, surface active substances, substances that bind chemically with sediment components, substances where Kd predicts high binding potential), the equilibrium partitioning method (EPM) is used in a modified way. For such substances, if the assessment is based on the EPM, the RCR for sediment and soil should be increased by a factor of 10 to account for the exposure of the organisms via ingestion of sediment or soil (see also Guidance R.7b, R.7c, R.10 and E).

Specific considerations for the RCR for water for intermittent release (see section R.16.2.2.6)

If intermittent release is identified, only short-term effects are considered for the aquatic ecosystem and no-effect levels are derived from short-term toxicity data only. Therefore, a specific PNEC for intermittent release may be derived (see Guidance R.10.3.3) and the RCR calculated on the basis of such PNEC intermittent.

Note that for sediments and soil, such rules do not apply. Therefore, when an equilibrium partitioning method is applied, it should be applied on the basis of the $PNEC_{water}$.

R.16.6 Summary of the assessment

In the following table the key determinants of release and exposure assessment are summarised, together with the assumptions/values for the default assessment and for a refined assessment. The detailed description of these assumptions can be found in sections R.16.3 to R.16.5.

The determinants correspond to the EUSES model regularly applied in chemical safety assessment in the EU. The model is available via a number of different tools, see Appendix A.16-4. Appendix A.16-4 also includes an overview on higher tier models complementing EUSES for certain environments or types of uses.

Table R.16-6: Overview on determinants for the default and refined exposure assessment

DETERMINANTS OF RELEASE AND EXPOSURE FOR THE DEFAULT AND REFINED ASSESSMENT		
Determinant	**Default assessment**	**Refined assessment**
Daily use amount at a site Annual use amount at the site [for uses at industrial site, ERC1-7, ERC 12]	They are calculated from the “tonnage per use” (see section R.16.2.2.1) It is assumed that the total tonnage for the use is processed by a single user. See R.16.2.2.1.1	The daily and annual use amount at a site for a use can be overwritten by the registrant, on the basis of: ▪ Site-specific information, such as the actual daily use in the manufacturing stage (readily accessible to the registrant)

DETERMINANTS OF RELEASE AND EXPOSURE FOR THE DEFAULT AND REFINED ASSESSMENT		
Determinant	**Default assessment**	**Refined assessment**
		▪ Information on the actual amount used by large downstream users (formulators and end uses at industrial site). Information may be provided by downstream user sectors. See R.16.2.2.1.1
Daily widespread use amount in standard town; [for uses by professional worker or consumer, ERC 8-11]	It is calculated from the "tonnage per use", corresponding to the consumption in a standard town of 10 000 inhabitants, multiplied by a safety factor of 4 (to take account of potential variations in time and space). See R.16.2.2.1.2	Registrants can overwrite this value, for example, if they have sufficient information to demonstrate that the use of the substance is evenly distributed in space and time throughout the region (e.g. for detergents); in this case, it is possible to divide the default tonnage by a factor of maximum 4.
Widespread use amount for agricultural use	The released amount per year is calculated from the application rate per hectare per year (kg/ha/year). See R.16.2.2.1.2	
Regional tonnage	For the uses at industrial sites (ERC1-7, 12), it is set equal to 100% of the tonnage for the use. For widespread uses, it is set equal to 10% of the tonnage for the use See R.16.2.2.1.3	Market data could be used to overwrite the default for the region with a percentage that corresponds to the actual situation.
Time pattern of release to water	Continuous (except in the case of direct release to agricultural soil widespread uses).	The pattern of release to water can be changed to *intermittent* (i.e. if the releases take place less than once per month and for no more than 24 hours). See R.16.2.2.6.

DETERMINANTS OF RELEASE AND EXPOSURE FOR THE DEFAULT AND REFINED ASSESSMENT		
Determinant	**Default assessment**	**Refined assessment**
Biological sewage treatment plant (STP)	By default, the releases to fresh and marine water are expected to be treated in a standard biological STP for all uses except in case of direct release to agricultural soil. Treatment efficiency and corresponding release factors are calculated by the SIMPLETREAT model, using substance properties and results of screening tests on biotic degradation as an input. See also R.16.2.2.4 and R.16.3.	For uses at industrial sites, in known situations, there may be no biological STP or there may be a specific biological STP (with specific discharge rate and specific treatment of the sludge, see parameters below). For a site-specific STP, treatment effectiveness and corresponding release factors may be refined based on measured data. It is also possible to refine the assumed treatment effectiveness in municipal STPs, if substance-specific evidence is available. See also R.16.3.2.2.
Discharge rate of the biological sewage treatment plant (STP)	2 000 m^3/day (see also R.16.3)	For site-specific assessment, the flow rate can be changed according to the site-specific data.
Application to agricultural soil of the sludge of the biological sewage treatment plant (STP)	The sludge is by default assumed to be applied to agricultural soil (see R.16.3)	For site-specific assessments, if incineration or other waste treatment of the sludge is foreseen, then agricultural application of sludge does not take place.
Receiving surface water flow rate	18 000 m^3/day (corresponding to a dilution factor of 10). For marine water, the dilution factor is set equal to 100 (see R.16.3). In case of direct releases to agricultural soil the receiving water compartment is a ditch with a residence time of 40 d.	For site-specific assessments, the flow rate or the dilution factor can be changed according to the site-specific data.
Release factors or rates (before biological STP)	ERCs correspond to default release factors (see R.16.2.3) which are listed in Appendix A.16-1. They are based on the assumption that no environmental risk management is in place.	The default release factor can be refined by taking into account i) release preventing techniques or ii) onsite RMM with set effectiveness. SPERCs, developed by industrial sector organisations, are meant to support such refinement. They are supposed to reflect releases based on OC/RMM typically existing at the DU sector level. Other possible sources to refine the release factors are: ▪ Emission Scenario Documents (ESDs) ▪ Permits from authorities, setting maximum releases to the environment ▪ Measured release rate at the site

DETERMINANTS OF RELEASE AND EXPOSURE FOR THE DEFAULT AND REFINED ASSESSMENT		
Determinant	**Default assessment**	**Refined assessment**
		The OC/RMM controlling the release should be described in the ES. See R.16.2.3.
Substance properties	Minimum substance properties information to run EUSES exposure assessment are: molecular weight, water solubility, vapour pressure, melting point, octanol-water partition coefficient, information on ready biodegradability, Koc and, if relevant, BCF. Registrants will have to decide when to rely on the QSARs included into EUSES and when more specific information needs to be generated. Nevertheless, reliable measured data should be used in preference to QSAR outputs, unless the weight of evidence indicates that the QSAR value is sufficiently representative (e.g. due to uncertainty in the measured value(s)).	Table R.16-24 in Appendix A.16-4 defines the substance properties that can be used for refining environmental assessment.
Characterisation of environmental compartments	Default assumption included in the Tier I models are reported in Appendix A.16-2.1 (Table R.16-8 for the local scale) and in Appendix A.16-3 (Table R.16-21 for the regional scale).	More specific information on environmental compartments close to the location of release sources can be provided by the user.

Based on the determinants above, EUSES (or complementary models) calculate the predicted environmental concentration (PEC) for various compartments.

In some circumstances, measured environmental concentrations can be used to establish PECs: If such data are i) of a suitable quality, (ii) representative of the OC/RMM that were in place when measurements were performed, (iii) supported by sufficient contextual information, and (iv) assigned to the appropriate spatial scale, they can be used for the exposure estimate (see Appendix A.16-6).

Appendix A.16-1 : Environmental Release Categories

Table R.16-7: Default parameters to derive the environmental release rate

DEFAULT PARAMETERS TO DERIVE THE ENVIRONMENTAL RELEASE RATE					
Note	**No**	**ERC**	**Default worst-case release factors resulting from the conditions of use described in the ERCs.**		
			to air	**to water (before STP)**	**to soil**
1,7	1	Manufacture of the substance	5%	6%	0.01%
2,7	2	Formulation into a mixture	2.5%	2%	0.01%
2,7	3	Formulation into a solid matrix	30%	0.2%	0.1%
3, 7	4	Use of non-reactive processing aid at industrial site (no inclusion into or onto article)	100%	100%	5%
4,7	5	Use at industrial site leading to inclusion into/onto article	50%	50%	1%.
5,7	6A	Use of intermediate	5%	2%	0.1%
5,7	6B	Use of reactive processing aid at industrial site (no inclusion into or onto article)	0.10%	5%	0.025 %
5,7	6C	Use of monomer in polymerisation processes at industrial site (inclusion or not into/onto article)	5%	5%	0%
5,7	6D	Use of reactive process regulators in polymerisation processes at industrial site; (inclusion or not into/onto article)	35%	0.005%	0.025 %
6,7	7	Use of functional fluid at industrial site	5%	5%	5%
3,7	8A	Widespread use of non-reactive processing aid (no inclusion into or onto article, indoor)	100%	100%	n.a.
5,7	8B	Widespread use of reactive processing aid (no inclusion into or onto article indoor)	0.10%	2%	n.a.
4,7	8C	Widespread use leading to inclusion into/onto article (indoor)	15%	30% [46]	n.a.
3,7,8	8D	Widespread use of non-reactive processing aid (no inclusion into or onto article, outdoor)	100%	100%	20%
4,7	8E	Widespread use of reactive processing aid (no inclusion into or onto article outdoor)	0.10%	2%	1%
4,7	8F	Widespread use leading to inclusion into/onto article (outdoor)	15%	5%	0.5%
6,7	9A	Widespread use of functional fluid (indoor)	5%	5%	n.a.
6,7	9B	Widespread use of functional fluid (outdoor)	5%	5%	5%

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[46] The default release factor of 30% applies to activities/processes where the substance is dissolved/dispersed in a surplus of water and applied to an article via dipping/immersion or spreading (e.g. textile dyeing/finishing or application of polishes with floor cleaning water). For other widespread uses (e.g. use of paints and adhesives, including water based products) the release factor of 5% is applicable.

DEFAULT PARAMETERS TO DERIVE THE ENVIRONMENTAL RELEASE RATE					
Note	No	ERC	Default worst-case release factors resulting from the conditions of use described in the ERCs.		
			to air	to water (before STP)	to soil
8	10A	Widespread use of articles with low release (outdoor)	0.05%	3.2.%	3.2%
9,10	10B	Widespread use of articles with high or intended release (outdoor)	100%	100%	100%
8	11A	Widespread use of articles with low release (indoor)	0.05%	0.05%	n.a.
9,10	11B	Widespread use of articles with high or intended release (indoor)	100%	100%	n.a.
10	12A	Processing of articles at industrial with low release	2.5%	2.5%	2.5%
10	12B	Processing of articles at industrial processing with high release	20%	20%	20%
8	12C	Use of articles at industrial sites with low release	0.05%	0.05%	n.a.

Notes

General

Each environmental release category is linked to default parameters to estimate the release rates to the relevant environmental compartments. For each environmental release category, the release factors are based on the highest release factors available for representative use patterns. A use pattern represents the use of a chemical that has its specific function during a process within a certain type of industry or sector or has a specific function in a material or article. The highest release factors have been selected from general release information contained in the A-Tables in Appendix 1 of the Technical Guidance Document (TGD) on Risk Assessment PART II (EC, 2003) for representative cases. In the conservative design of the release factors, it is assumed that no risk management measures are included. The physico-chemical properties of a substance are not taken into account. The distribution between air, water and soil is therefore not based on the properties of the substance. The potential waste treatment route is also not considered. These characteristics lead to conservative values for release to all compartments. The background to, and the rationale for, the default parameters to derive environmental release rates are based on the exposure assessment principles detailed in section R.16.1.4. In this section, the different spatial scales of assessment are explained.

For industrial production, formulation and use (ERC 1-7), air and water releases are considered for exposure at both the local and the regional scale. Direct releases to soil are however only taken into account at the regional scale. This is due to the fact that industrial soil is not considered a protection target for direct releases in the framework of chemicals assessment. The same assumptions apply to industrial processing of articles (ERC 12).

For wide dispersive uses (i.e. a large number of users, including private use) and non-industrial article service life (a large number of product sources), it is assumed that a certain fraction of the estimated volume for that use is used in a standard town of 10 000 inhabitants.

At the local scale, the corresponding releases in such a standard town go to surface water, via a municipal sewage treatment plant (STP), resulting in a point source release. The direct releases to air and to soil are considered for exposure at the regional scale.

Note that the default release factors are not applicable to agricultural uses. For these uses SpERCs developed by Fertilizers Europe[47] and CropLife Europe[48] associations can be used. They might include release factors due to direct releases to soil, water (via drift) and air (e.g. vaporisation during spray application).

Annotations per environmental release category

1) Manufacture of chemicals

The release factors are based on the information for the manufacture of basic chemicals and chemicals used in synthesis (including monomers and catalysts). Besides basic (organic) chemicals both the production of chemicals in the petrochemical industry and the metal extraction and refining industry are included. Release factors are derived from the general release factors for the production of chemicals provided in EC (2003).

2) Formulation

For the life-cycle stage formulation, a distinction is made between mixing and blending of substances (processing aids) in mixtures like liquids, pastes or (compressed) gases for instance in aerosol cans, and on the other hand processes of mixing, which result in inclusion on a matrix, for instance, in the plastics industry. To meet the requirements of specific applications for plastics materials, the polymers are blended or mixed with various types of additives, including fillers, pigments, plasticisers etc.

In the polymers industry, this process of compounding takes place before conversion of the plastic material into finished articles. Often the processes of compounding and conversion are performed as successive process steps at the same facility. The production of master batches, which are made up to contain high concentrations of specific additives, is also considered as a process of mixing and blending resulting in inclusion into or onto a matrix. The production of photographic films is also considered as formulation into a matrix. Release factors are derived from the general release factors for formulation from EC (2003). The highest release factors for formulation resulting in inclusion into or onto a matrix have been selected for mixing of plastic additives, pigments, fillers and plasticisers with the polymer matrix (compounding) and the production of photographic films (EC 2003).

3) Processing aids

Processing aids are substances that facilitate a process and will usually not be consumed (reacted) or included into or onto the matrix of an article. It should be stressed though that processing aids might be converted by high temperature processes like metal cutting and combustion of fuels (fuel additives). Processing aids are, for instance, detergents in fabric washing products, which facilitate the washing process and will be directly released to waste streams after use. Solvents in cleaners, paints or adhesives are another example of processing aids which are released with waste air, wastewater or as waste from the application process.

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[47] https://www.reachfertilizers.com/#spercs

[48] https://croplifeeurope.eu/

Without release abatement or waste treatment, 100% of this type of processing aid applied will be emitted via air or water.

Release factors for industrial use of processing aids have been derived from the release factor tables for industrial use of processing aids (processing). For each compartment, the highest release factors for this specific use pattern are taken from EC (2003).

In addition to industrial use, release factors have been derived for use by the public at large (households). Release factors for widespread use of processing aids have been derived from EC (2003) for the sector personal or domestic use. For air, the release factor is set at 100%, for instance, to represent the use of propellants in aerosol cans. For water, the release factor is also set a 100% for instance for the use of cleaning and washing agents and surface-active agents in all kinds of cleaning products. The release of these types of chemicals is assumed to be complete to either air or water.

4) Substances processed into or onto an article matrix

Besides the specific use of chemicals as processing aids, chemicals are also processed with the specific goal of being included into or onto a matrix. For example, pigments or fillers in paints will be included in the paint layer (matrix) after the painting process, fabric softeners will be included in the textile matrix during washing, and dyes will be included into the fibre matrix during the dyeing process. The highest release factors for air and water for this specific type of use have been taken from EC (2003), which is related, for instance, to dyeing of textiles/leather or spray coating with wet scrubber.

For releases to water from widespread indoor uses a differentiation is made between i) water-based applications (i.e. where the substance is dissolved/dispersed in a surplus of water and applied to an article via dipping/immersion or spreading) and ii) non such water-based applications (e.g. use of adhesives or paints, including water based products). The release factor for water-based applications is the default, but it can be replaced by a lower release factor for other types of applications. The release factors refer to i) the "private use" of dye-stuff and ii) to the use of viscosity adjustors/plasticisers in paints (see Table A4.1 and A4.5 in TGD Part II, EC 2013).

Please note: If a processing aid remains in the matrix without function after processing, it should be assessed under ERC 5 (ERC 8C) rather than ERC 4. An example for such a case is a heat stabiliser remaining in the polymer matrix although increased temperature was only relevant at the formulation or conversion stage.

5) Substances reacting on use

Substances reacting on use have been categorised into intermediates, reactive processing aids and monomers used in the polymers industry.

Reactive processing aids have so far not been covered in the default release factors in the Technical Guidance Document (EC 2003). Several assumptions have been made to provide release rates for air and water. Generally, these types of substances are highly soluble in water and therefore release to air has been considered to be negligible and a release factor of 0.1% has been assumed. A default half-life of 10 minutes has been assumed. For industrial use, a residence time of four hours in a recirculation system has been assumed. For wide dispersive use, a residence time of one hour has been assumed in the sewer (once-through system). Furthermore, a distinction has been made between monomers in a polymerisation processes for the production of thermoplastics and thermosetting resins, and auxiliaries for polymer processing of rubbers and thermosetting resins (pre-polymers). The release factors for intermediates have been taken from available release factors for the chemical industry and the specific use of intermediates in the synthesis of other chemicals. Release factors for the use of monomers in the polymer industry have also been taken from EC (2003) for this specific type of use (polymerisation processes). Releases to air and water from the processing of rubbers and thermosetting resins are provided by EC (2003) (polymer processing) for the following types of chemicals, curing agents and cross-linking agents.

6) Release from closed systems

The release factors have been based on leakage of cooling liquids from refrigerators and leakage of engine oil from cars. A leakage rate of 5% per year to air is assumed based on Matthijsen and Kroeze (1996) and Folkert and Peek (2001). The leakage rates do not include losses from recharging or filling of machinery (about 0.2% to air and 0.1% to water) but in general this is negligible compared to the annual leakage rate.

Release to soil and water is based on leakage rates for engine oil as this is thought to be a representative case for this type of use. Based on an average leakage rate, annual number of kilometres travelled per vehicle and the amount of engine oil per vehicle the release factor can be calculated as follows: a leakage rate of 10 mg/km and a mileage of 20 000 km per year and four litres of engine oil per vehicle results in a release factor of about 5% per year; the figures have been taken from Klein et al. (2004) and are in line with the figures provided by OECD (2004a). For hydraulic fluids, leakage rates are very similar. They vary from 1% up to about 15% per year (two applications) for soil. For water, leakage rate values are somewhat lower at about 0.5% up to 7% (OECD, 2004a). Releases to water have also been taken into account for indoor use because of the possible spills to (waste) water and the potential release of substances used in central heating systems where the heat transfer fluid is water.

7) Indoor and outdoor use

Industrial

Industrial activities are primarily considered to be indoor processes. The relevant life-cycle stages are production, formulation and industrial use (ERC 1-7). However this is not strictly the case for large industrial installations (e.g. refineries) that are usually not inside a covered building.

Release to industrial soil assumed in the ERCs may result from spilling during transfer or delivery procedures or leakage from equipment like pumps, pipes (above and below ground), reactors and storage tanks (above and below ground). They may also result from the transport of waste streams like wastewater due to leakage of the drain pipe (cracks, loose connections etc.) or the outside (open) storage of raw materials on the site. Releases might also result from the industrial application of certain products like hydraulic fluids and lubricants, for instance, in industrial transport or material handling equipment such as conveyer belts.

In many EU countries, the releases to soil will be lower due to special provisions which are compulsory to prevent them. Some typical spill prevention systems are liquid proof floors, concrete containment pits, curbs, dykes or bunds, containment buckets etc.

Widespread uses

For outdoor use of processing aids (ERC 8D), the release factor for soil refers to private use (consumers) of solvents. Release factors for the soil compartment for outdoor use of reactive processing aids (ERC 8E) refer to, for example, the use of a bleaching aid in cleaning products by the public at large. For outdoor use of substances, which results in inclusion into or onto a matrix (ERC 8F), the release factors have been taken for the private use of paints and specifically refers to substances like plasticisers and viscosity adjustor.

8) Release from articles/materials during service life, low release

Release factors are taken from the OECD emission scenario document on plastic additives (OECD, 2004b). If relevant, the registrant should assess whether the default assumptions also apply to other materials. The release factors presented in the ERC table take into account the service lifetime of the article; they are based on the assumption that a steady state has been reached in the market between the amounts of an article produced, the amount in use (stock) and the amount becoming waste per year. Under such an assumption, the annual release is not driven by the actual use of a substance for production of an article but by the stock of article in use. Thus, the annual release is derived from the release factor multiplied by the service life of the article. Note that for new substances recently placed on the market, there is no steady-state situation yet.

For outdoor use, the release factor to water and soil is based on a worst-case release of 0.16% multiplied by the service lifetime period of the article ($T_{service\ life}$). In Tier 1, $T_{service\ life}$ is set at 20 years, resulting in a release factor of 3.2%.

For indoor use, the release factors (0.05%) are also taken from the OECD emission scenario document on plastic additives (OECD, 2004b). This factor is also applied for articles that are used or processed at industrial sites under conditions where releases are expected to be low or very low.

9) Release from articles during service life, high release

Release factors to air and water for indoor use are taken from the emission scenario document for the textile processing industry, industrial category (IC) 13. For indoor wide dispersive use, the soil compartment is not considered to be relevant, and the same release factors are used for air and water.

For outdoor use, the release factors are set to 100% per year for all compartments (steady-state situation and total release of substance over service life). The reasoning behind this assumption is that complete release over the service life for outdoor applications may occur either to air, water or soil.

10) Release from processing of articles with abrasive techniques

The processes to be addressed here are high and low energy manipulation or hot work operations with articles, resulting in releases of substances contained in these articles. The release from the articles may occur in the form of a substance as such or as particles (larger particles, dust, aerosols) where the substance is still embedded in a more or less intact solid matrix. The processes potentially relevant may include treatment of article surfaces (polishing, sanding), sawing and cutting of semi-finished articles (mechanical cutting, flame cutting) or welding and soldering. This often corresponds to PROC 21, 24 and 25.

Typical examples would be cutting of textile in the fabric industry, metal cutting, or sanding and planing of polyurethane-foam blocks in the production of surfboards. Chemical/mechanical paint stripping and other surface treatments of e.g. buildings or vehicles are also processes to be covered under ERCs 10B, 11B or 12.

Particles from abrasive techniques can be quite large (fibres, wood shaving, chips, iron curls etc.), and thus unlikely to become airborne or potentially give rise to intensified leaching of substances due to the increase of surface. If dusts and aerosols are formed indoor, they are expected to be removed by local ventilation (efficiency not included in the release factors) or to precipitate on the ground/floor, and become waste (floor cleaning), or go to wastewater if cleaned with water. This is comparable to the considerations on handling powders in paint manufacture and plastics compounding and conversion. Two different situations can be discerned, related to the type of abrasive process. When cutting or coarse grinding of textile, polymers or metals is involved, larger particles are formed as a relatively small fraction of the original material. In the low release situation (ERC 12A), the release factors of 2.5% are based on the OECD ESD for plastic additives (OECD 2004), based on grinding/machining. The release might either be to air, water or soil or a combination of these.

When surfaces are treated with high energy abrasive techniques such as sanding or shot blasting, ERC 12b is applicable. The worst-case release is based on dust releases due to shot blasting without any RMM, where a high release factor of 20% is estimated (Verstappen 1993). The release might either be to air, water or soil or a combination of these.

If surfaces are treated with abrasive techniques under outdoor, non-industrial conditions (e.g. sanding of bridges, high pressure cleaning of walls, paint stripping of ships) substances contained in the removed surface may be completely released into the environment if no RMMs are applied (OECD 2006). Thus, such conditions can be covered under ERC 10B.

If surfaces are treated with abrasive techniques under indoor, non-industrial conditions (e.g. paint stripping of walls, doors, floors), substances contained in the removed surface or surface coatings could be released totally when no RMMs are in place (OECD, 2006). These activities are taken into account under ERC 11B when they are in a non-industrial setting with many release sources constituting wide dispersive release.

Appendix A.16-2 Model calculations

This appendix is an integration of the main body of the Guidance. The latter describes the process to estimate the environmental exposure to substances by outlining the different steps and main elements currently implemented in EUSES as implemented in Chesar Platform. This appendix provides more technical details and explains the calculations behind the assessment method. It is addressed mainly to experienced users and those who need to explore refinement options.

A.16-2.1 Characterisation of environmental compartments

In this section, the following parameters are derived:

- definition of the standard environmental characteristics; and
- bulk densities for soil, sediment, and suspended matter.

For the derivation of PECs at the local and regional scales, one 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 R.16-8, average or typical default values are given for the parameters characterising the environmental compartments (the values are chosen equal on all spatial scales). The standard assessment needs to be performed with the defaults, as given in Table R.16-8. When more specific information is available on the location of the release sources, this information can be applied in refinement of the PEC by deviating from the parameters of Table R.16-8 and justification should be provided.

Several other generic environmental characteristics, mainly relevant for the derivation of PECregional (e.g. the sizes of the environmental compartments, mass transfer coefficients) are given in Appendix A.16-3.3 (Table R.16-21).

Table R.16-8: Characterisation of environmental compartments

CHARACTERISATION OF ENVIRONMENTAL COMPARTMENTS			
Parameter	**Symbol**	**Unit**	**Value**
General			
Density of the solid phase	RHOsolid	$[kg_{solid} \cdot m_{solid}^{-3}]$	2 500
Density of the water phase	RHOwater	$[kg_{water} \cdot m_{water}^{-3}]$	1 000
Density of air	RHOair	$[kg_{air} \cdot m_{air}^{-3}]$	1.3
Environmental temperature (12°C)	TEMP	[K]	285.15
Surface water			
Concentration of suspended matter (dry weight)	$SUSP_{water}$	$[mg_{solid} \cdot l_{water}^{-1}]$	15
Suspended matter			
Volume fraction solids in susp. matter	$Fsolid_{susp}$	$[m_{solid}^{3} \cdot m_{susp}^{-3}]$	0.1
Volume fraction water in susp. matter	$Fwater_{susp}$	$[m_{water}^{3} \cdot m_{susp}^{-3}]$	0.9
Weight fraction organic carbon in susp. solids	Foc_{susp}	$[kg_{oc} \cdot kg_{solid}^{-1}]$	0.1
Sediment			
Volume fraction solids in sediment	$Fsolid_{sed}$	$[m_{solid}^{3} \cdot m_{sed}^{-3}]$	0.2
Volume fraction water in sediment	$Fwater_{sed}$	$[m_{water}^{3} \cdot m_{sed}^{-3}]$	0.8
Weight fraction organic carbon sediment solids	Foc_{sed}	$[kg_{oc} \cdot kg_{solid}^{-1}]$	0.05
Soil			
Volume fraction solids in soil	$Fsolid_{soil}$	$[m_{solid}^{3} \cdot m_{soil}^{-3}]$	0.6
Volume fraction water in soil	$Fwater_{soil}$	$[m_{water}^{3} \cdot m_{soil}^{-3}]$	0.2
Volume fraction air in soil	$Fair_{soil}$	$[m_{air}^{3} \cdot m_{soil}^{-3}]$	0.2
Weight fraction organic carbon in soil solids	Foc_{soil}	$[kg_{oc} \cdot kg_{solid}^{-1}]$	0.02
Weight fraction organic matter in soil solids	Fom_{soil}	$[kg_{om} \cdot kg_{solid}^{-1}]$	0.034

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:

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

Equation R.16-1

Explanation of symbols

Fx_{comp}	fraction of phase x in compartment comp	$[m^3 \cdot m^{-3}]$	Table R.16-8
$RHOx$	density of phase *x*	$[kg \cdot m^{-3}]$	Table R.16-8
RHO_{comp}	wet bulk density of compartment comp	$[kg \cdot m^{-3}]$	

Application of the formulas above for the values mentioned leads to the following bulk densities of each standard environmental compartment:

Total bulk density of the environmental compartments

RHO_{susp}	Bulk density of (wet) suspended matter	$[kg \cdot m^{-3}]$	1,150
RHO_{sed}	Bulk density of (wet) sediment	$[kg \cdot m^{-3}]$	1,300
RHO_{soil}	Bulk density of (wet) soil	$[kg \cdot m^{-3}]$	1,700

Conversion of concentration from wet weight todry weightsoil or sediments

In this guidance the concentrations in soil and sediment are expressed on a wet-weight basis. As the PNECsed and PNECsoil are expressed in dry weight, also the respective concentrations need to be expressed in dry weight.

The conversion factors CONVsoil, and CONVsusp, for soil and suspended matter respectively, are derived with the following formula:

$$CONV_{comp} = \frac{RHO_{comp}}{Fsolid_{comp} \cdot RHO_{solid}} \quad with\ comp \in \{soil, susp\}$$

Equation R.16- 2

Explanation of symbols

$CONV_{comp}$	Conversion factor for concentrations in compartment comp: wet weight to dry weight	$[kg \cdot kg^{-1}]$	
RHO_{comp}	wet bulk density of compartment comp	$[kg \cdot m^{-3}]$	Equation R.16-1
RHO_{solid}	density of the solid phase	$[kg \cdot m^{-3}]$	Table R.16-8
$Fsolid_{comp}$	fraction of solid phase in compartment comp	$[m^3 \cdot m^{-3}]$	Table R.16-8

A.16-2.2 Fate and distribution in the environment

The main principles and elements related to substance’s fate and distribution in the environment, which play an important role in the exposure assessment, are presented in section R.16.4.2. In this appendix, more details are provided on the calculation of the main parameters.

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.).

A.16-2.2.1 Partition coefficients

In this section, the following processes are described:

A. fraction of substance in air associated with aerosol;

B. partitioning between air and water;

C. partitioning between solids and water in soil, sediment and suspended matter.

D. partitioning between water/solids and biota (bioconcentration and biomagnification)

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 R.16.4.2.1 of the main body 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 will also 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, air distribution may also 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.

A) Adsorption to aerosol particles (gas-aerosol partitioning)

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.

$$Fass_{aer} = \frac{CONjunge \bullet SURF_{aer}}{VPL + CONjunge \bullet SURF_{aer}}$$

Equation R.16-3

Explanation of symbols

CONjunge	constant of Junge equation	[Pa·m]	*
$SURF_{aer}$	surface area of aerosol particles	[$m^2 \cdot m^{-3}$]	*
VPL	sub-cooled liquid vapour pressure	[Pa]	
$Fass_{aer}$	fraction of the substance associated with aerosol particles	[-]	

* as a default, the product of CONjunge and SURFaer 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):

$$VPL = \frac{VP}{e^{6.79 \bullet (1-\frac{TEMP_{melt}}{TEMP})}}$$

Equation R.16-4

Explanation of symbols

TEMP	environmental standard temperature	[K]	285.15
$TEMP_{melt}$	melting point of substance	[K]	data set
VPL	sub-cooled liquid vapour pressure	[Pa]	
VP	vapour pressure	[Pa]	data set

B) Volatilisation (air-water partitioning)

The transfer of a substance from the aqueous phase to the gas phase (e.g. stripping in the aeration tank of an 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 $K_{air\text{-}water}$ (also known as the "dimensionless" Henry's Law constant) can be estimated from the ratio of the vapour pressure to the water solubility (Equation R.16-5 and Equation R.16-6). For water miscible compounds, direct measurement of the Henry's Law constant is recommended. For detailed information, see Appendix A.7.1-1 to *Chapter R.7a of the Guidance on IR&CSA.*

$$HENRY = \frac{VP \bullet MOLW}{SOL}$$

Equation R.16-5

$$K_{air\text{-}water} = \frac{HENRY}{R \bullet TEMP}$$

Equation R.16-6

Explanation of symbols

VP	vapour pressure	[Pa]	data set
MOLW	molecular weight	[$g \cdot mol^{-1}$]	data set
SOL	solubility	[$mg \cdot l^{-1}$]	data set
R	gas constant	[$Pa \cdot m^3 \cdot mol^{-1} \cdot k^{-1}$]	8.314
TEMP	temperature at the air-water interface	[K]	285.15
HENRY	Henry's law constant	[$Pa \cdot m^3 \cdot mol^{-1}$]	
$K_{air\text{-}water}$	air-water partitioning coefficient	[-]	

If no reliable data for vapour pressure and/or solubility can be obtained, QSPRs models (quantitative structure-property relationship models) are available, see chapters R.7.1.5. and R.7.1.7 *of Chapter R7.a of the Guidance on IR&CSA*.

C) Adsorption/desorption (solids-water partitioning)

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 soil, sediment, suspended matter and sludge can be obtained from experimental data or estimated.

More explanation and information on the requirements for this property is given in section R.7.1.15. of *Chapter R7.a of the Guidance on IR&CSA.*

For water soluble, highly adsorptive substances, the use of K_{ow} as input into the SimpleTreat model (see section A.16-2.3.1 of this appendix) 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 ionisable substances, specifically bases, the measured / predicted Koc for sediment/soil should not be used as the Koc for sewage sludge, as the different medium (sewage sludge vs. sediment/soil) can make a significant difference in the Koc value. For this reason, specific QSARs to determine the Koc in sewage sludge for ionisable substances have been included in SimpleTreat 4[49].

The solid-water partition coefficient (K_p) in each compartment (soil, freshwater sediment, marine water sediment, freshwater suspended matter, marine water suspended matter) can be calculated from the Koc 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 R.16-8.

$$Kp_{comp} = Foc_{comp} \bullet Koc \qquad with\ comp \in \{soil\ ,\ sed\ ,\ susp\}$$ **Equation R.16-7**

Explanation of symbols

Koc	partition coefficient organic carbon-water	$[l \cdot kg^{-1}]$	
Foc_{comp}	weight fraction of organic carbon in compartment *comp*	$[kg \cdot kg^{-1}]$	Table R.16-8
$Kp_{susp,freshwater}$	partition coefficient solid-freshwater in suspended matter	$[kg \cdot kg^{-1}]$	
$Kp_{susp,seawater}$	partition coefficient solid-seawater in suspended matter	$[kg \cdot kg^{-1}]$	
$Kp_{sed,freshwater}$	partition coefficient solid-freshwater in sediment	$[kg \cdot kg^{-1}]$	
$Kp_{sed,seawater}$	partition coefficient solid-seawater in sediment	$[kg \cdot kg^{-1}]$	
Kp_{soil}	partition coefficient solid-water in soil	$[l \cdot kg^{-1}]$	

If no specific information on Kp in marine water is available, $Kp_{susp,seawater}$ and $Kp_{sed,seawater}$ can be set equal to $Kp_{susp,freshwater}$ and $Kp_{sed,freshwater}$, respectively.

K_p is expressed as the concentration of the substance sorbed to solids (in $mg_{chem} \cdot kg_{solid}^{-1}$) divided by the concentration dissolved in porewater ($mg_{chem} \cdot l_{water}^{-1}$). The dimensionless form of

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[49] The available QSARs in SimpleTreat 4 estimate log Koc in sewage sludge for ionisable substances on the basis of Log Dow. The Dow considers the solubility of the charged and neutral species in pure water and octanol at a specific pH and octanol is used as the surrogate for the soil matrix and all molecular interactions. Furthermore, for ionisable substances, octanol:water is not a good surrogate for the soil matrix, as octanol does not contain charged groups. As neither the pH dependence nor the ionic interactions between the solute and the soil matrix are accounted for in this approach the use of DOW approach may be followed with caution (Sigmund et al., 2022).

Kp, or the total compartment-water partitioning coefficient in $(mg \cdot m_{comp}^{-3})/(mg \cdot m_{water}^{-3})$, can be derived from the definition of the soil in three phases:

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

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

Equation R.16-8

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

Explanation of symbols

$Fwater_{comp}$	fraction water in compartment *comp*	$[m^3 \cdot m^{-3}]$	Table R.16-8
$Fsolid_{comp}$	fraction solids in compartment *comp*	$[m^3 \cdot m^{-3}]$	Table R.16-8
$Fair_{comp}$	fraction air in compartment comp (only relevant for soil)	$[m^3 \cdot m^{-3}]$	Table R.16-8
RHOsolid	density of the solid phase	$[kg \cdot m^{-3}]$	2,500
Kp_{comp}	solids-water part. coeff. in compartment *comp*	$[l \cdot kg^{-1}]$	Equation R.16-7
$K_{air\text{-}water}$	air-water partitioning coefficient	[-]	Equation R.16-6
$K_{soil\text{-}water}$	soil-water partitioning coefficient	$[m^3 \cdot m^{-3}]$	
$K_{susp,freshwater}$	suspended matter-freshwater partitioning coefficient	$[m^3 \cdot m^{-3}]$	
$K_{susp,seawater}$	suspended matter-seawater partitioning coefficient	$[m^3 \cdot m^{-3}]$	
$K_{sed,freshwater}$	sediment-freshwater partitioning coefficient	$[m^3 \cdot m^{-3}]$	
$K_{sed,seawater}$	sediment-seawater partitioning coefficient	$[m^3 \cdot m^{-3}]$	

D) Bioconcentration and biomagnification (biota-water/solids partitioning)

Bioconcentration and bioaccumulation may be of concern for lipophilic organic substances and some metal compounds as both direct and indirect toxic effects may be observed upon long-term exposure. Secondary poisoning is concerned with toxic effects in organisms in higher trophic levels of the food web, either living in the aquatic or terrestrial environment, which result from ingestion of organisms from lower trophic levels that contain accumulated substances. The subject of aquatic bioaccumulation and the corresponding information requirements is discussed in section R.7.10.1 of *Chapter R.7c of the Guidance on IR&CSA*.

Bioaccumulation in aquatic species is described by the bioconcentration factor (BCF). The static bioconcentration factor is the ratio between the concentration in the organism and the concentration in water in a steady-state (sometimes also called equilibrium) situation. When uptake and depuration kinetics are measured, the dynamic bioconcentration factor can be calculated from the quotient of the uptake and depuration rate constants:

Equation R.16-9

$$BCF_{org} = \frac{C_{org}}{C_{water}} \text{ or } \frac{k_1}{k_2}$$

Explanation of symbols

C_{org}	concentration in aquatic organism	$[mg \cdot kg^{-1}]$
C_{water}	concentration in water	$[mg \cdot l^{-1}]$
k_1	uptake rate constant from water	$[l \cdot kg^{-1} \cdot d^{-1}]$
k_2	Elimination rate constant	$[d^{-1}]$
BCF_{org}	bioconcentration factor	$[l \cdot kg^{-1}]$

The testing strategy for aquatic bioaccumulation is described in section R.7.10.6 of *Chapter R7c of the Guidance on IR&CSA*.

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 indirect uptake via the food may also contribute significantly to the bioaccumulation. Bioaccumulation of metallic species is not considered explicitly in this section.

Experimentally derived bioconcentration factors

REACH Annex IX indicates that information on bioaccumulation in aquatic – preferably fish – species is required for substances manufactured or imported in quantities of 100 t/y or more. For these substances, an experimentally derived BCF will be present (unless mitigating factors apply, see section R.7.10.3.1 of *Chapter R7.c of the Guidance on IR&CSA* on testing data for aquatic bioaccumulation).

Calculation of BCF fish

If measured BCF values are not available, the BCF for fish or other organisms can be predicted from the relationship between K_{ow} and BCF (QSARs), see section R.7.10.3.2 *of Chapter R.7c of the Guidance on IR&CSA* on non-testing data for aquatic bioaccumulation.

Calculation of BCF earthworm

When measured data on bioconcentration in worms is available, the measured BCF earthworm can be used. If data are not available, the BCF can be estimated with a QSAR. For more information on terrestrial bioaccumulation and biomagnification, see *Chapter R.7c of the Guidance on IR&CSA*[50].

Biomagnification factor

In a relatively simple food chain with one or two trophic levels, the concentration in the fish (i.e. the food for the fish-eater) should ideally 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, a simple correction factor for potential biomagnification on top of the bioconcentration through the water phase can be applied for very hydrophobic substances. For

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[50] https://echa.europa.eu/guidance-documents/guidance-on-information-requirements-and-chemical-safety-assessment

a more in-depth discussion on biomagnification, see section R.7.10 of *Chapter R.7c of the Guidance on IR&CSA*.

The biomagnification factor (BMF) should ideally be based on measured data. However, the availability of such data is usually very limited and therefore, the default values given in Table R.16-9 can be used (see also section R.7.10.4.5 of *Chapter R.7c of the Guidance on IR&CSA*). For further explanation, see section R.16.4.3.8 on secondary poisoning. When measured BCF values are available, these should form the basis for deciding on the size of the BMF_1.

Food chains of the marine environment can be very long and complex and may consist of five or more trophic levels. Since very hydrophobic substances may biomagnify in the tissue and organs of the predator, an additional biomagnification factor (BMF_2) must be applied for calculating the internal concentration of the predator. Default values for BMF_2 are given in Table R.16-9 as well.

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. If further data are also 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.

Table R.16-9: Default BMF values for organic substances with different log Kow or BCF in fish

DEFAULT BMF VALUES FOR ORGANIC SUBSTANCES WITH DIFFERENT LOG K_{OW} OR BCF IN FISH			
log Kow	**BCF (fish)**	**BMF_1**	**BMF_2**
< 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 substances 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 Kow, 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 should be provided.

A.16-2.2.2 Degradation rates in the environment

In this section of the appendix, the following processes, which are mentioned in section R.16.4.2.2, are described in more detail:

- 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 processes include 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.

Detailed guidance on the collection, selection and evaluation of data to assess the degradability of substances is provided in *Chapter R.7b of the Guidance on IR&CSA*.

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. Nevertheless, if stable degradation products are formed, the risk assessment should include these. It is possible that the rate of reaction is such that only the 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.

A) Hydrolysis

Values for the hydrolytic half-life (DT50) of a hydrolysable substance can be converted to degradation rate constants, which may be used in the models for calculating PEC_{local} and especially $PEC_{regional}$. The results of a ready biodegradability study will show whether or not the hydrolysis products are themselves biodegradable. Similarly, for substances where hydrolytic DT50 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. See *Chapter R.6* and section R.7.9 in *Chapter R.7b of the Guidance on IR&CSA* and R.7.1.7 in *Chapter R.7a of the Guidance on IR&CSA* for more details on hydrolysis.

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 freshwater, sediment and soil, a pH of 7 and a temperature of 12°C (285.15 K) will normally be established which conforms to the standard environmental parameters of Table R.16-8. 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 applying the Arrhenius equation:

$$DT50X = DT50test \cdot e^{\left(\left(\frac{Ea}{R}\right)\cdot\left(\frac{1}{TX}-\frac{1}{Ttest}\right)\right)}$$

Equation R.16-10

Explanation of symbols

DT50X	half-life for hydrolysis or biodegradation at absolute temperature X	[d]	
DT50test	half-life for hydrolysis or biodegradation at test absolute temperature	[d]	data set
Ea	enthalpy of activation	[J.mol^{-1}]	default: 65400 for (bio)degradation (when Ttest is in the range of 273.15-303.15 K)
R	gas constant	[Pa·m^3·mol^{-1}.K^{-1}]	8.314
TX	standard environmental / STP absolute temperature	[K]	285.15 / 288.15
Ttest	test absolute temperature	[K]	data set

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 R.16-11

Explanation of symbols

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

B) 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 ($^{1}O2$, 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). For more details on this property, see section R.7.9.4 *Chapter R.7b of the Guidance on IR&CSA*.

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. Computer programs have been developed for facilitating the complex calculation of phototransformation processes in natural waters (See chapter R.7.9). 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 R.16-12

Explanation of symbols

$DT50photo_{water}$	half-life for photolysis in surface water	[d]	data set
$kphoto_{water}$	first order rate constant for photolysis in surface water	[d^{-1}]	

C) Photochemical reactions in the atmosphere

Although direct photolysis may be an important breakdown process for some substances, 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 $cm^3.molecule^{-1}.s^{-1}$) can either be determined experimentally or estimated, see chapters R.7.9.3 and R.7.9.4.

By relating k_{OH} to the average OH-radical concentration in the atmosphere, the pseudo-first order rate constant in air is determined:

$$kdeg_{air} = k_{OH} \bullet OHCONC_{AIR} \bullet 24 \bullet 3600$$ **Equation R.16-13**

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	$[d^{-1}]$	

*The global annual average OH-radical concentration can be assumed to be $5 \cdot 10^5$ $molecules.cm^{-3}$ (BUA, 1992).

Degradation in the atmosphere is an important process and it is essential to consider whether it can affect the outcome, particularly for high tonnage substances when the regional concentration may be significant. 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 substance 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.

D) 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. For further guidance on use of sewage treatment plant (STP) simulation test results, see section A.16-2.3.1 of this appendix and R.7.8.17. Temperature influences the activity of microorganisms and thus the biodegradation rate in the STP. When biodegradation rates or half-lives have been determined in simulation tests, the degradation rates obtained should be recalculated to reflect an average STP temperature (i.e. 15°C, 288.15 K) by Equation R.16-10.

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, 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. As 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 an STP, the rate constants of Table R.16-10 and Table R.16-11 were derived from the biodegradation screening tests. All constants in Table R.16-10 and Table R.16-11 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 before the application of the rate constant;

- 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.

Table R.16-10: Elimination in sewage treatment plants: Extrapolation from test results from OECD 301 series, 310 and 302 series to rate constants in STP model (SimpleTreat)

ELIMINATION IN SEWAGE TREATMENT PLANTS: EXTRAPOLATION FROM TEST RESULTS TO RATE CONSTANTS IN STP MODEL (SIMPLETREAT)	
Test result	**Rate constant k·(h^{-1})**
Readily biodegradable	1
Readily, but failing 10-d window	0.3
Inherently biodegradable, fulfilling specific criteria	0.1
Inherently biodegradable, not fulfilling specific criteria	0
Not biodegradable	0

Table R.16-11: Elimination in sewage treatment plants: Extrapolation from percentage removal due to biodegradation from OECD 303 A tests to rate constants in STP model (SimpleTreat)

ELIMINATION IN SEWAGE TREATMENT PLANTS: EXTRAPOLATION FROM TEST RESULTS TO RATE CONSTANTS IN STP MODEL (SIMPLETREAT)	
Test result (% removal in OECD 303 A)	**Rate constant k·(h^{-1})**
95 – 100	3
90 - 95	1
50	0.1
25	0.03

In addition the first order degradation rate constant can be generated directly from OECD 314 B simulation test.

E) Biodegradation in surface water, sediment and soil

The rate of biodegradation in surface water, soil and sediment is related to the structure of substances, adequate concentration to induce microbial enzyme systems, 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.

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

Normally, specific information on biodegradability in sediment or soil is not available. Hence, rate constants for these compartments have to be estimated from the results of standardised tests. For an in-depth discussion of biodegradation testing strategies, see section R.7.9 *Chapter R.7b of the Guidance on IR&CSA*.

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 R.16-10. 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.

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 R.16-12 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 R.16-12) and 300 – 30 000 days in soil and sediment (Table R.16-13) will only affect 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 Table R.16-12 and Table R.16-13.

Table R.16-12: 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	∞[51]

Notes to Table R.16-12:

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.

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[51] Depending on the tool used, various high numbers may be used. EUSES upper boundary for a half-life is 10E+40.

c) Only those inherently degradable substances that fulfil the criteria described in note b) to Table R.16-12 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 R.16-12) should therefore be regarded as a "the realistic worst-case concept".

An OECD guidance document for classification of substances hazardous for the aquatic environment (OECD, 2001) contains a chapter on interpretation of degradation data. Even though the OECD 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 and a solid phase, and soil containing air, porewater and 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.

When no data from tests simulating the conditions in soil or sediment are available, the use of screening test data may be considered (see chapter R.7.9). The guidance for use of such data is based on the general recognition that for substances with low Kp values at present not enough empirical data are available to assume some sort of dependence of the soil biodegradation half-life on the solids/water partition coefficient. Nevertheless, for substances with high Kp-values there is evidence that some sort of Kp dependence exists. Therefore, degradation half-life classes for (bulk) soil, partly based on Kp are presented in Table R.16-13. 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-lives indicated in the table are considered to be conservative.

Table R.16-13: Half-lives (days) for (bulk) soil based on results from standardised biodegradation test results

Kp_{soil} [$l \cdot kg^{-1}$]	Readily biodegradable	Readily biodegradable, failing 10-d window	Inherently biodegradable
≤ 100	30	90	300
>100, ≤ 1 000	300	900	3 000
>1 000, ≤ 10 000	3 000	9 000	30 000
etc.	etc.	etc.	etc.

The following equation can be used to convert DT50 to a rate constant for biodegradation in soil:

$$kbio_{soil} = \frac{\ln 2}{DT50\, bio_{soil}}$$ **Equation R.16-14**

Explanation of symbols

$DT50bio_{soil}$	half-life for biodegradation in bulk soil	[d]	Table R.16-13
$kbio_{soil}$	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 10 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 R.16-15**

Explanation of symbols

$DT50bio_{soil}$	half-life for biodegradation in bulk soil	[d]	Table R.16-13
$Faer_{sed}$	fraction of the sediment compartment that is aerobic	[$m^3 \cdot m^{-3}$]	0.10
$kbio_{sed}$	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.

F) 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 PECregional, 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 also 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. 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 the degradation product(s) formed in the particular process (e.g. hydrolysis) should also be assessed. If this cannot be done or is not practical, the rate constant for the process should be set to zero.

$$k\deg_{water} = khydr_{water} + kphoto_{water} + kbio_{water}$$

Equation R.16-16

Explanation of symbols

khydrwater	first order rate constant for hydrolysis in surface water	$[d^{-1}]$	Equation R.16-12
kphotowater	first order rate constant for photolysis in surface water	$[d^{-1}]$	Equation R.16-11
kbiowater	first order rate constant for biodegradation in surface water	$[d^{-1}]$	Table R.16-12
Kdegwater	Total first order rate constant for degradation in surface water	$[d^{-1}]$	

G) Biodegradation in the marine environment

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 substance 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. For more information on (bio)degradation in marine environments, see chapter R.7.9.

Use of marine biodegradation screening test data

For many substances, no test data from marine simulation tests are yet available. For many substances, only data from screening tests are available. This may be data from marine biodegradation screening tests or freshwater biodegradation screening tests (see chapter R.7.9.4.1).

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 R.16-14.

Table R.16-14: 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	N/a.	15	50
Readily degradable 2)	15	15	50
Readily degradable, but failing 10-d window	50	50	150
Inherently degradable 3)	150	150	∞[52]
Persistent	∞	∞	∞

Notes to Table R.16-14:

1) Half-lives from Table R.16-12
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 (see chapter R.7.9). The half-life of 150 days is not fully scientifically justifiable (see chapter R.7.9), 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 normally to be used in the regional assessment (coastal model) as described in Appendix A.16-3.

The half-lives for the marine environments that are described in Table R.16-14 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 R.16-14).

A.16-2.3 Exposure and intake estimation

This section of the appendix provides details on the calculation of the PECs in the sewage treatment plant (STP) and in each environmental compartment. General underpinning principles and role of the PECs in the overall assessment approach are presented in the main body of this guidance and in particular in section R.16.4.3.

A.16-2.3.1 Wastewater treatment – estimation of effluent concentrations and PECstp

In this section, the following parameters are derived:

- release from a sewage treatment plant to air (to be further used in PECair estimation);
- concentration in sewage sludge (to be further used in PECsoil estimation);

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[52] Depending on the tool used, various high numbers may be used. EUSES upper boundary for a half-life is 10E+40.

- concentration in the effluent of a sewage treatment plant (to be further used in PECwater estimation).
- Calculation of the STP concentration for evaluation of inhibition to microorganisms (PECstp estimation)

Elimination refers to the reduction in the concentration of substances in gaseous or aqueous discharges before their release to the environment. Elimination from the water phase may occur by physical as well as chemical or biochemical processes. In 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. The percentage connection rate across the Community has improved following the implementation of the Urban Waste Water Treatment Directive (UWWTD, 91/271/EEC). This directive required 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. The time limit for implementation of the directive was 31 December 1998, 31 December 2000 or 31 December 2005 depending on the size of the agglomeration and the sensitivity of the receiving water body.

An interim figure of 80% connection to wastewater treatment was proposed for the regional standard environment. This value was thought to be representative for the actual situation in large urban areas at the time of revision of the TGD and is still implemented in the version of EUSES currently available. 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 can vary. Many of the larger industrial installations are usually 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%. The above-described situation is taken into account as follows:

- on a local scale, wastewater may or may not pass through an STP before being discharged into the environment. Depending on the exposure scenarios, an aquatic PEClocal with or without STP can be calculated. In some cases, both may be needed if it cannot be ascertained that local releases will pass through the STP. The PEC without considering an STP-treatment will only be used in the exposure estimation, when the substance considered has a specific identified use where direct discharge to water is widely practised;
- for a standard regional scale environment (for definition, see Appendix A.16-3) it is assumed that 80% of the wastewater is treated in a biological STP and the remaining

20% 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.

Modelling STP

The degree of removal can be estimated by means of a wastewater treatment plant model using log Kow (Koc or more specific partition coefficients can also be used; see section A.16-2.2 of this appendix), 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 the sewage treatment plant model SimpleTreat (Struijs, 2014) in the screening phase of exposure estimation. 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 nine compartments (see Figure R.16-10).

Depending on the test results for ready and/or inherent biodegradability of a substance (screening tests, and simulation tests), specific first order biodegradation rate constants are assigned to the compound (see Table R.16-10 and Table R.16-11).

Typical characteristics of the standard sewage treatment plant are given in Table R.16-15. The amount of surplus sludge per person equivalent and the concentration of suspended matter in the influent are taken from SimpleTreat (run at low loading rate and with suspended solids concentration in the effluent of 30 mg dry weight/L). At a higher tier in the risk assessment process, more specific information on the biodegradation behaviour of a substance may be available.

Table R.16-15: Standard characteristics of a municipal sewage treatment plant

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	$[kg \cdot d^{-1} \cdot eq^{-1}]$	0.0212
Concentration susp. matter in influent	$SUSPCONC_{inf}$	$[kg \cdot m^{-3}]$	0.45

The input-output parameters are:

Input

HENRY	Henry's law constant	[$Pa \cdot m^3 \cdot mol^{-1}$]	Equation R.16-5
Kow	octanol-water partitioning coefficient	[-]	data set
$kbio_{stp}$	first-order rate constant for biodegradation in STP	[d^{-1}]	Table R.16-10 and Table R.16-11

Output

$Fstp_{air}$	fraction of release directed to air by STP	[-]
$Fstp_{water}$	fraction of release directed to effluent by STP	[-]
$Fstp_{sludge}$	fraction of release directed to sludge by STP	[-]

Calculation of the STP influent concentration

For local scale assessments, it is assumed that one point source is releasing its wastewater to one STP.

In some situations, removal in the sewer can be taken into account. This is the case for rapidly reacting substances, substances following fast abiotic degradation as well as for substances for which biodegradation in the sewer is proven by OECD 314 A or similar literature or monitoring data, when the release takes place to a municipal STP. If applicable, removal in the sewer will also be considered at reginal scale on the standard fraction (80%) connected to an STP. Sewer degradation is not taken into account for releases to an industrial (on site) STP.

The following equation is to be used to calculate the sewer effluent concentration taking into account removal in the sewer:

$$Csewer_{eff} = \frac{Csewer_{inf}}{1 + kdeg_{sewer} \cdot HRT_{sewer}}$$ **Equation R.16-17**

Explanation of symbols

$Csewer_{eff}$	sewer effluent concentration (entering the STP)	[$mg \cdot l^{-1}$]	
$Csewer_{inf}$	sewer influent concentration	[$mg \cdot l^{-1}$]	
$kdeg_{sewer}$	degradation rate constant in raw sewage (at 285.15 K)	[h^{-1}]	1
HRT_{sewer}	average hydraulic residence time in sewer	[h]	1

Note that when removal in the sewer is taken into account the above equation gives the concentration in STP influent (hence $Csewer_{eff} = Clocal_{inf}$).

When there is no removal in the sewer the concentration in the influent of the STP, i.e. the untreated wastewater, can be calculated from the local release 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 R.16-18**

Explanation of symbols

$Clocal_{inf}$	concentration in untreated wastewater	**[mg·l⁻¹]**	
$Elocal_{water}$	local release rate to (waste) water during episode	**[kg·d⁻¹]**	Section R.16.2.1
$EFFLUENT_{stp}$	effluent discharge rate of STP	**[l·d⁻¹]**	Equation R.16-20

Calculation of the STP-effluent concentration

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

$$Clocal_{eff} = Clocal_{inf} \cdot Fstp_{water}$$ **Equation R.16-19**

Explanation of symbols

$Clocal_{eff}$	concentration of substance in the STP effluent	[mg·l⁻¹]	
$Clocal_{inf}$	concentration in STP influent	[mg·l⁻¹]	Equation R.16-18
$Fstp_{water}$	fraction of release directed to water by STP	[-]	

If no specific data are known, EFFLUENTstp should be based on an averaged wastewater flow of 200 l per capita per day for a population of 10 000 inhabitants (see Table R.16-15):

$$EFFLUENT_{stp} = CAPACITY_{stp} \cdot WASTEWinhab$$ **Equation R.16-20**

Explanation of symbols

$EFFLUENT_{stp}$	effluent discharge rate of STP	[l·d⁻¹]	
$CAPACITY_{stp}$	capacity of the STP	[eq]	Table R.16-15
WASTEWinhab	sewage flow per inhabitant	[l·d⁻¹·eq⁻¹]	Table R.16-15

For calculating the PEC in surface water without sewage treatment, the fraction of the release to wastewater, directed to the effluent (Fstpwater) should be set to 1. The fractions to air and sludge (Fstpair and Fstpsludge resp.) should be set to zero.

Calculation of the release to air from the STP

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

$$Estp_{air} = Fstp_{air} \cdot Elocal_{water}$$ **Equation R.16-21**

Explanation of symbols

$Fstp_{air}$	fraction of the release to air from STP	[-]	
$Elocal_{water}$	local release rate to water during release episode	$[kg \cdot d^{-1}]$	Section 16.2.1
$Estp_{air}$	local release to air from STP during release episode	$[kg \cdot d^{-1}]$	

Calculation of the STP sludge concentration

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

$$C_{sludge} = \frac{Fstp_{sludge} \cdot Elocal_{water} \cdot 10^6}{SLUDGERATE}$$ **Equation R.16-22**

Explanation of symbols

C_{sludge}	concentration in dry sewage sludge	$[mg \cdot kg^{-1}]$	
$Fstp_{sludge}$	fraction of release directed to sludge by STP	[-]	
$Elocal_{water}$	local release rate to water during episode	$[kg \cdot d^{-1}]$	Section R.16.2.1
SLUDGERATE	rate of sewage sludge production	$[kg \cdot d^{-1}]$	Equation R.16-23

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 R.16-23**

Explanation of symbols

SLUDGERATE	rate of sewage sludge production	$[kg \cdot d^{-1}]$	
$SUSPCONC_{inf}$	concentration of suspended matter in STP influent	$[kg \cdot m^{-3}]$	Table R.16-15
$EFFLUENT_{stp}$	effluent discharge rate of STP	$[m^3 \cdot d^{-1}]$	Equation R.16-20
SURPLUSsludge	surplus sludge per inhabitant equivalent	$[kg \cdot d^{-1} \cdot eq^{-1}]$	Table R.16-15
$CAPACITY_{stp}$	capacity of the STP	[eq]	Table R.16-15

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 modelling, the removal of a substance 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, volatilisation and outflow of activated sludge into the secondary settler.

Activated sludge flowing out of the aeration tank contains the substance 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 the 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 R.16-24**

Explanation of symbols

$Clocal_{eff}$	total concentration of substance in STP effluent	$[mg \cdot l^{-1}]$	Equation R.16-19
PEC_{stp}	PEC for microorganisms in the STP	$[mg \cdot l^{-1}]$	

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. Such a situation is not considered as an intermittent release and the PEC_{STP} can still be considered equal to Clocaleff. After longer intervals the specific bacteria that are capable to biodegrade the compound, may be completely lost.

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

$$PEC_{stp} = Clocal_{inf}$$ **Equation R.16-25**

Explanation of symbols

$Clocal_{inf}$	total concentration of substance in STP influent	[$mg \cdot l^{-1}$]	Equation R.16-19
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 release periods, care must be taken that the release rates are in fact calculated over the actual release period (as kg.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 wastewater 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.

A.16-2.3.1.1 Refinement based on further substance properties

Simulation test data

There is insufficient information available on the applicability of elimination data from the laboratory test to the processes of a real sewage 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. If no mass balance study has been performed, the percentage of transport to air or sludge should be estimated.

Measured data in full scale STP

The percentage removal could be based upon measured influent and effluent concentrations (when they are available). As with measured data from the environment, measured data from the 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 long period of time. Furthermore, consideration should be given to the fact that removal may be due to stripping or adsorption (not degradation). If no mass balance study has been performed, the percentage of transport to air or sludge should be estimated.

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.

A.16-2.3.2 Calculation of PEClocal for the atmosphere

In this section, the following parameters are derived:

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

A standardised exposure estimation is carried out making a number of explicit assumptions and using a number of fixed default parameters. The gaussian plume model OPS, as originally described by Van Jaarsveld (1990) and updated by Sauter et al. (2020) is proposed using the standard parameters as described by Toet and de Leeuw (1992). The OPS model was used to carry out a number of default calculations 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 calculations were re-done in 2020 with the version of the model available at that time.-The following assumptions/model settings are made:

- realistic average atmospheric conditions are used, obtained from long term annual average meteorological conditions (2005-2014) for the Netherlands and a receptor height of 1.5 metres;
- 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 R.16-3);
- the atmospheric reaction rate is set at a fixed value of 5% per hour. However, on the spatial scale that is regarded (i.e. a distance of 100 m from the source), atmospheric reactions do not play any role in the removal of the substance (even at very high reaction rates) (Toet and De Leeuw, 1992);
- 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 metres, 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 metres; 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 metres from the point source is estimated. This distance is chosen to represent the average distance between the release 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 the help of the OPS model. The deposition flux to soil is averaged over a circular area around the source, with a radius of 1 000 m to represent the local agricultural area. Deposition velocities are used for three different categories:

- dry deposition of gas/vapour: determined using the classical two-film resistance model (Mackay et al., 1992) (Table R.16-16);
- 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 release from a point source is known, the concentration at 100 metres from the source can be estimated from a simple linear relationship.

In the calculation of PEClocal for air, both the release from a point source as well as the release from an STP is taken into account. The concentration on the regional scale (PECregional) is used as a background concentration and therefore, summed to the local concentration. The STP is assumed as a point source and the concentration of the substance 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 R.16-26**

$$Clocal_{air,ann} = Clocal_{air} \cdot \frac{Temission}{365}$$ **Equation R.16-27**

Explanation of symbols

$Elocal_{air}$	local direct release rate to air during episode	$[kg \cdot d^{-1}]$	Section R.16.2.1
$Estp_{air}$	local indirect release to air from STP during episode	$[kg \cdot d^{-1}]$	Equation R.16-21
$Cstd_{air}$	concentration in air at source strength of 1 $kg \cdot d^{-1}$	$[mg \cdot m^{-3}/(kg.d^{-1})]$	Default $3.2*10^{-4}$ ($3.18*10^{-4}$ for gaseous substances and $3.23*10^{-4}$ for aerosol-bound substances)
T emission	number of emission days equal to: annual use ($kg \cdot y^{-1}$) / daily use ($kg \cdot d^{-1}$)	$[d \cdot y^{-1}]$	Section R.16.2.2
$Clocal_{air}$	local concentration in air during release episode	$[mg \cdot m^{-3}]$	
$Clocal_{air,ann}$	annual average concentration in air, 100 m from point source	$[mg \cdot m^{-3}]$	

$$PEClocal_{air,ann} = Clocal_{air,ann} + PECregional_{air}$$ **Equation R.16-28**

Explanation of symbols

$Clocal_{air,ann}$	annual average local concentration in air	$[mg \cdot m^{-3}]$	Equation R.16-27
$PECregional_{air}$	regional concentration in air	$[mg \cdot m^{-3}]$	Appendix A.16-4
$PEClocal_{air,ann}$	annual average predicted environmental conc. in air	$[mg \cdot m^{-3}]$	

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 releases 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 R.16-29**

$$DEPtotal_{ann} = DEPtotal \cdot \frac{Temission}{365}$$ **Equation R.16-30**

Explanation of symbols

$Elocal_{air}$	local direct release rate to air during release episode	$[kg \cdot d^{-1}]$	Section R.16.2.1
$Estp_{air}$	local indirect release to air from STP during episode	$[kg \cdot d^{-1}]$	Equation R.16-21
$Fass_{aer}$	fraction of the substance bound to aerosol	[-]	Equation R.16-3
$DEPstd_{aer}$	standard deposition flux of aerosol-bound compounds at a source strength of 1 $kg \cdot d^{-1}$	$[mg.m^{-2}/(kg.d^{-1})]$	$1.1 \cdot 10^{-2}$
$DEPstd_{gas}$	deposition flux of gaseous compounds as a function of Henry's Law constant, at a source strength of 1 $kg \cdot d^{-1}$	$[mg.m^{-2}/(kg.d^{-1})]$	Table R.16-16
T emission	number of emission days equal to: annual use $(kg \cdot y^{-1})$ / daily use $(kg \cdot d^{-1})$	$[d \cdot y^{-1}]$	Section R.16.3.2.1
DEPtotal	total deposition flux during release episode	$[mg \cdot m^{-2}.d^{-1}]$	
$DEPtotal_{ann}$	annual average total deposition flux	$[mg.m^{-2}.d^{-1}]$	

The default values for the deposition flux of gaseous compounds ($DEPstd_{gas}$) as a function of the Henry's Law constant to be used in Equation R.16-29 are included in the below table.

Table R.16-16: Deposition flux of a gaseous substance to soil as a function of the Henry coefficient (H) (J.Bakker et al. 2021, not published)[53]

H ($Pa.m^{-3}.mol^{-1}$)	Dep.flux ($g.m^{-2}.s^{-1}$)
≤ 1,0E-06	4,16E-09
3,0E-06	4,15E-09
1,0E-05	4,12E-09
3,0E-05	4,05E-09
1,0E-04	3,81E-09
3,0E-04	3,26E-09
1,0E-03	2,21E-09
3,0E-03	1,23E-09
1,0E-02	6,21E-10
3,0E-02	3,84E-10
1,0E-01	2,05E-10
3,0E-01	9,40E-10
1,0E00	3,99E-11
3,0E00	2,34E-11
1,0E+01	1,76E-11
3,0E+01	1,60E-11
1,0E+02	1,54E-11
3,0E+02	1,52E-11
≥ 1,03E+03	1,52E-11

Note that if the Henry's Law constant falls between two values in the table above, the most conservative value (i.e. the higher value) should be used for the estimation of deposition.

A.16-2.3.3 Calculation of PEClocal for the aquatic compartment (freshwater)

In this section, the following parameters are derived:

- local concentration in surface water during release episode;
- annual average local concentration 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 ecosystem;
- 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.

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[53] 1 g/s = 86.4 kg/d

As introduced in section R.16.4.1.3, the starting point is the concentration of the substance in the STP effluent. Dilution in the receiving surface water and adsorption to suspended matter are then considered.

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 is generally linked to the release scenario of the use category. For example, an average dilution factor for sewage from municipal treatment plants of 10 is recommended for consumer products. 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), this may lead to overestimation of PEC for surface water and underestimation of PEC for 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 release 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 releases 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 release as well as the impact of degradation, volatilisation, etc. in the derivation of the PEC. Normally, only dilution and adsorption to suspended sediments 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 higher concentrations will occur in the mixing zone. 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, for site-specific assessments, the dilution factor that is applied for calculating the local concentration in surface water should not be greater than 1 000.

If no measured data are available on the partition coefficient between suspended matter and water, Kpsusp, it can be estimated from the Koc of the substance, determined for other sorbents like soil or sediments (A.16-2.2 in this appendix) 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 are in excess of the water solubility. 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 (1992)) which address the specific release pattern as well as river parameters.

The local concentration in surface water is calculated as follows:

$$Clocal_{water} = \frac{Clocal_{eff}}{(1 + Kp_{susp,freshwater} \cdot SUSP_{water} \cdot 10^{-6}) \cdot DILUTION}$$ **Equation R.16-31**

Explanation of symbols

$Clocal_{eff}$	concentration of the substance in the STP effluent	[mg·l^{-1}]	Equation R.16-19
$Kp_{susp,freshwater}$	solids-freshwater partitioning coefficient of suspended matter	[l·kg^{-1}]	Equation R.16-7
$SUSP_{water}$	concentration of suspended matter in the river	[mg·l^{-1}]	15
DILUTION	dilution factor	[-]	10
$Clocal_{water}$	local concentration in surface water during release episode	[mg·l^{-1}]	

When considering the available dilution, 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 R.16-32**

Explanation of symbols

$EFFLUENT_{stp}$	effluent discharge rate of stp	[l·d^{-1}]	Equation R.16-20
FLOW	flow rate of the river	[l·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 R.16-33**

Explanation of symbols

$Clocal_{water}$	local concentration in surface water during release episode	[$mg \cdot l^{-1}$]	Equation R.16-31
T emission	number of emission days equal to: annual use ($kg \cdot y^{-1}$) / daily use ($kg \cdot d^{-1}$)	[$d \cdot y^{-1}$]	Section R.16.3.2.1
$Clocal_{water,ann}$	annual average local concentration in surface water	[$mg \cdot l^{-1}$]	

The concentration at the regional scale ($PECregional_{freshwater}$) is used as a background concentration for the local scale.

For naturally occurring substances also the natural background concentration may have to be taken into account. This depends also on whether the natural background is already accounted for when deriving the PNEC (see added risk approach in Appendix A.7.13-2[54]). Note that in any case, when using measured data for the regional concentration, the natural background concentration is generally already considered part of the regional concentration. Therefore, care should be taken not to include the background concentration twice.

Therefore, these concentrations are summed (when applicable, as explained above):

$$PEClocal_{water} = Clocal_{water} + PECregional_{water} + Cnatural_{water}$$ **Equation R.16-34**

$$PEClocal_{water,ann} = Clocal_{water,ann} + PECregional_{water} + Cnatural_{water}$$ **Equation R.16-35**

Explanation of symbols

$Clocal_{water}$	local concentration in surface water during episode	[$mg \cdot l^{-1}$]	Equation R.16-31
$Clocal_{water,ann}$	annual average concentration in surface water	[$mg \cdot l^{-1}$]	Equation R.16-33
$PECregional_{freshwater}$	regional concentration in surface water	[$mg \cdot l^{-1}$]	Appendix A.16-3
$PEClocal_{water}$	predicted environmental concentration during episode	[$mg \cdot l^{-1}$]	
$PEClocal_{water,ann}$	annual average predicted environmental concentration	[$mg \cdot l^{-1}$]	
$Cnatural_{water}$	natural background concentration in surface water	[$mg \cdot l^{-1}$]	Default = 0

A.16-2.3.4 Calculation of PEClocal for the sediment compartment (freshwater and marine water)

In this section, the following parameter is derived:

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[54] https://echa.europa.eu/documents/10162/17224/information_requirements_r7_13_2_en.pdf/0497e68d-4bb5-4b12-a4db-52ce0c1bc237?t=1322594777855

- local concentration in sediment during the release 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).

The concentration at the regional scale is used as a background concentration for the local scale and for naturally occurring substances also the natural background concentration may have to be taken into account (as explained for the water compartment, see A.16-2.3.3):

$$PEClocal_{sed,freshwater} = \frac{K_{susp-freshwater}}{RHO_{susp}} \cdot Clocal_{freshwater} \cdot 1000 + PECregional_{sed,freshwater} + Cnatural_{sed,freshwater}$$

Equation R.16-36

$$PEClocal_{sed,seawater} = \frac{K_{susp-seawater}}{RHO_{susp}} \cdot Clocal_{seawater} \cdot 1000 + PECregional_{sed,seawater} + Cnatural_{sed,seawater}$$

Equation R.16-37

$PECregional_{sed,freshwater}$ and $PECregional_{sed,seawater}$ are by default calculated by equilibrium partitioning (using suspended matter characteristics) using the equations below. However, when measured data for $PECregional_{sed,freshwater}$ and/or $PECregional_{sed,seawater}$ are available, the calculated values can then be overwritten. In this case the measured data should reflect the concentration in freshly deposited sediment (top layer) to ensure consistency between PEC and PNEC.

$$PECregional_{sed,freshwater} = \frac{K_{susp-freshwater}}{RHO_{susp}} \cdot PECregional_{freshwater} \cdot 1000$$

Equation R.16-38

$$PECregional_{sed,seawater} = \frac{K_{susp-seawater}}{RHO_{susp}} \cdot PECregional_{seawater} \cdot 1000$$

Equation R.16-39

Explanation of symbols

$K_{susp\text{-}freshwater}$	suspended matter-water partition coefficient in freshwater	[$m^3.m^{-3}$]	Equation R.16-8
$K_{susp\text{-}seawater}$	suspended matter-water partition coefficient in seawater	[$m^3.m^{-3}$]	Equation R.16-8
RHO_{susp}	bulk density of suspended matter	[$kg.m^{-3}$]	Equation R.16-1
$Clocal_{freshwater}$	local concentration in freshwater during emission episode	[$mg.l^{-1}$]	Equation R.16-31
$Clocal_{seawater}$	local concentration in seawater during emission episode	[$mg.l^{-1}$]	Equation R.16-40
$PECregional_{sed,freshwater}$	predicted environmental regional concentration in freshwater sediment	[$mg.kg^{-1}$]	Equation R.16-38
$PECregional_{sed,seawater}$	predicted environmental regional concentration in seawater sediment	[$mg.kg^{-1}$]	Equation R.16-39
$Cnatural_{sed,freshwater}$	natural background concentration in freshwater sediment	[$mg.kg^{-1}$]	Default = 0
$Cnatural_{sed,seawater}$	natural background concentration in seawater sediment	[$mg.kg^{-1}$]	Default = 0
$PECregional_{freshwater}$	regional concentration in surface water	[$mg.l^{-1}$]	Appendix A.16-3
$PECregional_{seawater}$	regional concentration in seawater	[$mg.l^{-1}$]	Appendix A.16-3

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.

When release to the surface water predominately occurs as particles, 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).

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 to be taken into account especially when comparing measured concentrations to estimated concentrations.

A.16-2.3.5 Calculation of PEClocal for the marine aquatic compartment

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 seas, 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).

In site-specific assessments, due account can be taken of the true dilution available to the given release as well as the impact of degradation, volatilisation, etc. in the derivation of the PEC.

Normally, only dilution and adsorption to suspended sediment needs be considered but site-specific conditions may indicate that valid local distribution models can be used. A realistic worst-case dilution factor for discharges to a coastal zone of 100 may be assumed if no further information is available. The same estimation method as for inland exposure estimation can then be used to obtain the local concentration in seawater ($Clocal_{seawater}$).

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. Specific approaches (using higher tier models) can be used if needed.

Then, the local concentration in seawater can be obtained with:

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

Equation R.16-40

Explanation of symbols

$Clocal_{eff}$	concentration of the substance in the STP effluent	[mg·l^{-1}]	Equation R.16-19
$Kp_{susp-seawater}$	solids-water partitioning coefficient of suspended matter	[l·kg^{-1}]	Equation R.16-8
$SUSP_{water}$	concentration of suspended matter in the seawater	[mg·l^{-1}]	15
DILUTION	dilution factor	[-]	100
$Clocal_{seawater}$	local concentration in seawater during release episode	[mg·l^{-1}]	

$Kp_{susp-seawater}$ is derived as for inland risk assessment. For a specific estimation of the partitioning behaviour of substances in saltwater environments, see section R.16.4.2.1

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 before discharge.

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

$$Clocal_{seawater,ann} = Clocal_{seawater} \cdot \frac{Temission}{365}$$

Equation R.16-41

Explanation of symbols

$Clocal_{seawater}$	local concentration in seawater during release episode	[mg·l^{-1}]	Equation R.16-40
T emission	number of emission days equal to: annual use (kg·y^{-1}) / daily use (kg·d^{-1})	[d·y^{-1}]	Section R.16.2.2
$Clocal_{seawater,ann}$	annual average local concentration in seawater	[mg·l^{-1}]	

The concentration at the regional scale ($PECregional_{seawater}$) is used as a background concentration for the local scale. For naturally occurring substances also the natural background concentration may have to be taken into account. This depends, as explained in A.16-2.3.3 for the freshwater compartment, on whether the natural background is already accounted for when deriving the PNEC (see added risk approach in Appendix A.7.13-2[55]). Note that in any case, when using measured data for the regional concentration, the natural background concentration is generally already considered part of the regional concentration. Therefore, care should be taken not to include the background concentration twice.

Therefore, these concentrations are summed (when applicable, as explained above):

$$PEClocal_{seawater} = Clocal_{seawater} + PECregional_{seawater} + Cnatural_{seawater}$$ **Equation R.16-42**

$$PEClocal_{seawater,ann} = Clocal_{seawater,ann} + PECregional_{seawater} + Cnatural_{seawater}$$ **Equation R.16-43**

Explanation of symbols

$Clocal_{seawater}$	local concentration in seawater during episode	[mg·l^{-1}]	Equation R.16-40
$Clocal_{seawater,ann}$	annual average concentration in seawater	[mg·l^{-1}]	Equation R.16-41
$PECregional_{seawater}$	regional concentration in seawater	[mg·l^{-1}]	Appendix A.16-3
$PEClocal_{seawater}$	predicted environmental concentration during episode	[mg·l^{-1}]	
$PEClocal_{seawater,ann}$	annual average predicted environmental concentration	[mg·l^{-1}]	
$Cnatural_{seawater}$	natural background concentration in seawater	[mg·l^{-1}]	0

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:

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[55] https://echa.europa.eu/documents/10162/17224/information_requirements_r7_13_2_en.pdf/0497e68d-4bb5-4b12-a4db-52ce0c1bc237?t=1322594777855

- substances released from platforms. A harmonised mandatory control system for the use and reduction of the discharge of offshore substances 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[56];
- 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.

A.16-2.3.6 Calculation of PEClocal for the soil compartment

In this section, the following parameters are derived:

- local concentration in arable land (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.

A model for estimation of release and exposure of agricultural soil to substances directly released to soil is included in Appendix A.16-2.4. This model is largely based on the Crop Life Europe (CLE) Local Environment Tool (LET) to assess direct application of co-formulants to soil and more information can be found in Appendix A.16-4.2.

For sludge application to arable land, an application rate of 5 000 kg/ha dry weight per year is assumed while for grassland a rate of 1 000 kg/ha/year should be used. Sludge application is treated as a single event once a year. The contribution to the overall impact from wet and dry deposition is based on the release calculation of a point source (section R.16.4.3.7and A.16-2.3.2 of this appendix) and is related to a surrounding area within 1 000 m from that source. The deposition is averaged over the whole area.

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 release episode. Averaging is done to facilitate calculation of a steady-state level. Furthermore, it is impossible to indicate when the release 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.

The PEC in agricultural soil is used for two purposes:

- for risk characterisation of terrestrial ecosystems;
- as a starting point for the calculation of indirect human exposure via crops and cattle products (see A.16-2.3.9 of this appendix and Appendix A.16-5).

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[56] 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.

There are several extensive numerical soil and groundwater models available (mainly for pesticides). These models, however, require a detailed definition of soil and environmental characteristics. This makes these types of models less appropriate for a generic risk assessment at EU-level. For the initial assessment, 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.

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 R.16-44**

Explanation of symbols

D_{air}	aerial deposition flux per kg of soil	[mg·kg^{-1}·d^{-1}]	Equation R.16-45
t	time	[d]	
k	first order rate constant for removal from topsoil	[d^{-1}]	Equation R.16-49
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 R.16-45**

Explanation of symbols

$DEPtotal_{ann}$	annual average total deposition flux	[mg·m^{-2}·d^{-1}]	Equation R.16-30
$DEPTH_{soil}$	mixing depth of soil	[m]	Table R.16-17
RHO_{soil}	bulk density of soil	[kg·m^{-3}]	Equation R.16-1
D_{air}	aerial deposition flux per kg of soil	[mg·kg^{-1}·d^{-1}]	

The differential Equation R.16-44 has an analytical solution, given by:

$$C_{soil}(t) = \frac{D_{air}}{k} - \left[\frac{D_{air}}{k} - C_{soil}(0)\right] \cdot e^{-kt}$$ **Equation R.16-46**

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

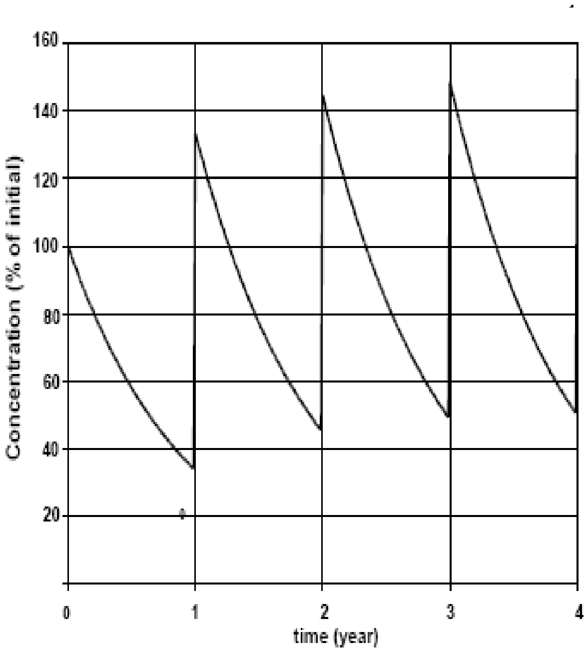

Figure R.16-16: Accumulation in soil due to several years of sludge application

Accumulation of the substance may occur when sludge is applied over consecutive years. This is illustrated in Figure R.16-16. As a realistic worst-case exposure scenario, it is assumed that sludge is applied for 10 consecutive years.

To indicate for potential persistency of the substance, the percentage of the steady-state situation is calculated. As shown in Figure R.16-16, the concentration in soil is not constant in time.

The concentration will be higher just after sludge application (in the beginning of the growth season), and lower at the end of the year due to removal processes. Therefore, for exposure of the endpoints, the concentration needs to be averaged over a certain time period. Different averaging times should be considered for these endpoints: for the ecosystem a period of 30 days after application of sludge is used[57]. To determine biomagnification effects and indirect human exposure, it is more appropriate to use an extended period of 180 days.

This averaging procedure is illustrated in Figure R.16-17 where the average concentration is given by the area of the shaded surface, divided by the number of days.

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[57] However, when the terrestrial ecotoxicity tests are based on the initial nominal concentration, the initial concentration in soil (immediately after the last sludge application) should be considered.

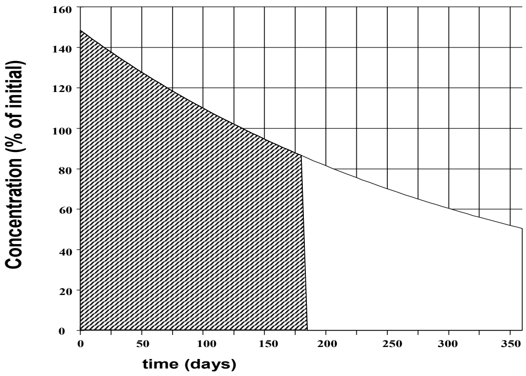

Figure R.16-17: The concentration in soil after 10 years. The shaded area is the integrated concentration over a period of 180 days

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 R.16-47

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

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

Equation R.16-48

Explanation of symbols

D_{air}	aerial deposition flux per kg of soil	$[mg \cdot kg^{-1} \cdot d^{-1}]$	Equation R.16-45
T	averaging time	[d]	Table R.16-17
k	first order rate constant for removal from topsoil	$[d^{-1}]$	Equation R.16-49
C_{soil} (0)	initial concentration (after sludge application)	$[mg \cdot kg^{-1}]$	Equation R.16-56
$Clocal_{soil}$	average concentration in soil over T days	$[mg \cdot kg^{-1}]$	

Derivation of the removal rate constants

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

- biodegradation rate constant;

- volatilisation of substance from soil;
- leaching to deeper soil layers.

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 R.16-49

Explanation of symbols

k_{volat}	pseudo-first order rate constant for volatilisation from soil	[d^{-1}]	Equation R.16-50
k_{leach}	pseudo-first order rate constant for leaching from topsoil	[d^{-1}]	Equation R.16-51
$kbio_{soil}$	pseudo-first order rate constant for biodegradation in soil	[d^{-1}]	Equation R.16-14
k	first order rate constant for removal from topsoil	[d^{-1}]	

The diffusive transfer from soil to air is estimated using the classical two-film resistance model. The soil-side of the interface is treated as a pair of parallel resistances (air phase and water phase of soil) (Mackay et al., 1992). The rate constant for volatilisation from soil is given by:

$$\frac{1}{k_{volat}} = \left(\frac{1}{kasl_{air-soil} \cdot K_{air-water}} + \frac{1}{kasl_{soil-air} \cdot K_{air-water} + kasl_{soil-water}}\right) \cdot K_{soil-water} \cdot DEPTH_{soil}$$

Equation R.16-50

Explanation of symbols

$kasl_{air-soil}$	partial mass transfer coefficient at air side of the air-soil interface	[m.d-1]	Table R.16-22
$kasl_{soil-air}$	partial mass transfer coefficient at soil side of the air-soil interface	[m.d-1]	0.48 [58]
$kasl_{soil-water}$	partial mass transfer coefficient at soil side of the water-soil interface	[m.d-1]	$4.8 \cdot 10^{-5}$ [59]
$K_{air-water}$	air-water equilibrium distribution constant	[$m^3.m^{-3}$]	Equation R.16-6
$K_{soil-water}$	soil-water partitioning coefficient	[$m^3.m^{-3}$]	Equation R.16-8
$DEPTH_{soil}$	mixing depth of soil	[m]	
k_{volat}	pseudo first-order rate constant for volatilisation from soil	[d-1]	

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[58] TGD (2003) part II

[59] TGD (2003) part II

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

Equation R.16-51

$$kleach = \frac{Finf_{soil} \cdot RAINrate}{K_{soil-water} \cdot DEPTH_{soil}}$$

Explanation of symbols

$Finf_{soil}$	fraction of rainwater that infiltrates into soil	[-]	0.25
RAINrate	rate of wet precipitation (700 mm/year)	$[m.d^{-1}]$	$1.92 \cdot 10^{-3}$
$K_{soil-water}$	soil-water partitioning coefficient	$[m^3 \cdot m^{-3}]$	Equation R.16-8
$DEPTH_{soil}$	mixing depth of soil	[m]	
k_{leach}	pseudo first-order rate constant for leaching from soil layer	$[d^{-1}]$	

<u>Derivation of the initial concentration after 10 years of sludge application</u>

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 R.16-48), 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 R.16-52 with an initial concentration of zero and 10 years of input:

Equation R.16-52

$$Cdep_{soil\,10}(0) = \frac{D_{air}}{k} - \frac{D_{air}}{k} \bullet e^{-365 \bullet 10 \bullet k}$$

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:

Equation R.16-53

$$Csludge_{soil\,1}\ (0) \ = \ \frac{C_{sludge} \ \bullet \ APPL_{sludge}}{DEPTH_{soil} \ \bullet \ RHO_{soil}}$$

Explanation of symbols

C_{sludge}	concentration in dry sewage sludge	$[mg \cdot kg^{-1}]$	Equation R.16-22
$APPL_{sludge}$	dry sludge application rate	$[kg \cdot m^{-2} \cdot yr^{-1}]$	Table R.16-21
$DEPTH_{soil}$	mixing depth of soil	[m]	Table R.16-21
RHO_{soil}	bulk density of soil	$[kg \cdot m^{-3}]$	Equation R.16-1
$Csludge_{soil\,1}$ (0)	concentration in soil due to sludge in first year at t=0	$[mg \cdot kg^{-1}]$	

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

$$Facc = e^{-365\,k}$$ **Equation R.16-54**

Explanation of symbols

k	first order rate constant for removal from topsoil	[d^{-1}]	Equation R.16-49
Facc	fraction accumulation in one year	[-]	

At the end of each year, a fraction Facc 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 R.16-55**

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 R.16-56**

This initial concentration can be used in Equation R.16-49 to calculate the average concentration in soil over a certain time period.

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 R.16-57**

Explanation of symbols

C_{soil} 10 (0)	initial concentration after 10 years	[$mg \cdot kg^{-1}$]	Equation R.16-56
$C_{soil\,\infty}$ (0)	initial concentration in steady-state situation	[$mg \cdot kg^{-1}$]	Equation R.16-58
Fst-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 R.16-58**

Explanation of symbols

D_{air}	aerial deposition flux per kg of soil	$[mg \cdot kg^{-1} \cdot d^{-1}]$	Equation R.16-45
k	first order rate constant for removal from topsoil	$[d^{-1}]$	Equation R.16-49
Facc	fraction accumulation in one year	[-]	Equation R.16-54
$Csludge_{soil\ 1}(0)$	concentration in soil due to sludge in first year at t=0	$[mg \cdot kg^{-1}]$	Equation R.16-53
$C_{soil\infty}(0)$	initial concentration in steady-state situation	$[mg \cdot kg^{-1}]$	

Calculation of $PEClocal_{soil}$

For soil, three different PECs are calculated, for different endpoints (Table R.16-17).

Table R.16-17: Characteristics of soil and soil-use for the three different endpoints

CHARACTERISTICS OF SOIL AND SOIL-USE FOR THE THREE DIFFERENT ENDPOINTS				
	Depth of soil compartment [m]	Averaging time [days]	Rate of sludge application $[kg_{dwt} \cdot m^{-2} \cdot year^{-1}]$	Endpoint
$PEClocal_{arableland}$	0.20	30	0.5	terrestrial ecosystem
$PEClocal_{arableland}$	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 topsoil 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 arable land and grassland is also the relevant period for the derivation of pore water concentrations. For the ecosystem, a period of 30 days after the last sludge application is taken as a relevant time period with respect to chronic exposure of soil organisms. However, when the terrestrial ecotoxicity tests are based on the initial nominal concentration, the initial concentration in soil (immediately after the last sludge application) should be considered.

The concentration at the regional scale is used as background concentration for the local scale. 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.

For naturally occurring substances also the natural background concentration may have to be taken into account. This depends also on whether the natural background is already accounted for when deriving the PNEC (see added risk approach in Appendix A.7.13-2[60]). Note that in any case, when using measured data for the regional concentration, the natural background concentration is generally already considered part of the regional concentration. Therefore, care should be taken not to include the background concentration twice.

$$\boldsymbol{PEClocal_{soil} = Clocal_{soil} + PECregional_{natural\ soil} + Cnatural_{soil}}$$ **Equation R.16-59**

Explanation of symbols

$Clocal_{soil}$	local concentration in soil	[$mg \cdot kg^{-1}$]	Equation R.16-48
$PECregional_{natural\ soil}$	regional concentration in natural soil	[$mg \cdot kg^{-1}$]	Appendix A.16-3
$PEClocal_{soil}$	predicted environmental concentration in soil	[$mg \cdot kg^{-1}$]	
$Cnatural_{soil}$	natural background concentration in soil	[$mg \cdot kg^{-1}$]	0

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

$$PEClocal_{soil,porew} = \frac{PEClocal_{soil} \cdot RHO_{soil}}{K_{soil\text{-}water} \cdot 1000}$$ **Equation R.16-60**

Explanation of symbols

$PEClocal_{soil}$	predicted environmental concentration in soil	[$mg \cdot kg^{-1}$]	Equation R.16-59
$K_{soil\text{-}water}$	soil-water partitioning coefficient	[$m^3 \cdot m^{-3}$]	Equation R.16-8
RHO_{soil}	bulk density of wet soil	[$kg \cdot m^{-3}$]	Equation R.16-1
$PEClocal_{soil,porew}$	predicted environmental concentration in porewater	[$mg \cdot l^{-1}$]	

A.16-2.3.7 Calculation of concentration in groundwater

In this section, the following parameter is derived:

- local concentration in groundwater.

$$PEClocal_{grw} = PEClocal_{soil,porew}$$ **Equation R.16-61**

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[60] https://echa.europa.eu/documents/10162/17224/information_requirements_r7_13_2_en.pdf/0497e68d-4bb5-4b12-a4db-52ce0c1bc237?t=1322594777855

Explanation of symbols

$PEClocal_{soil,porew}$	predicted environmental concentration in porewater	$[mg \cdot l^{-1}]$	Equation R.16-60
$PEClocal_{grw}$	predicted environmental concentration in groundwater	$[mg \cdot l^{-1}]$	

A.16-2.3.8 Predators (secondary poisoning)

In this section, the following parameters are calculated:

A. Predicted environmental concentration in food (fish) of fish-eating predators (aquatic food chain).

B. Concentration in food (worms) of worm-eating predators (terrestrial food chain).

These are used for the assessment of secondary poisoning via the aquatic food chain and of secondary poisoning via the terrestrial food chain.

A) Assessment of secondary poisoning via the aquatic food chain

The concentration of contaminants in food (fish) of fish-eating predators ($PECoral_{predator}$) and top-predators ($PECoral_{top\ predator}$) is calculated from the PEC for surface water (fresh or marine water), the measured or estimated BCF for fish and the biomagnification factor (BMF):

$$PEC_{oral,predator} = PEC_{water} \cdot BCF_{fish} \cdot BMF$$ **Equation R.16-62**

$$PEC_{oral,toppredator} = PEC_{oral,predator} \cdot BMF_2 = PEC_{water\cdot} \cdot BCF_{fish} \cdot BMF_1 \cdot BMF_2$$ **Equation R.16-63**

Explanation of symbols

$PEC_{oral,predator}$	predicted environmental concentration in food	$[mg \cdot kg_{wet\ fish}^{-1}]$
$PEC_{oral,top\ predator}$	predicted environmental concentration in the food of the top predator	$[mg \cdot kg_{wet\ fish}^{-1}]$
PEC_{water}	predicted environmental concentration in water (seawater or freshwater)	$[mg \cdot l^{-1}]$
BCF_{fish}	bioconcentration factor for fish on wet weight basis	$[l \cdot kg_{wet\ fish}^{-1}]$
BMF_1	biomagnification factor in fish	[-]
BMF_2	biomagnification factor in the predator	[-]

The BMF is defined as the relative concentration in a predatory animal compared to the concentration in its prey (BMF = Cpredator/Cprey). The concentrations used to derive and report BMF values should, where possible, be lipid normalised. For the assessment of the risks to the top-predator, an additional biomagnification factor is used.

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 also forage on fish from other sites than the area around the point of discharge. Biodegradation in surface water is also not taken into account using PEClocal. However, using PECregional may have the opposite effect, as there may be large areas in the region with higher concentrations. It has therefore been decided that for a first trophic level of predators, a scenario where 50% of the diet comes from a local area (represented by the annual average PEClocal) and 50% of the diet comes from a regional area (represented by the annual average PECregional) is the most appropriate for the assessment:

$$\boldsymbol{PEC_{oral,predator} = 0.5 \cdot (PEC_{local,water} + PEC_{regional,water}) \cdot BCF_{fish} \cdot BMF}$$

Equation R.16-64

For the second trophic level of predators, the top predators, it can be assumed that they obtain their prey mainly from the larger-scale marine environment. 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:

$$\boldsymbol{PEC_{oral,toppredator} = (0.1 \cdot PEC_{local,seawater} + 0.9 \cdot PEC_{regional,seawater}) \cdot BCF_{fish} \cdot BMF_1 \cdot BMF_2}$$

Equation R.16-65

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) 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 only gives an indication that secondary poisoning is a critical process in the aquatic risk characterisation of a substance.

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 rates 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 substances: 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.

B) Assessment of secondary poisoning via the terrestrial food chain

For the terrestrial food chain, a similar approach as for the aquatic route can be used. The food-chain soil → earthworm → worm-eating birds or mammals is used as has been described by Romijn et al. (1994).

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 $PECoral_{predator}$ is calculated as:

$$PEC_{oral,\,predator} = C_{earthworm}$$

Equation R.16-66

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.
For $PEC_{soil,}$ the PEClocal is used in which the concentration is averaged over a period of 180 days (see section A.16-2.3.6 of this appendix) with respect to sludge application. The same scenario is used as for the aquatic food chain, 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):

$$PEC_{oral,predator} = \frac{BCF_{earthworm} \cdot 0,5 \cdot (PEClocal_{porewater} + PECregional_{porewater}) + 0,5 \cdot (PEClocal_{soil} + PECregional_{soil}) \cdot W_{gut}}{W_{earthworm} + W_{gut}}$$

Equation R.16-67

Explanation of symbols

$PECoral_{predator}$	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	$[mg \cdot kg_{wet\ earthworm}^{-1}]$
$PEC_{local,\ porewater}$	Local concentration in porewater	$[mg \cdot L^{-1}]$
$PEC_{regional,\ porewater}$	Regional concentration in porewater	$[mg \cdot L^{-1}]$
$PEC_{local,\ soil}$	Local concentration in soil	$[mg \cdot kg_{wwt}^{-1}]$
$PEC_{regional,\ soil}$	Regional concentration in soil	$[mg \cdot kg_{wwt}^{-1}]$
$W_{earthworm}$	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:

$$W_{gut} = W_{earthworm} \cdot F_{gut} \cdot CONV_{soil}$$

Equation R.16-68

Explanation of symbols

$CONV_{soil}$	conversion factor for soil concentration wet-dry weight soil	$[kg_{wwt} \cdot kg_{dwt}^{-1i}]$	Equation 16.2
F_{solid}	volume fraction of solids in soil	$[m^3 \cdot m^{-3}]$	Table R.16-8
F_{gut}	fraction of gut loading in worm	$kg_{dwt} \cdot kg_{wwt}^{-1}$	0.1
RHO_{soil}	bulk density of wet soil	$[kg_{wwt} \cdot m^{-3}]$	Equation R.16-1
RHO_{solid}	density of solid phase	$[kg_{dwt} \cdot m^{-3}]$	Table R.16-8Table R.16-9

Using this equation, the concentration in a full worm can be written as:

$$\boldsymbol{PEC_{oral,predator} = \frac{BCF_{earthworm} \cdot 0,5 \cdot (PEClocal_{porewater} + PECregional_{porewater}) + 0,5 \cdot (PEClocal_{soil} + PECregional_{soil}) \cdot F_{gut} \cdot CONV_{soil}}{1 + F_{gut} \cdot CONV_{soil}}}$$

Equation R.16-69

When measured data on bioconcentration in worms is available, the BCF factors can be inserted in the above equation. For most substances, however, these data will not be present and BCF will have to be estimated. For organic substances, 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):

$$BCF_{earthworm} = (0.84 + 0.012K_{ow})/RHO_{earthworm}$$ **Equation R.16- 70**

where for $RHO_{earthworm}$ by default a value of 1 ($kg_{wwt} \cdot L^{-1}$) can be assumed. Jager (1998) has demonstrated that this approach performed very well in describing uptake in an 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[61].

Earthworms are also able to take up substances from food and it has been hypothesised that this process may affect accumulation at log Kow>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 the 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 substances in soil within the range log Kow 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 Kow 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 Kow of the neutral species. The underlying data are, however, too limited to propose this approach in general for ionised substances.

A.16-2.3.9 Humans exposed indirectly via the environment

Assessment of indirect exposure via the environment comprises the following steps:

- Assessing the concentrations in intake media (food, drinking water, air);

- Assessing the intake rate of each medium (using a standard consumption pattern);

- Combining the concentrations in the media with the intake of each medium.

A) Input

The required PEC-values are given in Table R.16-18.

In addition to the data required for the environmental exposure estimation (as mentioned in section R.16.4.3), the bioconcentration factor (BCF), soil accumulation factors (BSAFs) and human intake rates for crops, milk and meat are required. Default values for the latter (from EUSES) are given in

Table R.16-19.

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[61] 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 logKow > 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

Table R.16-18: Environmental concentrations used as input for indirect exposure to humans via the environment calculations

ENVIRONMENTAL CONCENTRATIONS USED AS INPUT FOR INDIRECT EXPOSURE CALCULATIONS		
Compartment	**Local assessment**	**Regional assessment**
surface water	annual average concentration after complete mixing of STP-effluent	steady-state concentration in surface water
air	annual average concentration at 100 m from source or STP (maximum)	steady-state concentration in air
agricultural soil	concentration averaged over 180 days after 10 years of sludge application and aerial deposition	steady-state concentration in agricultural soil
porewater	concentration in porewater of agricultural soil as defined above	steady-state concentration in porewater of agricultural soil
groundwater	concentration in porewater of agricultural soil as defined above	steady-state concentration in porewater of agricultural soil

Table R.16-19: Human daily intake of food and water (from EUSES)

HUMAN DAILY INTAKE OF FOOD AND WATER (FROM EUSES)	
Food	**Intake**
Drinking water	2 l/d
Fish	0.115 kg/d
Leaf crops (incl. fruit and cereals)	1.2 kg/d
Root crops	0.384 kg/d
Meat	0.301 kg/d
Dairy products	0.561 kg/d

B) Assessment of the concentrations in intake media (food, water, air and soil)

Currently, the scenario for indirect human exposure cannot take into account exposure from aquatic organisms apart from fish. This is because, to date, an internationally validated bioaccumulation standard test is only available for fish and consumption data on aquatic organisms other than fish are scarce.

A general description of the different relevant exposure routes and guidance for the assessment of the resulting indirect exposure is given in the following sections.

C) Exposure via environmental compartments

Exposure via inhalation of air

This exposure route can contribute significantly to the total exposure for volatile compounds.

The concentration in the intake medium (air) can be calculated using the distribution models of section A.16-2.3.2 of this appendix.

Only the intake scenario chosen has important consequences on the exposure via this route. It is proposed to follow a worst-case, but transparent, scenario: continuous, chronic exposure of humans to the air concentration (which is assumed to be constant). Exposure through inhalation will be summed with exposure via the oral route.

Exposure via soil ingestion and dermal contact

Exposure through these routes is usually very unlikely. Only in cases of extremely polluted soils (e.g. in dump sites or through accidents) can these routes provide significant contributions to the total exposure.

Exposure via drinking water

Drinking water can be obtained from surface water or from groundwater sources. Groundwater can be contaminated through leaching from the soil surface, whilst surface water can be polluted through direct or indirect release of the substance. Hrubec and Toet (1992) evaluated the predictability of the fate of organic substances during drinking water treatment. One of their conclusions was that groundwater treatment, which is generally not intended for removal of organic substances, can be neglected in the assessment. The accuracy of the predicted removal efficiencies for surface water treatment was rather low. This was mainly due to uncertainties in the most effective treatment processes (such as activated carbon filtration).

D) Exposure via food consumption

Assessing concentrations in food products (in this context; fish, leaf crops, root crops, meat and dairy products) in initial or intermediate screening stages usually involves calculation of bioconcentration (BCF) or biotransfer factors (BTF). These are defined as the external exposure (as a concentration or a dose) divided by the internal concentration in the organisms. The use of fixed factors implies a steady-state situation in which the exposure period is assumed long enough to reach a steady-state. Reliable (and relevant) experimental bioconcentration factors should always be preferred to estimated factors.

Bioconcentration in fish

Fish, residing in contaminated surface water, are able to take up appreciable amounts of (especially lipophilic) substances through their gills (or from their food, for which the bioaccumulation factor (BMF) is used). The concentration in fish may be orders of magnitude greater than the concentration in water. The bioconcentration factor (BCF) in fish has been found, for some substances, to be well correlated with the octanol-water partitioning coefficient (Kow), indicating that lipid or fat is the main dissolving medium. Estimating fish-water bioconcentration is more specifically discussed in section A.16-2.2 of this appendix.

Biotransfer from soil and air to plants

Plant products are a major component of the diet of humans and cattle. Uptake of substances in plants will therefore have a significant influence on the exposure of humans via the environment. When trying to predict concentrations in plants there are several important conceptual issues to consider:

- there are hundreds of different plant species forming the heterogeneous group of food crops. Furthermore, varietal differences can also account for large differences in biotransfer rates;
- different tissues from plants are consumed, which may have different biotransfer rates (roots, tubers, fruit, leaves);
- crops differ in their potential for exposure via different routes, for instance, many crops are grown in greenhouses, which limits the potential for biotransfer via aerial deposition;
- substances may biotransfer to crops through uptake from the soil, but also through gas uptake and aerial deposition.

Therefore, based on the consideration above, it is clear that a modelling approach can only give a rough approximation of the concentration of a substance in plants. To account for the variety in plant products, tuberous plants are distinguished from leaf crops. Furthermore, the exposure of plants incorporates both the soil and air routes.

Uptake from soil is, in general, a passive process governed by the transpiration stream of the plant (in the case of accumulation in leaves) or physical sorption (in the case of roots). Uptake into the leaves from the gaseous phase can also be viewed as a passive process, in which the leaves components (air, water, lipids) equilibrate with the air concentration. A general form of steady state partitioning coefficient between these compartments is given by Riederer (1990). Kow and Kaw (the air-water partitioning coefficient) are used to assess the distribution between the air and the plant. The modelling approach of Trapp and Matthies (1995) is used to estimate levels in leaves and roots due to uptake from soil and air.

Biotransfer to meat and milk

Lipophilic substances are known to accumulate in meat, and can be subsequently transferred to milk. Cattle can be exposed to substances in grass (or other feed) with adhering soil, drinking water, and through inhalation of air. Biotransfer factors can be defined as the steady-state concentration in meat, divided by the daily intake of the substance. Travis and Arms (1988) calculated biotransfer factors for cow's meat and milk by log-linear regression on a number of substances (28 for milk and 36 for beef).

Even though the theoretical background is limited, these factors provide a useful tool in risk assessment.

It should be noted that no distinction is made between different milk products like cheese or yoghurt. The concentration in milk is used for all dairy products.

E) Total daily intake for humans

The total daily intake for humans via the environment can be estimated by summing the daily intake rates for each contributing medium.

A.16-2.4 Direct emissions to agricultural soil

A specific model to cover direct releases to agricultural soil is described here. It can be used, for example, for substances used in fertilizer products or as a co-formulant in plant protection products. This scenario is based on EUSES, LET tool[62] (developed by CropLife Europe) and FEE tool[63] (developed by Fertilizers Europe).

A.16-2.4.1 Release and exposure in the atmosphere

When emission to air takes place, i.e. due to volatilisation during spray application, air concentrations need to be estimated.

The exposure estimation is to be carried out as explained in Appendix A.16-2.3.2 with the following differences:

- For the calculation of PECair the averaging time should be 30 days instead of 365 days, due to the reduced number of emission days. This means that in Equation R.16-27 the value 30 should be used instead of 365;
- $PEClocal_{air,annual}$ is therefore replaced by $PEClocal_{air,average}$ (averaged over 30 days);
- For the calculation of the deposition flux, the only release is that from the application ($Estp_{air}=0$ in Equation R.16-29).

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[62] Local Environmental Tool https://croplifeeurope.eu/pre-market-resources/reach-in-registration-evaluation-authorisation-and-restriction-of-chemicals/

[63] Fertilisers Environmental Exposure tool https://www.reachfertilizers.com/

A.16-2.4.2 Release and exposure to soil

A.16-2.4.2.1 Release to the soil compartment

A differentiation is made between arable land and grassland. This differentiation enables the assessment of exposure of humans via the environment in the same systematic way as for the application of sludge on agricultural soil: via the cattle (meat, milk) grazing in grassland and food crops growing on arable soil.

The release to soil from one application is then calculated using the following equation (see also appendix A.16-4.2):

$$Elocal_{soil} = \frac{APPLrate_{year}}{APPL_{number}} \cdot RF_{soil}$$

Equation R.16-71

Explanation of symbols

$Elocal_{soil}$	amount released per hectare in one application	[kg.ha^{-1}]
$APPLrate_{year}$	amount of substance applied to the soil in a year	[kg.ha^{-1}.yr^{-1})]
$APPL_{number}$	number of applications per year	[yr^{-1}]
RF_{soil}	release factor to soil	[-]

A.16-2.4.2.2 Exposure in soil compartment

The default scenario assumes 10 years of application. The calculation of the soil concentration accounts for the removal from soil (volatilisation, leaching, biodegradation and runoff).

The depth of mixing soil should be set as follows:

Arable land:

- With ploughing: 20 cm
- Without ploughing: 5 cm

Grassland:

- 10 cm

(To be noted that for the STP sludge application the soil depth remains 20 cm for arable land and 10 cm for grassland).

The following local concentrations in soil are then calculated.

- For risk assessment for the soil compartment, depending on the type of PNEC[64]
    - *Clocal_soil_initial* (calculated after the last application in the 10th year) or
    - *Clocal_soil_30 days* (calculated over 30 days after the (last) application in the 10th year)

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[64] PNEC_initial if based on the nominal initial test concentration or PNEC_twa if the actual concentration is taken into account in the test. By default it is assumed that the PNEC provided is based on actual concentration.

- For calculation of groundwater concentration as well as for terrestrial secondary poisoning and human exposure via food consumption and drinking water *Clocal_soil_180 days* (calculated over 180 days after the (last) application in the 10th year) is used

Like for the application of sewage sludge to 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 as explained in Equation R.16-57 and R.16-58.

Table R.16-20: Parameters used in the model application on agricultural soil

Type of soil	Concentration calculated	Depth (m)	Used for
Arable land	$Clocal_{soil,initial}$ (calculated after the last application in the 10th year) or $Clocal_{soil,30\ days}$ (calculated over 30 days after the (last) application in the 10th year)	0.2 or 0.05 (when ploughing is used the soil depth should be set to 0.2)	Terrestrial ecosystem, terrestrial secondary poisoning (30d)
Arable land	$Clocal_{soil,180\ days}$ (calculated over 180 days after the (last) application in the 10th year)	0.2 or 0.05 (same as above)	Crops for human consumption, groundwater
Grassland	$Clocal_{soil,180\ days}$ (calculated over 180 days after the (last) application in the 10th year)	0.1	Grass for cattle, groundwater

After one year of application (one or more applications per year) the amount of substance remaining in the soil, taking removal into account between applications, is calculated using the following equation:

$$Elocal_{soil\_1} = Elocal_{soil} \cdot \frac{1 - e^{-Time_{appl} \cdot k \cdot APPL_{number}}}{1 - e^{-Time_{appl} \cdot k}}$$

Equation R.16-72

Explanation of symbols

$Elocal_{soil\_1}$	amount remaining per hectare after one year of application	$[kg.ha^{-1}]$	
$Elocal_{soil}$	amount released per hectare in one application	$[kg.ha^{-1}]$	
$Time_{appl}$	time between applications	[d]	
$APPL_{number}$	number of applications (in 1 year)	[-]	
k	first order rate constant for removal from topsoil	$[d^{-1}]$	Equation R.16-49

The model considers that four days after the last application (on year 10) a runoff event takes place. The runoff is calculated using the following equation:

$$\text{runoff\%} = 100 - 100 \times e^{-30 \cdot ks\_w}$$ **Equation R.16-73**

Where $k_{s\text{-}w}$ (d^{-1})= transfer rate from regional, continental and global soils to the freshwater (estimated in SimpleBox).

The runoff% is bounded: should not be higher than 5% nor lower than 0.5%. If the result of Equation R.16-73 falls outside this range, the runoff% used in subsequent calculations should be 5% (if the calculated value is above 5%) or 0.5% (if the calculated value is below 0.5%). This is to avoid, on one hand, overestimation of runoff (for low Koc) and, on the other hand, avoid an underestimation of the contribution related to erosion (for high Koc).

The runoff is taken into account in the calculation of the initial concentration in soil after 10 years of subsequent application. This is calculated using the following equation:

$$Csoil_{initial} = \frac{Elocal_{soil\_1}}{DEPTH_{soil} \cdot RHO_{soil}} \cdot \frac{100 - runoff\%}{100} \cdot \frac{1 - e^{-365 \cdot k \cdot 10}}{1 - e^{-365 \cdot k}}$$ **Equation R.16-74**

Explanation of symbols

$Csoil_{initial}$	initial concentration in soil after 10 years of subsequent application (taking removal into account)	[$mg.kg^{-1}$]	
$Elocal_{soil\_1}$	released amount at local scale	[$mg.m^{-2}$]	Equation R.16-72*
$DEPTH_{soil}$	depth of mixing soil	[m]	
RHO_{soil}	bulk density soil	[$kg.m^{-3}$]	Equation R.16-1
runoff%	runoff from soil	[%]	Equation R.16-73
k	first order rate constant for removal from topsoil	[d^{-1}]	Equation R.16-49

*Note that Equation R.16-72 result (in $kg.ha^{-1}$) must be converted into $mg.m^{-2}$ in order to be used in this equation

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:

$$Csoil_{T\ days} = Csoil_{initial} \cdot \frac{1 - e^{-k \cdot T}}{k \cdot T}$$ **Equation R.16-75**

Explanation of symbols

$Csoil_{T\ days}$	average concentration in soil over T days	[$mg.kg^{-1}$]	
$Csoil_{initial}$	initial concentration in soil after 10 years of subsequent application (taking account removal)	[$mg.kg^{-1}$]	Equation R.16-74
T	averaging time	[d]	Table R.16-17
k	first order rate constant for removal from top soil	[d^{-1}]	Equation R.16-49

Calculation of $PEClocal_{soil}$

For calculating the PECs, the approach described in Appendix A.16-2.3.6 should be followed, using Equation R.16-75.

A.16-2.4.3 Calculation of concentration in groundwater

The calculation of concentration in groundwater should be carried out as explained in Appendix A.16-2.3.7.

A.16-2.4.4 Release and exposure to surface water

A.16-2.4.4.1 Release to surface water compartment

There are two sources of releases to water:

- Direct release via drift when the application method is spraying
- Indirect release via runoff

The release amount to water from drift is estimated as:

$$Input\_drift = APPL\_eq \times Drift\% \qquad \textbf{Equation R.16-76}$$

Where:

$$APPL\_eq = \frac{APPLrate_{year}}{\mathrm{APPLnumber}}$$

Explanation of symbols

Input_drift	release amount to water from drift	[$mg.m^{-2}$]
APPL_eq	equivalent application rate (single application)	[$kg.ha^{-1}$]
Drift%	release factor to water via drift	[%]
$APPLrate_{year}$	amount of substance applied to the soil per year	[$kg.ha^{-1}.yr^{-1}$)]
$APPL_{number}$	number of applications per year	[yr^{-1}]

In case of application by spraying, the release from drift is taken into account on each application day,.

The input due to runoff from soil is assumed to take place on day four after the last application and is estimated as:

$$\text{Input\_runoff} = \text{Elocal}_{soil} \times \frac{F\_1}{F\_2} \times \text{runoff\%} \times \text{FW\_RATIO}$$ **Equation R.16-77**

Where:

$F\_1\ [-] = 1 - e^{-APPL_{number} \cdot Time_{appl} \cdot \mathrm{k}}$

$F\_2\ [-] = 1 - e^{-Time_{appl} \cdot \mathrm{k}}$

Explanation of symbols

Input_runoff	release amount to water from runoff	[$mg.m^{-2}$]	
$Elocal_{soil}$	amount released per hectare in one application	[$kg.ha^{-1}$]	Equation R.16-71
F1 and F2	factors for removal in soil	[-]	
runoff%	runoff % from soil	[%]	Equation R.16-73
FW_RATIO	Surface ratio of treated field and adjacent water body	[-]	10 (FOCUS)
$APPL_{number}$	number of applications per year	[yr^{-1}]	
$Time_{appl}$	time between applications	[d]	
k	first order rate constant for removal from topsoil	[d^{-1}]	Equation R.16-49

A.16-2.4.4.2 Exposure in water/sediment compartments

The exposure in water takes into account both release via drift (for spraying application only) and runoff and accounts for degradation of the substance in water. The surface water is represented by a ditch surrounding a 1 hectare field (1:10 surface ratio between field and water), with a depth of 30 cm and where the residence time of water is 40 d (Table R.16-8).

The exposure estimation of the surface water concentration (to be used in the risk assessment) is as follows:

1. The concentration in surface water is calculated for each day during 365 days (not an average) taking into account the releases from drift (when applicable) and runoff, as indicated above, dilution in the water body and removal processes in water:

$$Clocal_{water}\,(t) = \frac{\frac{Input\ runoff + Input\ drift}{DEPTHwater} \cdot e^{-kwater \cdot t}}{1 + Kp_{susp} \cdot SUSP_{water} \cdot 10^{-6}}$$ **Equation R.16-78**

Where:

Equation R.16-79

$$kwater = \frac{\ln(2)}{DT50bio\ water\ sed} + \frac{1}{time\ res}$$

Explanation of symbols

$Clocal_{water}(t)$	concentration in surface water at day t	$[mg \cdot m^{-3}]$	
Input runoff		$[mg.m^{-2}]$	Equation R.16-80
Input drift		$[mg.m^{-2}]$	Equation R.16-81
t		[d]	
kwater	first order rate constant for removal from water phase at 12 °C	$[d^{-1}]$	
DT50bio_water_sed	half-life for biodegradation in surface water	[d]	
$Time_{res}$	residence time of water	[d]	40 Table R.16-21
DEPTHwater	water depth	[m]	0.3
Kp_{susp}	solids-water partitioning coefficient of suspended matter	$[l \cdot kg^{-1}]$	Equation R.16-7
$SUSP_{water}$	concentration of suspended matter in surface water (dry weight)	$[mg \cdot l^{-1}]$	15 Table R.16-21

2. The maximum daily exposure value is then identified and is used as the surface water concentration (Clocal) in the risk assessment. That is, the maximum concentration in surface water over 365 days is used in the risk assessment.

For the sediment compartment the equilibrium partitioning method between water and suspended solids (section A.16-2.3.4) is used to calculate Clocal_sed_freshwater from $Clocal_{water}$.

A.16-2.4.5 Secondary poisoning and humans exposed indirectly via the environment

The calculations explained in A.16-2.3.8 and A.16-2.3.9 are applicable also in case of the direct release to agricultural soil other than via sludge, with the differences described below:

- Instead of PECwater, the annual average concentration in surface water is used to estimate fish concentration used for freshwater secondary poisoning and human's consumption of fish:

  Clocalwater,annual = sum of C(t) (calculated for each day for 365 days)/365, with C(t) calculated as explained above.

- The indirect exposure of humans will be considered via the standard humans via environment exposure model taking into account the exposure in the various compartments. However, only groundwater is considered as drinking water, not the surface water from the ditch.

- The concentration in groundwater is calculated for both the arable land and the grassland, and the higher value should be used in the assessment.

Appendix A.16-3 Model for Regional assessment

A.16-3.1 Releases at regional level

All regional releases associated with the different identified uses, both industrial and wide disperse sources, are cumulated to estimate the total regional release (kg/day) to surface water, wastewater, air and soil. The regional releases associated with the different identified uses are based on the tonnage at regional level for each use and the same release factors used at local scale.

By default, the tonnage at the regional level for the industrial settings (i.e. manufacture, formulation and industrial uses) is set equal to 100% of the tonnage at EU level, while for wide dispersive uses it is set equal to 10% of the registrant's supply volume at EU level. Releases at the regional scale are assessed for water, air and soil (including industrial soil). At this scale, direct releases to soil are also considered.

The default regional releases are therefore calculated, for each use, according to the following formula:

$$E_{\text{regional,IU,j}} = Q_{\text{regional daily,IU}} \cdot RF_{\text{IU,j}} \cdot 1\,000$$

Where:

J = environmental compartment (air, soil, wastewater)

$E_{regional,IU,j}$ (kg/day): release rate to the compartment "j" at the regional scale for an identified use (IU);

$Q_{regional\ daily,IU}$ (tonnes/day): average daily use at the regional scale for an identified use (IU) = regional tonnage for each use/365 days;

Regional tonnage for each use (tonnes/year) = 100% × total registrant's tonnage at EU level (for industrial setting);

Regional tonnage for each use (tonnes/year) = 10% × total registrant's tonnage at EU level (for widespread uses);

$RF_{\text{IU, j}}$: Release factor (% or kg/kg) to compartment "j" for identified use. The default value is set by ERCs (see Appendix A.16-1 and *Chapter R.12 of the Guidance on IR&CSA*).

If the registrant has more information (market data), the volume to be used for the regional calculation could be refined.

As stated before, when calculating the total regional releases, by default, 80% (representing the EU average) of the wastewater is assumed to be treated in an STP and 20% to go directly to surface water without any treatment, regardless of the assumptions made about STP connection at local scale.

The formulas to be applied for the calculation of the total regional release to air, surface water, wastewater and soil are the following:

$$E_{total,regional,air} = \sum E_{regional,IU,air}$$

$$E_{total,regional,soil} = \sum E_{regional,IU,soil}$$

$$E_{total,regional,wastewater} = \sum E_{\text{regional,IU,wastewater}} \times 80/100$$

$$E_{total,regional,surface\ water} = \sum E_{regional,IU,wastewater} \times 20/100$$

where:

$E_{total,regional,wastewater}$ passes through an STP and, subsequently, is discharged in surface water.

A.16-3.2 Continental release estimation

As long as the activities related to a specific stage of the life-cycle of a substance can be assumed to take place within a region, as it is often the case for manufacture, formulation and industrial uses, 100% of the whole registrant's tonnage at EU level is attributed to the regional scale.

When activities are more widely distributed over the EU, as is assumed for wide dispersive uses, only a fraction of the whole registrant's tonnage at EU level is attributed to the region (10% by default) while most of it (90% by default) is attributed to the continental scale. Therefore, for these life-cycle stages, releases at continental scale will contribute as a background to the regional concentration.

The continental release for each environmental compartment and for each stage can be calculated multiplying the continental tonnage by the release factor:

Continental release (kg/day) = continental tonnage (tonnes/year) × release factor × 1 000 / 365

where continental tonnage = total registrant's tonnage at EU level – regional tonnage.

The total continental release for each environmental compartment is obtained by summing overall life-cycle stages. If the fraction going to the region is changed in iteration, the continental release will also change.

A continental release estimation is also carried out for PBT substances. In this case, the whole EU-level tonnage is used for each life-cycle stage to estimate the overall releases to the continental scale, due to registered tonnage as a whole.

A.16-3.3 Calculation of PECregional

Regional computations are done by means of multimedia fate models based on the fugacity concept. 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 R.16-6) 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. Several types of fate processes are distinguished in the regional assessment, as drawn in Figure R.16-18:

- release, 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, 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, e.g. deposition, runoff, 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.

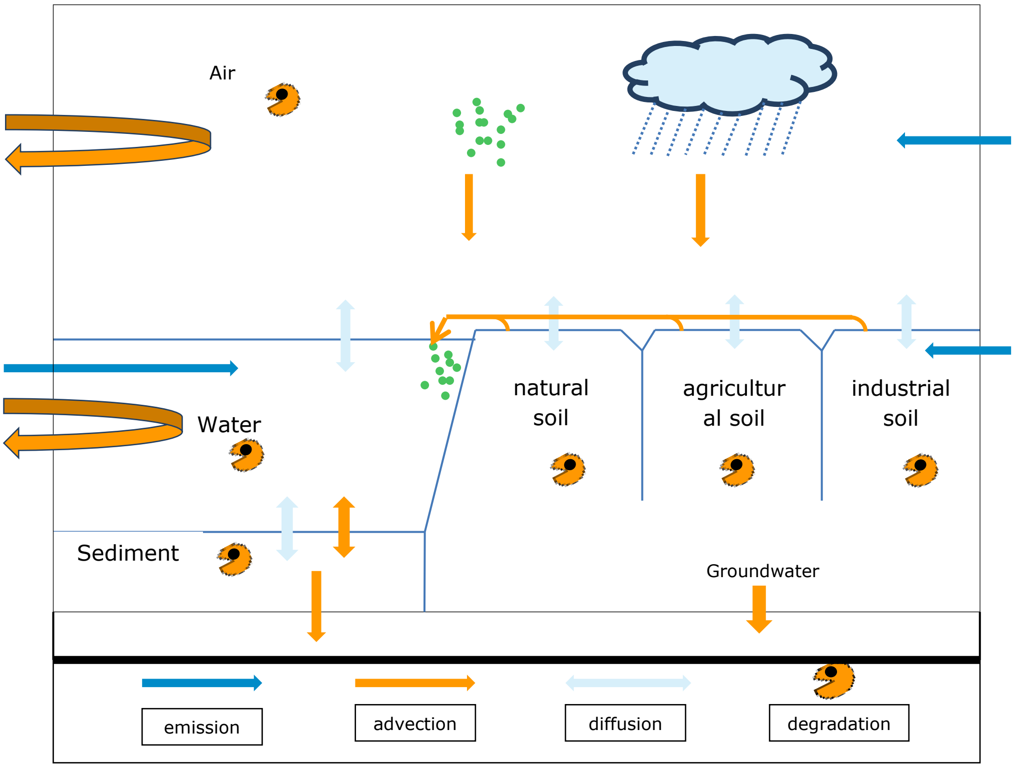

Figure R.16-18: Regional calculations

Substance input to the model is regarded as continuous and equivalent to continuous diffuse release. 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 release 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.

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, an STP connection rate of 80% (the EU average according to data available before the implementation of the Urban Waste Water Treatment Directive and currently used in EUSES) 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 to consider which modelling parameters are chosen and what fraction of the total releases is used as release 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/release 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. The model parameters proposed for this standard region are given in Table R.16-21. 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 R.16-21 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 R.16-21.

Table R.16-21: Proposed model parameters for regional model

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	0.27
area fraction of agricultural soil	0.60
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	3 m·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 (1994), supplemented with data received from Sweden and Finland. Data for Norway and Austria are obtained from the FAO statistical databases (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) 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 river water, 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 R.16-22.

Table R.16-22: Intermedia mass transfer coefficients

INTERMEDIA MASS TRANSFER COEFFICIENTS	
Parameter	**Value**
air-water interface: air side partial mass transfer coefficient (kaw_{air})	Equation R.16-91
air-water interface: water side partial mass transfer coefficient (kaw_{water})	Equation R.16-92
Aerosol deposition rate	$0.001\ m\cdot s^{-1}$
air-soil interface: air side partial mass transfer coefficient ($kasl_{air}$)	$1.05\cdot 10^{-3}\ m\cdot s^{-1}$
air-soil interface: soil side partial mass transfer coefficient ($kasl_{soil}$)	Equation R.16-82
sediment-water interface: water side partial mass transfer coefficient (Ksw_{water})	$2.78\cdot 10^{-6}\ m\cdot s^{-1}$
sediment-water interface: pore water side partial mass transfer coefficient ($Ksw_{pore\ water}$)	$2.78\cdot 10^{-8}\ m\cdot s^{-1}$
net sedimentation rate	$3\ mm\cdot yr^{-1}$

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:

$$\boldsymbol{kasl_{soil} = \left(Veff_{soil} + \frac{Deff_{soil}}{d_p}\right)}$$ **Equation R.16-82**

In undisturbed soil, processes of downward advection (pore water + small particles), diffusion (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 R.16-83**

In which:

$$Veff_{soil} = FRw.soil\frac{RAINRATE\cdot F\inf_{soil}}{Fwater_{soil}} + FRs.soil.\frac{SOLIDadv.soil}{Fsolid_{soil}}$$ **Equation R.16-84**

$$Deff_{soil} = FRa.soil\frac{DIFFgas\cdot Fair_{soil}^{\ 1.5}}{Fair_{soil}} + FRw.soil.\frac{DIFFwater\cdot Fwater_{soil}^{\ 1.5}}{Fwater_{soil}}$$ **Equation R.16-85**

$$+ FRs.soil\cdot\frac{SOLIDdiff.soil}{Fsolid_{soil}}$$

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

Equation R.16-86

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

Equation R.16-87

$$FRa.soil = 1 - FRw.soil - FRs.soil$$

Equation R.16-88

$$DIFFgas = 2.57 \cdot 10^{-5} \sqrt{\frac{18}{MOLW}}$$

Equation R.16-89

$$DIFFwater = 2.0 \cdot 10^{-9} \sqrt{\frac{32}{MOLW}}$$

Equation R.16-90

Explanation of symbols

MOLW	molecular weight of the substance	$[kg_c \cdot mol^{-1}]$	
$kdeg_{soil}$	rate constant for degradation in bulk soil	$[d^{-1}]$	
RAINRATE	average daily rate of wet precipitation	$[m \cdot d^{-1}]$	$1.92 \cdot 10^{-3}$
$Finf_{soil}$	fraction of precipitation that penetrates into the soil	[-]	0.25
d_p	substance-dependent penetration depth	[m]	Equation R.16-83
$Veff_{soil}$	effective advection (with penetrating porewater)	[m]	Equation R.16-84
Deffsoil	effective diffusion coefficient	$[m^2 \cdot d^{-1}]$	Equation R.16-85
FRa.soil	mass fraction of the substance in the air phase of soil	[-]	Equation R.16-88
FRw.soil	mass fraction of the substance in the water phase of soil	[-]	Equation R.16-86
FRs.soil	mass fraction of the substance in the solid phase of soil	[-]	Equation R.16-87
$Fair_{soil}$	volume fraction of air in the soil compartment	$[m_{air}^3 \cdot m_{soil}^{-3}]$	Table R.16-8

$Fwater_{soil}$	volume fraction of water in the soil compartment	$[m_{water}^3 \cdot m_{soil}^{-3}]$	Table R.16-8
$Fsolid_{soil}$	volume fraction of solids in the soil compartment	$[m_{solid}^3 \cdot m_{soil}^{-3}]$	Table R.16-8
$K_{air\text{-}water}$	air-water partitioning coefficient	$[m^3 \cdot m^{-3}]$	Equation R.16-6
$K_{soil\text{-}water}$	soil-water partitioning coefficient	$[m^3 \cdot m^{-3}]$	Equation R.16-8
DIFFgas	molecular diffusivity of the substance in the gas phase	$[m^2 \cdot d^{-1}]$	Equation R.16-89
DIFFwater	molecular diffusivity of the substance in the water phase	$[m^2 \cdot d^{-1}]$	Equation R.16-90
SOLIDadv.soil	rate of advective downward transport of soil particles	$[m \cdot d^{-1}]$	$6.34 \cdot 10^{-12}$
SOLIDdiff.soil	solid phase diffusion coefficient in the soil compartment	$[m^2 \cdot d^{-1}]$	$6.37 \cdot 10^{-12}$
$kasl_{soil}$	partial mass-transfer coefficient at soil side at the air-soil interface	$[m \cdot d^{-1}]$	Equation R.16-82

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 R.16-21).

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:

$$kaw_{air} = 0.01 \cdot (0.3 + 0.2 \cdot WINDSPEED) \cdot \left(\frac{0.018}{MOLW}\right)^{0.335}$$ **Equation R.16-91**

$$kaw_{water} = 0.01 \cdot (0.0004 + 0.0004 \cdot WINDSPEED^2) \cdot \left(\frac{0.032}{MOLW}\right)^{0.25}$$ **Equation R.16-92**

Explanation of symbols

MOLW	molecular weight of the substance	$[kg_c \cdot mol^{-1}]$	
WINDSPEED	average wind speed	$[m \cdot d^{-1}]$	Table R.16-21
kaw_{air}	partial mass-transfer coefficient at the air side of the air-water interface	$[m \cdot d^{-1}]$	Equation R.16-91
kaw_{water}	partial mass-transfer coefficient at the water side of the air-water interface	$[m \cdot d^{-1}]$	Equation R.16-92

PEC regional for the marine environment

The impact of substances on the marine situation that are released from point and diffuse sources over a wider area can be assessed in a similar way as for the freshwater environment.

To assess the potential impacts of multiple point and diffuse sources of substances on the marine environment, a river plume in coastal sea water 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 substances 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 releases 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 releases 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 can be modelled with a multi-media fate model that is used for the freshwater PEC calculations, modified to allow dispersive exchange between the coastal zone to the continental sea water. 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 substances) or more (for substances that react, volatilise or sediment) lower than in river water. The extent of degradation, volatilisation, etc. in this coastal sea scenario is also incorporated in the multimedia model.

The calculation of $PECregional_{seawater}$ according to this standard scenario may be sufficient for generic risk assessment. If additional information is available on sources and releases and site-specific information on the suspended matter concentration, the flow rate and the dispersion velocity, the generic assessment can be made more site-specific by overriding some of the default parameters or can even 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 substances with a 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.

Model parameters for the continental concentration

The continental box in principle covers all 27 EU countries and Norway and similar percentages for water and natural, agricultural and industrial/urban soils as given in Table R.16-21. All other parameters are similar to the ones given in the preceding tables.

Release estimations 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 R.16-18, it is assumed that no inflow of the substance into the continental system takes place. More recent versions of multimedia models also contain 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 substance.

Table R.16-23: Parameters for the continental[65] model

PARAMETERS FOR THE 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	0.27
area fraction of agricultural soil	0.60
area fraction of industrial/urban soil	0.10

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[65] The parameters for the continental model are still based on the current 15 EU Member States and Norway.

Appendix A.16-4 Models for environmental assessment

A.16-4.1 EUSES

EUSES was introduced in section R.16.4.1.2. This appendix provides technical details on the functioning of the model and some of the information needed to run it.

Note that when EUSES is referred to in this guidance this mainly refers to the models for estimating the fate and distribution of the substance in the biological STP and in the environment. EUSES (version 2.1/2.2) also contains a release module which is considered outdate under REACH and is to be replaced by the information contained in this guidance.

EUSES provides calculation of exposure in a standardly defined environment covering all compartments and different scales (local, regional, continental).

Chesar Platform embeds the latest improvement of the EUSES algorithm for the fate and distribution of the substance have their own release modules.

Input

The information necessary to run EUSES is described here below.

For Tier 1 assessments of environmental distribution, the information described in Table R.16-22 should be collected (more information on fate may be needed for metals and metal compound, see Appendix A.7.13-2).

Table R.16-24: Information on substance properties needed for Tier 1 assessment of environmental distribution

Parameter	Description	Source
MOLW	Molecular weight	Technical dossier – chapter 1.1
MP	Melting point of substance	Technical dossier–chapter 4
BP	Boiling point of substance	Technical dossier–chapter 4
VP	Vapour pressure of substance	Technical dossier–chapter 4[66]
SOL	Water solubility of substance	Technical dossier–chapter 4
K_{OW}	Octanol water partition coefficient of substance (not relevant for inorganics)	Technical dossier–chapter 4
Biodegradability	Results of screening test on biodegradability. Not relevant for inorganic substances.	Technical dossier–chapter 5 See also Appendix A.16-2.2
Koc	Organic carbon water partition coefficient	Technical dossier–chapter 5

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[66] The Vapour pressure is not provided for metals in technical dossier. However, registrants of metals compounds should introduce a fictitious (very low) Vapour Pressure in the Tier I algorithms as described here to correctly estimate exposure.

Parameter	Description	Source
		See also Appendix A.16-3.2
BCF (aquatic)	Bioaccumulation factor for aquatic organisms	

In addition to the substance properties, information on releases of the substance from each use (each contributing activity for the environment) is needed to carry out the exposure estimation. The parameters required are listed in the table below.

Parameter	Description	Source
$E_{local,j}$	Daily and annual local release to the release route j (j: (waste)water, air, soil) for a given contributing scenario	Release estimation based on use scenario See Section R.16.2
STP	Sewage Treatment Plant (STP) setting. STP Yes/No (default=Yes); Application of STP to agricultural soil Yes/No (default=Yes); STP flow rate (default=2000m3/day)	Biological Sewage Treatment Plant See Section R.16.3
Regional $Release_j$ by use	Regional release from use to the release route j (j: (waste)water, air, soil)	Release estimation based on exposure scenario See Section R.16.2

The following table gives an overview of additional substance property data used as input for EUSES exposure estimation. When not available specifically for the substance, these values are calculated automatically by EUSES.

Table R.16-25: Substance information for refined assessment

Parameter	Description	Source
Kpsoil	Soil-water partition coefficient. As a default, EUSES calculates the parameter from Koc. For inorganic substances however, Kpsoil should be measured directly, because other sorption mechanisms, like sorption to mineral surfaces play in important role. See also Appendix A.16-2.2	Technical dossier– chapter 5. See also Appendix A.16-2.2
Kpsed	Sediment-water partition coefficient. As a default, EUSES calculates the parameter from Koc. For inorganic substances however, Kpsed should be measured directly, because other sorption mechanisms, like sorption to mineral surfaces play in important role. See also Appendix A.16-2.2	Technical dossier– chapter 5. See also Appendix A.16-2.2
Kpsusp	Solids-water partition coefficient in suspended matter. As a default, EUSES calculates the parameter from Koc. For inorganic substances however, Kpsusp should be measured directly, because other sorption mechanisms, like sorption to mineral surfaces play in important role. See also Appendix A.16-2.2	Technical dossier– chapter 5. See also Appendix A.16-2.2
kdegsoil kdegsed	Total rate constant for biodegradation in bulk soil and sediment. In Tier 1 estimated from screening tests on biodegradation.	Technical dossier– chapter 5. See also Appendix A.16-2.2
$DT50hydr_{water}$	Half-life for hydrolysis in water at the temperature of the data set	Technical dossier– chapter 5. See also Appendix A.16-2.2
$DT50photo_{water}$	Half-life for photolysis in water at the temperature of the data set	Technical dossier– chapter 5. See also Appendix A.16-2.2
DT50air	Half life for degradation in air at the temperature of the data set	Technical dossier– chapter 5 .See also Appendix A.16-2.2

In particular, the Henry’s Law constant (HENRY), the octanol-water partitioning coefficient (Kow) and the first order rate constant for biodegradation ($kbio_{stp}$) can be used to refine the input into the STP calculations.

Output

The output of EUSES consists of the predicted environmental concentrations (PECs) for environmental risk assessment (see Table R.16-26). EUSES can prepare an electronic report of all the input and output data in a Word or Excel format.

1 **Table R.16-26: EUSES – output: Predicted environmental concentrations, PECs**

EUSES – OUTPUT: PREDICTED ENVIRONMENTAL CONCENTRATIONS, PECS		
Parameter	**Description**	**Destination**
PECstp	Concentration in the aeration tank of the sewage treatment plant	Assessment of whether the substance may inhibit processes in the STP
$PEClocal_{air,ann}$	Annual average local PEC in air (total)	Assessment for indirect exposure of humans (inhalation)
$PEClocal_{water}$	PEC in surface water during episode	Assessment for freshwater
$PEClocal_{water,ann}$	Annual average local PEC (dissolved)	Input to assessment for secondary poisoning
$PEClocal_{seawater}$	PEC in marine water during episode	Assessment for marine water
$PEClocal_{seawater,ann}$	Annual average local PEC in marine surface water (dissolved)	Input to assessment for secondary poisoning
$PEClocal_{sed}$	PEC in sediment	Assessment for freshwater sediments
$PEClocal_{sed,seawater}$	PEC in marine sediment	Assessment for marine water sediments
PEClocal.arableland,30	Local PEC in arable land (total) averaged over 30 days	Assessment for terrestrial environment
PEClocal.arable land,180	Local PEC in arable land (total) averaged over 180 days (to calculate concentration in crops)	Input to assessment for secondary poisoning Input to assessment for indirect exposure of humans
PEClocal.grass,180	Local PEC in grassland (total) averaged over 180 days	Input to assessment for secondary poisoning Input to assessment for indirect exposure of humans
$PECreg_{water,tot}$	Regional PEC in surface water (total)	Assessment for fresh water (regional contribution to local PEC)
$PECreg_{seawater,tot}$	Regional PEC in seawater (total)	Assessment for marine water (regional contribution to local PEC)
$PECreg_{air}$	Regional PEC in air (total)	Assessment for indirect exposure of humans (inhalation, regional contribution to local PEC)
$PECreg_{arableland}$	Regional PEC in arable land (total)	Input to assessment for secondary poisoning Input to assessment for indirect exposure of humans
$PECreg_{natural}$	Regional PEC in natural soil (total)	Assessment for terrestrial environment (regional contribution to local PEC)
$PECreg_{ind}$	Regional PEC in industrial soil (total)	
$PECreg_{sed}$	Regional PEC in sediment (total)	
$PECreg_{sed,seawater,}$	Regional PEC in seawater sediment (total)	

2

Boundary to EUSES

Although EUSES has been mainly developed for organic substances, it is possible to use it for a wide range of substances, including inorganic and metals. However, some exception should be mentioned:

- For certain substance properties, the EUSES exposure calculation is uncertain or is not provided at all (out of boundary of the tool):
    - In case the molecular weight is ≥ 700 g/mol, the concentration in the aquatic food chain and for humans via environment cannot be calculated.
    - If the log Kow>8, the parameter is considered to be outside the boundaries of the QSAR model for terrestrial bioaccumulation. Therefore, not reliable prediction for secondary poisoning can be made.
- For certain chemicals, some EUSES submodel is not suitable and therefore no reliable exposure can be estimated:

For example, for metals and more in general for inorganics, Kow is not provided; for environmental exposure, this absence can be compensated by providing the bioaccumulation factor (BCF) and the different partitioning coefficient between water and soil, sediments and suspended matter. However, Kow is also a key parameter to calculate exposure in the food basket, and therefore for these chemicals indirect exposure to humans cannot be calculated by EUSES.

A.16-4.2 Other exposure estimation tools

There is a wide range of exposure estimation models which can be used to simulate fate and distribution of substances among the different environmental compartments. These models vary in their complexity and purposes.

Other models have been developed for other purposes, for example for better describing the local environment where the releases take place for specific uses. These models demand expert knowledge to operate them, a characterization of the environmental compartment where they are applied and a high level of detail. However, they provide a more accurate estimate of environmental concentrations for specific use scenarios.

CropLife Europe LET (co-formulants in pesticides)

In order to assess local exposure estimation following from releases of co-formulants of pesticides to agricultural soil and to edge of field water bodies via spray drift and runoff/drainage, CropLife Europe has developed the Local Environment Tool (CLE LET) which is freely available at https://croplifeeurope.eu/pre-market-resources/reach-in-registration-evaluation-authorisation-and-restriction-of-chemicals/.

The CLE LET is a spreadsheet which calculates a local-scale exposure for all REACH relevant environmental compartments (including soil and surface water and secondary poisoning via the food chain). Conceptually, a treated 1 ha agricultural field with an adjacent shallow waterbody is simulated. Specifically, the LET uses the calculations described in the REACH R.16 (2012) guidance, as well as the "Step 2" calculation approach for surface water devised by the Forum for the Co-ordination of pesticides fate models and their use (FOCUS, 2003, see below).

Regional concentrations, taking into account all the uses of the substance, should be calculated outside the LET with appropriate tools (e.g. ECETOC TRA, EUSES in Chesar Platform etc), and can be imported into LET. In the LET the local and regional exposure estimates are combined.

Chesar Platform implements a model for exposure and risk assessment of direct releases to agricultural soil, which is based on the CLE LET and on the FEE tool (developed by Fertilizers Europe).

The calculation approach for the local scale is illustrated below:

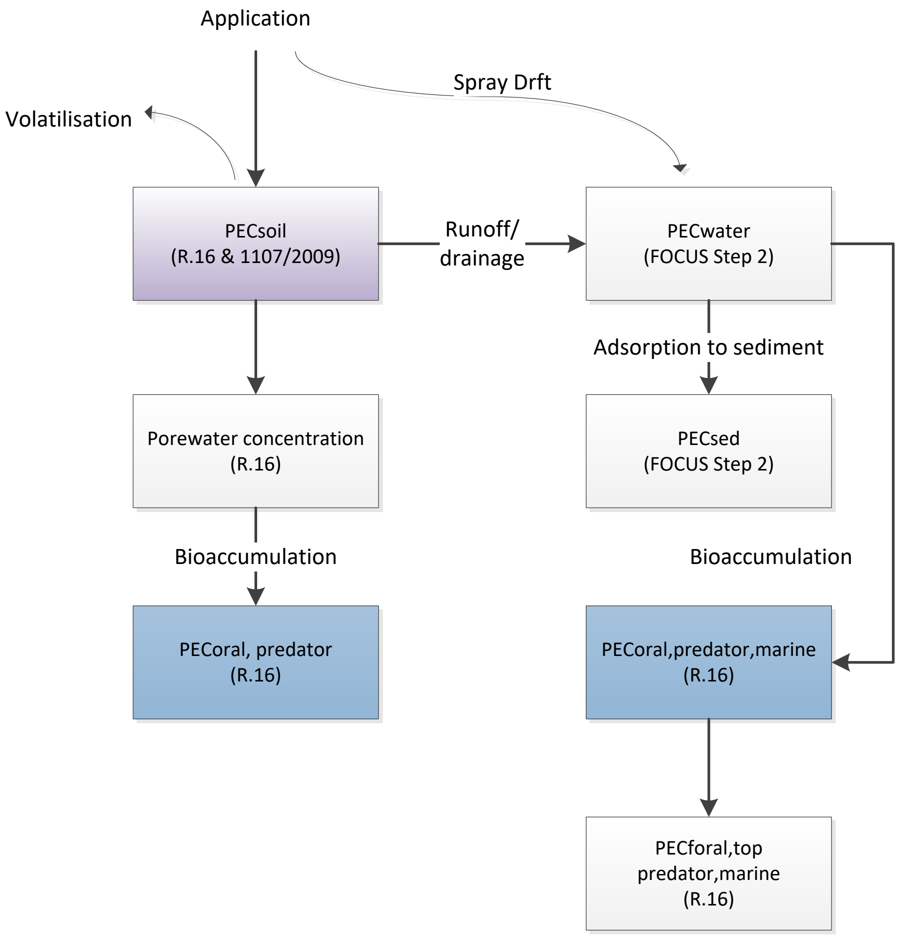

Figure R.16-19: The CLE LET Model concept

This scenario design is closely analogous to the established Tier 1 scenario used in the assessment of plant protection product active substances. It is considered to be a more appropriate representation of co-formulant uses than the industrial or municipal local settings implemented in the standard REACH models[67].

FOCUS (pesticides)

FOCUS is an abbreviation for FOrum for the Co-ordination of pesticide fate models and their USe. The organisation is an initiative of the European Commission to harmonise the calculation of predicted environmental concentrations (PEC) of active substances of plant protection products (PPP) in the framework of EU Directive 91/414/EEC.

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[67] See also https://setac.onlinelibrary.wiley.com/doi/10.1002/ieam.4755

FOCUS has recommended a number of models to be used for soil and ground water exposure estimation:

- MACRO,, PEARL, PELMO, PRZM_GW

and for surface water exposure estimation:

- STEPS1-2, which is a model that predicts PECs for surface water and sediment in European Tier 1 and 2 assessments of plant protection products based on harmonised scenario definitions;

- SWASH, which is a software shell used to perform Tier 3 and 4 European harmonised exposure modelling of pesticide applications to the surface water and sediment compartments. SWASH software includes a substance characteristics database (SPIN), spray drift calculations, soil drainage (MACRO), run off (PRZM) and surface water (incl. sediment) fate (TOXSWA) models.

More information on FOCUS is available at https://esdac.jrc.ec.europa.eu/projects/focus-dg-sante.

CHARM (Offshore platforms)

In order to assess releases from offshore platforms, the CHARM model (see Figure R.16-20) can be an alternative to EUSES in Chesar Platform for this specific use.

CHARM has been developed for screening level risk assessment of offshore substances, e.g. “drilling” and “production” chemicals or “completion/workover”. Since offshore drilling and production of oil and gas may result in environmental effects, it was decided to control the use and discharge of substances in the North Sea OSPAR area. Some of the participating countries within the framework of the Oslo and Paris Conventions agreed upon the development of a Harmonised Mandatory Control System (PARCOM Decision 96/3, now OSPAR Decision 2000/2). In this Control System, CHARM is referred to as a model for priority setting of substances.

The exposure estimates obtained with CHARM may be used within a REACH assessment for offshore uses. Long term exposure of persistent and bioaccumulative substances and inorganic substances cannot be assessed by CHARM.

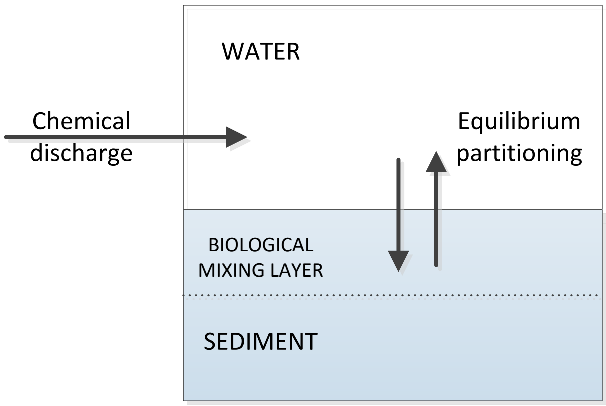


Figure R.16-20: The CHARM model

Most of the calculations within CHARM concern the estimation of the concentration of a substance in the waste stream, and different models are used depending on the process for which they are used, the amount of the substance, its partitioning characteristics, the oil (or condensate) and water production at the platform, the in-process degradation mechanisms and the residence time before release. Within CHARM the offshore environment is divided into two compartments: water and sediment. This is done in order to acknowledge the fact that a substance present in the environment will partition between the water and organic matrix in the sediment. The concentration of a substance may, therefore vary greatly from one compartment to another. Consequently, two PEC values are calculated: PECwater and $PEC_{sediment}$. For further details see https://eosca.eu/software/.

Appendix A.16-5 Release from articles

This appendix describes how to assess releases to and exposure of the environment from substances in articles which are produced or imported. Substances in articles can be assessed:

- as a part of the life cycle stage of a *substance* to be registered (Article 6);
- as a part of a registration for substances in articles in case *substances in the article* are intended to be released (Article 7.1 of REACH);
- if the Agency has grounds for suspecting that a substance in an article could be released and that this poses a risk (Article 7(5)). See the *Guidance on requirements for substances in articles* for details and definitions.

A.16-5.1 General work flow

Exposure estimation for substances in articles is structured by a general workflow. This is meant to streamline the process but it can be adapted according to the available information or tools.

1. Document the available information on the quantity or number of articles that are produced, imported and used, and the quantity of the substances incorporated in the articles. Consider that articles that are produced, and emissions of substances from these articles, can potentially accumulate in society over the service life of the article (see A.16-5.4). Consider the current measures to control the risk of substances in articles.
2. Consider the emission pathways (see section A.16-5.2). In general, the applicable life-cycle stages are ‘use’ and ‘service-life’. Service life relates to the use of an article containing the substance over a period of >1 year. Such activities include, for example, wear and maintenance of textiles, use and maintenance of vehicles or sport articles, etc.
3. Consider an exposure estimation strategy (see section A.16-5.3). Estimate release to the environment (see A.16-5.4) using the appropriate equations and tools described in section R.16.2. The categories applied for the description of uses can support tier 1 exposure estimates (see *Chapter R.12*). For environmental exposure, use can be made of the environmental release categories (ERCs, see *Chapter R.12* and Appendix A.16-1).
4. Environmental Tier 1 release estimates, whether derived from applying the ERCs or the equations in section A.16-5.4, are used as an input into calculating predicted environmental concentrations (PECs), as described in Appendix A.16-2, using the appropriate tools.
5. Based on the risk characterisation, define the operational conditions (OCs) and risk management measures (RMMs) that ensure control of risks for release of substances from articles for humans or the environment for inclusion in the exposure scenario. This could include product integrated RMMs that influence release or migration from the article, or recommendations of specific concentrations or migration limits.

A.16-5.2 Emission and exposure pathways

Emissions can in principle come from virtually any article. Emissions can be classified into four different groups:

- Release into surrounding air (by evaporation)
- Release into surrounding water (leaching)

- Release into surrounding solid material (by diffusion)
- Release in the form of material particles to various surroundings (e.g. due to wear and tear).

In the first three groups, the substance is emitted in molecular form. In the fourth group, the substance is emitted in the form of particles of material. It is assumed that the particles have the same composition as the original material.

The following questions will be helpful in determining the relevant environmental exposure pathways during use and handling of the article:

- Is the substance released intentionally from the article?
- Is evaporation of substances from the article matrix likely?
- Is leaching to (ground)water and redistribution to soil/sediment possible?
- Is particle abrasion or loss of particles likely at any stage?
- How are articles handled in the waste stage and does this lead to releases?

A.16-5.3 Release and exposure estimation for the environment

A.16-5.3.1 General considerations

To calculate exposure for the environment, the estimated loading of the environment is calculated from release rates and the tonnage of the substance contained in the articles. Subsequently, the calculated or measured overall emission is treated as any other environmental emission in the current exposure estimation.

The emissions during service life are considered to be diffuse emissions and are treated as widespread uses. Emission is greatly influenced by the total quantity of the article. If an article has been in use for a prolonged period of time, with a relatively constant consumption (with regard to volumes and areas of use), the maximum cumulative quantity has had time to become established.

At this stage, the annual quantity removed (by waste incineration, degradation etc.) is just as high as the quantity added annually. Then the chemical flow in society has reached an overall equilibrium (steady state). The cumulative quantity can be estimated in a simplified manner by multiplying the quantity added each year by the residence time of the chemical in years. Release into the environment (air, water, soil and indirectly, sediment) is calculated from the emission rate, the weight of the article(s) and the service life of the article.

A usual Tier 1 screening taking the service life of the article into account is to assume a constant release rate over time, called 'emission factor' [%] (Fservice life$_{\text{comp}}$) if the surface area is not the controlling factor for release:

$$\mathrm{Rtot}_{\mathrm{comp}} = \mathrm{F}_{\mathrm{comp}} \cdot \mathrm{Atot} \cdot \mathrm{Fc}_{\mathrm{article}} \cdot T_{SL\_article}$$

Equation R.16-93

Explanation of symbols

$Rtot_{comp}$	annual total release of the substance to a certain environmental compartment (comp) over the service life of the products at steady state	[kg/yr]
F_{comp}	annual emission factor to a certain environmental compartment [%] (estimated or measured)	[-]
Atot	yearly total input of the articles	[kg/yr]
$Fc_{article}$	weight fraction of substance in article	[-]
$T_{SL\_article}$	service life of articles	[yr]

This calculation can be repeated for each relevant environmental compartment. Note that the emission factor to each environmental compartment can be different depending on the properties of the substance and the article matrix. Losses of substances due to loss of particles (abrasion, wear and tear) can also be calculated in this way by defining a) an emission factor from the particles, and b) a separate particle loss fraction in addition [%].

An alternative method of estimating the emission from articles over their service life is to assume that the emission is directly proportional to the surface area of the objects exposed to water (leaching) or air (volatilisation). This approach needs area emission factors (F_{area} [mg.m^{-2}.year^{-1}]). If such emission factors are known or can be estimated for a substance in an article, the emissions of the substance can be estimated as follows:

$$\mathrm{Rtot\_Subst_{comp}} = F_{area,camp} \times Area_{article} \times T_{SL\_article}$$

Equation R.16-94

Explanation of symbols

$Rtot\_Subst_{comp}$	annual total release of the substance to a certain environmental compartment (comp) over the service life of the products at steady state	[kg.yr^{-1}]
$F_{area,\ comp}$	annual emission factor to an environmental compartment (comp) on an article- area basis	[kg.m^{-2}.year^{-1}]
$Area_{article}$	annual emitting surface area	[m^{2}.yr^{-1}]
$T_{SL\_article}$	service life of articles	[yr]

The relevant ERCs can be adapted for service life by applying Equation R.16-93 or Equation R.16-94 to the emission factors in the ERCs.

More detailed calculations of emissions from articles can be performed by using the equations in the next sections. This process is simplified by using the ERCs as described in Appendix A.16-1 and section R.16.2 for the relevant process and article category that is applicable to the articles.

The steps are explained in more detail in the next sections:

1. Estimate the service life of the article.
2. Consider the emission type (molecular and/or particulate).

3. Estimate emission factors for the substance from the actual material (e.g. fraction/tonne or mg.m^{-2} surface area). If emission data are missing:
    - Compare with similar articles described in ESD's or other sources;
    - Search for data in the literature;
    - Use a worst-case assumption or if necessary perform an emission study, leaching study etc.
4. Calculate the total releases of substance from articles at a steady state.
5. Calculate the regional releases representing a densely populated area.

A.16-5.3.2 Detailed release estimation for service life

Considerations

Although not required by the legislation, manufacturers, importers or article producers may want to know what their portion of the total market volume contributes to the overall release and whether there is any probability that a substance evaluation under REACH may conclude that additional risk management is needed. Hence, article producers may want to use the total EU market volume for their substance in their calculations.

Although not explicitly required, manufacturers, importers or article producers may want to know whether their market volume stocks up a base-line release from articles accumulated in society over the past. They can take account of this in using the default release rates referring to the whole service life as an annual release rate (see "steady state" concept later in this section).

Input data

Substance emissions during service life are assessed as widespread uses. It is assumed that the emissions homogenously disperse in the environment over time and that local emission at local scale happens via the municipal STP of a standard town. Hence, producers need different types of information:

1. Article types in which their substance is used; and

2. The average service life of these products;

3. The fraction of the marketed volume used in certain product types;

4. An emission factor (release rate) per year. In a Tier 1 assessment, a default emission factor can be used based on the ERCs (see section R.16.2). Specific information can be used to substitute the defaults, e.g. based on models (for example, for packaging materials) or based on testing.

Estimate the service life of the article

A list of examples for service life spans and release factors taken from the emission scenario document on plastic additives is presented in Table R.16-27. For an overview of available emission scenario documents, see references in section R.16.2.3.3.

Table R.16-27: Example of service life and release factors (per year) for polymer articles

Article type	Typical service life time	Release factor for a plasticizer, medium volatility	Release factor for a flame retardant or a stabiliser
Packaging materials, articles used in agriculture	1		
Sports articles, plastic used in electric devices	2 to 5 years		
Furniture, household appliances (e.g. refrigerator)	5 to 10 years		0.05% per year
Plastic used in electronic devices, cars, construction materials	10 to 20 years	0.16% per year	
Tyres	5 years		

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 estimation (see considerations made in section R.16.2.3.4).

Consider the emission type (molecular and/or particulate)

There are several mechanisms for diffuse emission such as evaporation, leaching, corrosion, abrasion and weathering effects. An additional release route that is important in some cases 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. However, in the absence of more detailed data concerning adsorption/bioavailability/persistence, the substance content in small particles can be handled as if it was distributed in molecular form.

For the molecular emission of additives from long-life materials, the emission can normally be expected to be highest in the beginning of the use period (due to diffusion mechanisms). The opposite situation occurs for solid metal products where the particle emission can be expected to be highest at the end of the use period. It is necessary to be aware that the emission factors are normally an average for the whole service life.

Emission factors

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 (i.e. fraction.tonne^{-1} or kg.m^{-2} surface area).

The emission factors are driven by the following main characteristics of the substance, the article and the environment:

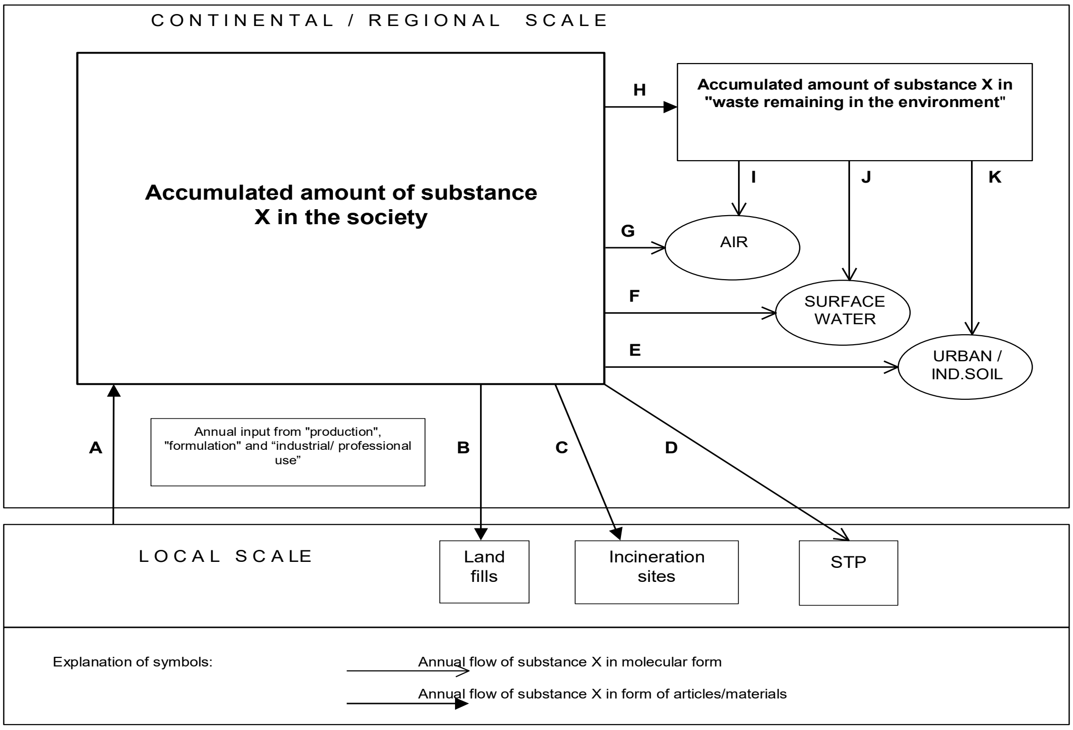
- geometric form of the material determining the content-to-surface-ratio;
- the chemical-physical properties of the substance (e.g. water solubility, vapour pressure);

- the environment of use (weathering, eroding forces, heat);
- the interaction between the matrix and the substance.

In particular, the geometric form of the finished material and the interaction between substance and matrix is difficult to predict for the producers of the substance, without having detailed knowledge on the type of article. Here they have to rely on conservative default assumptions in the ERCs (see section R.16.2) or emission scenario documents as, for example, available for plastic materials.

Calculate the total releases of substance

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 Figure R.16-21).



(A = B + C + D + E + F + G + H for society;

H = I + J + K for "waste remaining in the environment").

Figure R.16-21: Emissions from long-life articles at steady state

Releases from waste remaining in the environment (H) will also contribute to the total releases. Further details on emissions from the waste stage are given in *Chapter R.18*.

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:

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

Equation R.16-95

and:

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

Equation R.16-96

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

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

Equation R.16-97

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 16-84 to 16-85) can be simplified as:

$$RELEASEtot\_steadystate_{i,j,k} = F_{i,j} \cdot Qtot_k \cdot Tservice_k$$

Equation R.16-98

$$RELEASEtot\_steadystate_{i,total,k} = F_{i,total} \cdot Qtot_k \cdot Tservice_k$$

Equation R.16-99

$$Qtot\_accum\_steadystate_k = Qtot_k \cdot Tservice_k$$

Equation R.16-100

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)
$RELEASEtot\_steadystate_{i,j,k}$	annual total release during life-cycle state i to compartment j at steady state for product k	[tonnes·yr^{-1}]	
$RELEASEtot\_steadystate_{i,total,k}$	annual total releases during life-cycle state i 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
$Qtot\_accum\_steadystate_k$	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 R.16-104
2) Alternatively use Equation R.16-105

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 R.16-21) can be written as (assuming no degradation within the article):

$$QWASTEtot\_steadystate_k = Qtot_k - RELEASEtot\_steadystate_{i,total,k}$$ **Equation R.16-101**

Explanation of symbols

$QWASTEtot\_steady\ state_k$	total quantity of the substance in product k ending up as waste at steady state	[$tonnes \cdot yr^{-1}$]	
$Qtot_k$	annual input of the substance in product *k*	[$tonnes \cdot yr^{-1}$]	data set
$RELEASEtot\_steady\ state_{i,total,k}$	annual total releases during life-cycle stage i to all relevant compartments at steady state for product *k*	[$tonnes \cdot yr^{-1}$]	Equation R.16-96 Equation R.16-99

Calculate the regional releases

Using a 10% default (which can be substituted with any other percentage if indicated by e.g. market survey data) the annual regional release from article k to compartment j and for the total of all compartments can be calculated as:

$$RELEASEreg\_steadystate_{i,j,k} = RELEASEtot\_steadystate_{i,j,k} \cdot 0.1$$ **Equation R.16-102**

and:

$$RELEASEreg\_steadystate_{i,total,k} = RELEASEtot\_steadystate_{i,total,k} \cdot 0.1$$ **Equation R.16-103**

Explanation of symbols

RELEASEreg_steady $state_{i,j,k}$	annual regional release during life-cycle i to compartment *j* at steady state for product *k*	[tonnes·yr^{-1}]	
RELEASEreg_steady $state_{i,total,k}$	annual regional release during life-cycle i to all relevant compartments at steady state for product *k*	[tonnes·yr^{-1}]	
RELEASEtot_steady $state_{i,j,k}$	annual total release during life-cycle i to compartment *j* at steady state for product *k*	[tonnes·yr^{-1}]	Equation R.16-98
RELEASEtot_steady $state_{i,total,k}$	annual total release during life-cycle i to all relevant compartments at steady state for product *k*	[tonnes·yr^{-1}]	Equation R.16-96 Equation R.16-99

These regional diffuse releases are then added to the regional emissions calculated from non-diffuse emissions ($Eregional_j$).

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 R.16-104

and:

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

Equation R.16-105

Explanation of symbols

$F_{i,j}$	fraction of tonnage released per year (emission factor) during life-cycle stage *i* (service life) to compartment *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*	$[kg \cdot dm^{-3}]$	data set
$EMISSIONarea_{i,j,k}$	annual amount of substance emitted per area from product *k* to compartment *j*	$[g \cdot m^{-2} \cdot yr^{-1}]$	data set
$EMISSIONarea_{i,total,k}$	annual total amount of substance emitted per area from product *k*	$[g \cdot m^{-2} \cdot yr^{-1}]$	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 Equation R.16-101 and Equation R.16-102 above are used.

If the emission is expected to be independent of the remaining amount of the substance in the product, e.g. corroding metals, the simplified Equation R.16-104 and Equation R.16-105 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 contribute to the regional releases (see above equations). However, the emissions from indoor uses can be released to wastewater and therefore be regarded as a point source (stream D in Figure R.16-21).

Outdoor uses may also cause releases to STP if the storm water system is connected to the STP. This is considered in the general approach of widespread uses as described in section R.16.2.

A.16-5.4 Refined exposure estimation

A.16-5.4.1 Release rates of substances from articles

For more specific calculations, e.g. on losses during service life, calculations of the release rate of a substance from an article may be needed. The release rate may be constant, or change over time. This depends on the function of the article and the properties of the substance and the article matrix in which it is contained.

For screening purposes, simple worst-case assumptions may be sufficient. The producers or importers of articles that contain substances intended to be released should have more detailed, relevant information on estimating the release rate and the total amount released from their articles.

Two main possibilities are distinguished:

- The release is controlled by the user of the article (e.g. release of ink from a pen) and therefore dependent on use frequency and use time per event. The release is constant over the time of use to ensure its function.
- The release is controlled by the matrix of the article, e.g. scented objects. The release is declining over time because the total amount of substance in the object declines over time (usually approximated by first-order release kinetics).

The release rate of a substance from an article can be expressed on a weight basis ($mg.kg^{-1}.d^{-1}$) or on a surface basis ($mg.m^{-2}.d^{-1}$), depending on the type of substance and use characteristics of the object. Release rates can be:

- Based on worst-case assumptions, e.g. all substance contained in the article is released (almost) instantaneously, or released over a period of time representing the service-life, etc. This can be useful for screening purposes.
- Modelled using appropriate software.
- Measured under the relevant conditions.

For some classes of articles, release rates are given in relevant OECD emission scenario documents (e.g. on plastic additives; OECD 2004).

Appendix A.16-6 Selection of measured data

When measurements are available, to be used in release and exposure estimation, (normally in combination with modelled estimates) they have to be assessed first. The following aspects should be considered:

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

Registrants 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 R.16-28 (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.

Note that a general introduction to the use of measured data can also be found in Part D.5.2.

Table R.16-28: Quality criteria for use of existing measured data (based on OECD, 2000)

QUALITY CRITERIA FOR USE OF EXISTING MEASURED DATA (BASED ON OECD, 2000)		
Study category		
Criteria	1 Valid without restriction – may be used for measured PEC	2 Valid with restrictions - May be used to support Exposure estimation (difficult data interpretation)
What has been analysed? 1)	required	required
Analytical method 2)	required	required
Unit specified 3)	required	required
Limit of quantitation 4)	required	required
Blank concentration 5)	required	optional
Recovery 6)	required	optional
Accuracy 7)	required	optional
Reproducibility 8)	required	optional
Sample collection 9)	required	optional
One shot or mean 10)	required	required
Location 11)	required	required
Date dd/mm/yy 12)	required	Minimum is knowledge of year
Compartment characteristics 13)	required	optional
Sampling frequency and pattern	required	required
Proximity of discharge points 14)	required	required
Discharge emission pattern and volume 15)	required (for local scale)	required (for local scale)
Flow and dilution or application rate	required (for local scale)	required (for local scale)
Treatment of measurements below the limit of quantification	required	required

Notes to

Table R.16-28:

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 as to 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 substance. 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 substance under study is released as a discontinuous emission showing variations in both volume and concentration with time.

A.16-6.1 Quality of the sampling and analytical techniques

A quality check should be performed for both sampling and analytical techniques. The applied sampling techniques (e.g. use clean and appropriate containers to avoid contamination of the sample), sample shipping and storage, sample preparation for analysis and analysis must take into account the physico-chemical properties of the substance (e.g. the substance may degrade in presence of light, oxygen, may be volatile, etc.). For further information, see EC, 2009a. Measured data that are of insufficient quality should not be used in the release and exposure estimation.

A.16-6.2 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.

For the purpose of risk assessment, there are 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 the release should be used to describe the local scenario, while samples taken at larger distances may represent the regional concentrations.
- Whether the data are appropriate and relevant for the scenario being investigated i.e. is there sufficient information on RMMs and OCs that were in place when measurements were performed.

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, data that is too old 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 90th percentile if the distribution function has only one mode), and the required 90th percentile values, mean or median values of this distribution could be used in the PEC prediction. The mean of the 90th 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 90th 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 (Appendix A.16-2.3).

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 high quality concerning a list of pollutants are available in the European Pollutant Release and Transfer Register (E-PRTR)[68].

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 of whether or not production/import of the substance is in a 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 a steady state and the accumulation is ongoing, only a calculated PEC will represent the future situation. This should be considered when comparing such a PEC with measured data representing 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:

Location	Substance	Concentration	Period	Remark	Reference
Country Location	substance or metabolite	Units: [µg/L], [ng/L] [mg/kg], etc. Data - mean - average - range - percentile - daily - weekly - monthly - annual - etc.	month, year	limit of quantitation (LOQ) relevant information on analytical method analytical quality control Number of measured values and number of values above the LOQ.	Literature reference

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[68] https://environment.ec.europa.eu/topics/industrial-emissions-and-safety/european-pollutant-release-and-transfer-register-e-prtr_en .

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.

A.16-6.3 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
- an 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[69] (EC, 1999; US-EPA (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.

A.16-6.4 Treatment of measurements below the limit of quantification

A commonly encountered problem when working with monitoring data is the use of concentrations below the limit of quantification (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 an adequate method of analysis for the substance or if the substances are toxic in extremely low concentrations, one approach that could be considered would be to use a

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[69] For example, the following approach may be used: $\boldsymbol{log(X_i) > log(p_{75}) + K(log(p_{75}) - log(p_{25}))}$
Where Xi 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.

value corresponding to LOQ/2 (EC, 2009b). As this method could heavily influence the assessment (e.g. when calculating a mean or a standard deviation), other methods may also be considered (e.g. assuming same distribution of data below and above the LOQ) (EC, 1999).

A.16-6.5 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. However, 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. A specific guidance on chemical monitoring of sediment and biota is currently under preparation for the implementation of the Water Framework Directive.

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