European Union Risk Assessment Report

ETHYLBENZENE

CAS No: 100-41-4

EINECS No: 202-849-4

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RISK ASSESSMENT

environmental part only

Draft of April 2007

Germany

Rapporteur for the risk assessment of ethylbenzene is Germany

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Foreword

This Draft Risk assessment Report is carried out in accordance with Council Regulation (EEC) 793/93[1] on the evaluation and control of the risks of “existing” substances. “Existing” substances are chemical substances in use within the European Community before September 1981 and listed in the European Inventory of Existing Commercial Chemical Substances. Regulation 793/93 provides a systematic framework for the evaluation of the risks to human health and the environment of these substances if they are produced or imported into the Community in volumes above 10 tonnes per year.

There are four overall stages in the Regulation for reducing the risks: data collection, priority setting, risk assessment and risk reduction. Data provided by Industry are used by Member States and the Commission services to determine the priority of the substances which need to be assessed. For each substance on a priority list, a Member State volunteers to act as “Rapporteur”, undertaking the in-depth Risk Assessment and recommending a strategy to limit the risks of exposure to the substance, if necessary.

The methods for carrying out an in-depth Risk Assessment at Community level are laid down in Commission Regulation (EC) 1488/94[2], which is supported by a technical guidance document[3]. Normally, the “Rapporteur” and individual companies producing, importing and/or using the chemicals work closely together to develop a draft Risk Assessment Report, which is then presented at a Meeting of Member State technical experts for endorsement. The Risk Assessment Report is then peer-reviewed by the Scientific Committee on Toxicity, Ecotoxicity and the Environment (CSTEE), now renamed Scientific Committee on Health and Environmental Risks (SCHER) which gives its opinion to the European Commission on the quality of the risk assessment.

This Draft Risk Assessment Report has undergone a discussion in the Competent Group of Member State experts with the aim of reaching consensus by interpreting the underlying scientific information, or including more data, but this work has not yet been totally finalised. The information contained in this Draft Risk Assessment Report does not, therefore, necessarily provide a sufficient basis for decision making regarding the hazards, exposures or the risks associated with the priority substance.

This Draft Risk Assessment Report is under the responsibility of the Member State rapporteur. In order to avoid possible misinterpretations or misuse of the findings in this draft, anyone wishing to cite or quote this report is advised to contact the Member State rapporteur beforehand.

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[1] O.J. No L 084, 05/04/199 p.0001 – 0075

[2] O.J. No L 161, 29/06/1994 p. 0003 – 0011

[3] Technical Guidance Document, Part I – V, ISBN 92-827-801 [1234]

0 OVERALL RESULTS OF THE RISK ASSESSMENT[4]

CAS Number:	100-41-4
EINECS Number:	202-849-4
IUPAC Name:	Ethylbenzene

Environment

Conclusion (ii) There is at present no need for further information and/or testing and no need for risk reduction measures beyond those which are being applied already.

Conclusion (iii) There is a need for limiting the risks; risk reduction measures which are already being applied shall be taken into account.

Conclusion (ii) applies to

all production sites as well as all production and processing sites to *Surface water*, *Waste water treatment plants* and the *Terrestrial compartment*. It also applies to biotic effects of ethylbenzene in the *Atmosphere*.

Conclusion (iii) applies to

Atmosphere (indirect effects of ethylbenzene)

Conclusion (iii) applies to the contribution of the commercial product ethylbenzene to the formation of ozone. In the context of the consideration of which risk reduction measures that would the most appropriate, it is recommended that under the relevant Air Quality Directives a specific in-depth evaluation be performed. Such an evaluation should focus on the contribution of isolated as well as non-isolated ethylbenzene to the complex issue of ozone and smog formation and the resulting impact on air quality.

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[4]

Conclusion (i)	There is a need for further information and/or testing.
Conclusion (ii)	There is at present no need for further information and/or testing and no need for risk reduction measures beyond those which are being applied already.
Conclusion (iii)	There is a need for limiting the risks; risk reduction measures which are already being applied shall be taken into account.

CONTENTS

EUSES Calculations can be viewed as part of the report at the website of the European Chemicals Bureau: http://ecb.jrc.it

TABLES

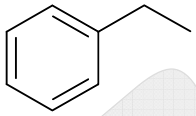
Fehler! Es konnten keine Einträge für ein Abbildungsverzeichnis gefunden werden.

1 GENERAL SUBSTANCE INFORMATION

1.1 IDENTIFICATION OF THE SUBSTANCE

CAS Number:	100-41-4
EINECS Number:	202-849-4
IUPAC Name:	Ethylbenzene
Molecular formula:	$C_8 H_{10}$

Structural formula:



Molecular weight: 106 g/mol

Synonyms: Ethylbenzol

Benezene, ethyl-

Phenylethane

.alpha.-Methyltoluene

EB

1.2 PURITY/IMPURITIES, ADDITIVES

The purity of Ethylbenzene was determined to be > 99.5 % by gas chromatography.

The following impurities have been identified and analyzed:

compound	**CAS-No.**
Benzene	71-43-2
Toluene	108-88-3
p-Xylene	106-42-3
m-Xylene	108-38-3

o-Xylene	95-47-6
Cumene	98-82-8
n-Propylbenzene	103-65-1
m-Ethyltoluene	620-14-4
p-Ethyltoluene	622-96-8
o-Ethyltoluene	611-14-3
tert-Butylbenzene	98-06-6
sec-Butylbenzene	135-98-8
Styrene	100-42-5
m-Diethylbenzene	141-93-5
p-Diethylbenzene	105-05-5
o-Diethylbenzene	135-01-3
Benzaldehyde	100-52-7
Acetophenone	98-86-2
Cyclohexylmethane	108-87-2
Ethylcyclohexane	1678-91-7
Methylbenzylalcohols	
Napthenes	
aliphatic compounds	
Unknowns	

1.3 PHYSICO-CHEMICAL PROPERTIES

Vapour Pressure

The vapour pressure of a substance is defined as the saturation pressure above a solid or liquid substance. At the thermodynamic equilibrium, the vapour pressure of a pure substance is a function of the temperature only.

Vapour pressures in the range of 1 mm mercury column (1.333 hPa) at –9.8 °C to 760 mm (1013.25 hPa) mercury column at 136.2 °C are listed in the CRC Handbook of Chemistry and Physics (Lide, 1991-1992)

A value of 9.3 hPa at 20 °C is listed in the Auer Technikum (1988) which is a collection of common tables of several chemical compounds and is often used in laboratories. This value has been used for further calculations. 16 hPa at 30 °C and 46 hPa at 50 °C are also mentioned in the Auer Technikum. These values are also in good agreement with the values mentioned in the CRC Handbook.

A value of 9.33 hPa at 20 °C is mentioned by Verschueren (1983) and Duve et al. (1976) which supports the value of the Auer Technikum (1988).

Moreover Verschueren (1983) mentions a value of 16 hPa at 30 °C. This value is in good agreement with the Auer Technikum and the CRC Handbook.

Water Solubility

The water solubility of a substance is specified by its saturation concentration in pure water at a certain temperature, preferably at 20 °C.

A water solubility of 160 mg/l at 25 °C is mentioned in the CRC Handbook of Chemistry and Physics (Lide, 1991-1992). This value is in very good agreement with other values and has been used for further calculations therefore.

A value of 152 mg/l at 20 °C is mentioned by Tewari et al. (1982) and Verschueren (1983) whereas the value of 186.7 mg/l at 25 °C has been mentioned by Crookes and Howe (1991).

Partition Coefficient

The partition coefficient (Pow) is defined as the ratio of the equilibrium concentrations of a dissolved substance in a two phase system consisting of two largely immiscible solvents. In the case of n-octanol and water:

$$\text{Pow} = \text{equilibrium } c_{\text{n-octanol}} : \text{equilibrium } c_{\text{water}}$$

The partition coefficient therefore is the quotient of two concentrations and is usually given in the form of its logarithm to base ten (logPow).

The logPow value at 25 °C was determined to be 3.13 by Tewari et al. (1982). This value was used for further calculations because the exact testing temperature was given. But nevertheless the value of 3.15 mentioned by Crookes and Howe (1991) and Verschueren (1983) correspond very well.

Table 1.1 **Summary of physico-chemical properties**

Property	Value	
Physical state	liquid at 25 °C	
Melting point	- 94.949 °C	Gerhartz (1987)
Boiling point (at 1013 hPa)	136.186 °C	Gerhartz (1987)
Relative density	0.8670 at 20 °C	Lide (1991-1992)
Vapour pressure	p(20 °C) = 9.3 hPa	Auer Technikum (1988)
Water solubility	160 mg/l at 25 °C	Lide (1991-1992)
Partition coefficient n-octanol/water (log value)	3.13 at 25 °C	Tewari et al. (1983)
Granulometry	not applicable (liquid)	
Conversion factors		
Flash point	23 °C	CHEMSAFE
Autoflammability	430 °C	CHEMSAFE
Flammability	highly flammable	CHEMSAFE
Explosive properties	not explosive	CHEMSAFE
Oxidizing properties	not oxidizing (structure)	
Viscosity		
Henry's constant	617 Pa m^3/mol	calculated
Surface tension	28.48 mN/m	Gerhartz (1987)
Index of refraction (nd)	1.49588 at 20 °C 1.49320 at 25 °C	Gerhartz (1987)

1.4 CLASSIFICATION

1.4.1 Current classification

- (Classification according to Annex I of the directive 67/548/EEC)

F	R 11	Highly flammable

Harmful	R 20	Harmful by inhalation

1.4.2 Proposed classification

According to the data presented below and the criteria of directive 67/548/EEC the substance has not to be classified as dangerous for the environment.

2 GENERAL INFORMATION ON EXPOSURE

2.1 PRODUCTION

Ethylbenzene is naturally present in crude oil. Commercially it is mainly produced by alkylating benzene with ethene. Ethylbenzene is primarily used in the manufacture of styrene. Due to its use in fuels and solvents it is widely distributed in the environment.

2.1.1 Production processes

The majority of ethylbenzene (~ 90 %) is produced by catalytic reaction of benzene with ethene. This Friedel-Crafts-alkylation is carried out in a closed continuous system. No water is involved in the process; the benzene is dried prior to entering the reactor. Additionally to the commonly used aluminium chloride catalyst, often catalyst promoters like ethyl chloride or hydrogen chloride are present in the reactor.

As a variation to this liquid phase process the alkylation can take place in the vapour phase. In this case the reaction mixture is passed over a fixed bed catalyst, such as phosphoric acid or zeolite.

Several fractions are produced from the ethylbenzene reactor. These are either recirculated (excess benzene, light fraction of polyethylbenzene), passed on for further processing (toluene to lower olefins unit) or incinerated (light components, heavy fraction of polyethylbenzene). Ethylbenzene is further refined by closed continuous distillation. The solid waste (catalyst waste containing traces of ethylbenzene and waste clay) is treated by 3rd parties. (Shell NL, 2001)

Another production method is the fractionation of mixed xylene streams which is, however, employed to a much lesser extent. These streams occur in petroleum refineries during distillation of crude oil into petroleum products and contain ~ 80 % o-, m-, p-xylenes ("mixed xylene stream") and ~15 – 20 % ethylbenzene.

2.1.2 Production capacity

There are 9 producers in the EU; one company is a trader only. The production volume in the European Union can be estimated to be **~ 5.28 x 10^6 t/a**. No information on export from or import in the EU is available. The known volume to be processed is **~ 5.10 x 10^6 t/a**. The discrepancy to the production volume of 1.82 x 10^5 t/a might be due to inaccuracies from figures round up. A total market volume of ethylbenzene of **~ 5.28 x 10^6 t/a** is assumed for the risk assessment. The above figures are based on specific information given by industry in 2001-2004.

2.2 USES

2.2.1 Introduction

Ethylbenzene is primarily employed for the production of styrene. A small percentage is used in the production of other chemicals.

2.2.2 Scenarios

Table 2.1 and Table 2.2 give an overview over uses, quantities and the assigned ICs/UCs. **MC I** is allocated as main category (closed systems) for production and processing.

Table 2.1 Quantity of ethylbenzene in different applications

Application	**Quantity used (tonnes/year)**	**Percentage of total use**
Polymer/Chemical industry	5,253,600	99.5 %
Chemical industry	26,400	0.5 %

Table 2.2 Use of ethylbenzene in Western Europe

		IC	**UC**	**%**
Processing	Production of styrene	Chemical industry **(3)**	Intermediate **(33)**	99.5
	Production of other chemicals	Chemical industry: chemicals used in synthesis **(3)**	Intermediate **(33)**	0.5

2.2.2.1 Chemical industry - production of styrene

The majority of ethylbenzene is used for the production of styrene. The quantities given vary between 95 and 99.8 % of the total ethylbenzene volume (ECB, 2002). Some of the companies giving specific information on production and processing stated that 100 % of their produced ethylbenzene is processed to styrene. Since the exact percentage for the total tonnage is not known it is assumed that 99.5 % of the ethylbenzene produced is used as intermediate in the styrene production.

According to RAR Styrene (EU, 2000) there are two routes to manufacture styrene from ethylbenzene. Firstly, ethylbenzene can react with air to ethylbenzene hydroperoxide, followed by reaction with propene to styrene. Alternatively, ethylbenzene can be catalytically dehydrogenated.

Styrene is further processed to polystyrene which is used in large volumes in the automobile industry (replacing metal parts), in the building industry and for packaging. Furthermore, styrene is a raw material for the manufacture of synthetic rubber.

It can be referred to RAR Styrene (EU, 2000) for more detailed information on styrene and polystyrene.

2.2.2.2 Chemical industry – production of other chemicals than styrene

A small fraction of the total ethylbenzene serves as chemical intermediate, e.g. in the manufacture of acetophenone, cellulose acetate, diethylbenzene, propylene oxide. It is also used as solvent/reactant in unsaturated polyesters. Quantities involved in this application are assumed to be 0.5 % of the total amount, derived from information of the IUCLID data set (ECB, 2002).

2.2.2.3 Paint industry - use as solvent (intentional)

Ethylbenzene is known to be used as a solvent, both on its own and blended with xylenes. The solvents are applied in paints, lacquers, inks, rubber and agricultural industry.

There is no precise information on the amount of ethylbenzene formulated to solvents. It was assumed that about 1.5 % of the total quantity of ethylbenzene produced is applied in the solvent sector (intentional use of ethylbenzene as solvent). It was further assumed that the produced solvents consist of 15 % ethylbenzene. This value is a mean of data on the content of ethylbenzene in technical solvents, mainly on the German market (INFU, 2003). It is not clear if this content relates to ethylbenzene in “mixed xylene” solvent.

The European Council of Paint, Printing Inks and Artist's Colours (CEPE, 2000) had launched a survey among its members and supplied recently more detailed information about the results. A questionnaire was sent to all major paint manufactures plus most of the medium-sized companies as well as a number of small companies asking for information on the use of ethylbenzene in paints and solvents.

It became apparent that > 99 % of ethylbenzene used in paints is stemming from “mixed xylene” solvent. A more detailed description of this unintentional use of ethylbenzene can be found in 2.2.3.2.

The intentional use of ethylbenzene in paints seems not to be of relevance anymore. That might also be due to higher flammability and higher price of ethylbenzene compared to the “mixed xylene” solvent. In addition industry has emphasised their endeavour to develop solvent free systems and water based paints.

In summary it is concluded that the intentional use of ethylbenzene in the solvent sector is only marginal and is not further considered in the risk assessment.

2.2.3 Unintential uses

Some petroleum refineries isolate a reformate stream during the distillation of crude oil into petroleum products. Reformate is a blending stream used in the production of gasoline and has several CAS numbers. The final concentration of ethylbenzene in gasoline is approximately 2 % (by weight). CONCAWE estimate 20 million tons of reformate are produced annually for use in gasoline blending (CEFIC, 2004).

The reformate stream may be further processed to isolate a mixed xylene stream. "Mixed xylenes" contain generally about 80 % o-, m-, and p-xylenes and 15 to 20 % ethylbenzene (range of 10 – 45 % (CEFIC, 2004)). Ethylbenzene can be separated from the stream as means of production; however, this technology is economically not favourable.

The "mixed xylenes" (also called xylene-range aromatic solvent) is a commercial product (CAS: 1330-20-7). There are other processes which can be used to produce mixed xylene, e.g. gasoline pyrolysis and toluene disproportionation. "Mixed xylenes" is used mainly for blending into gasoline. The remainder is used as solvent to make coatings, agrochemicals and miscellaneous products (car cleaning and household). Smaller applications are in the manufacture of perfumes, pesticides, pharmaceuticals as well as in the production of the individual isomers (ECETOC, 1986; Crookes and Howe, 1991; Lundberg et al., 1997).

For the risk assessment, the two main sources of ethylbenzene emissions stemming from unintentional uses of mixed xylenes are taken into account. Firstly, petrol-related emissions to the gas phase (2.2.3.1) are considered in the calculation of the regional background concentration. Secondly, a generic local scenario is calculated for the formulation and use of mixed xylenes as solvent (2.2.3.2).

It is known that ethylbenzene can be released during combustion processes other than combustion of gasoline, i.e. power stations and waste incinerators. Only very few measurements exist.

In BUA (1997), the quantity ethylbenzene released by coal-fired power stations is estimated to be 3 – 25 t/a for Germany. This amount is only 2 % of that from traffic (worst case).

It can be concluded that emissions from waste incineration and power stations are minor compared to releases by traffic, and will be neglected in this RAR.

2.2.3.1 Ethylbenzene in Petrol

The majority of the mixed xylenes produced is blended into gasoline (ECETOC, 1986). Ethylbenzene serves as a "anti-knock" agent (octane enhancer) (Fishbein, 1985). Although not strictly part of the risk assessment of ethylbenzene this application is discussed here since estimated emissions are used in the calculation of the background concentrations.

Leseman (1986) cites the following quantities of ethylbenzene in different types of fuels:

Table 2.3 Quantity of ethylbenzene in different types of petrol (Leseman, 1986)

	% ethylbenzene (by weight)
petrol, regular	1.5 – 3.1
petrol, unleaded	1.8 – 4.7
aviation fuel	0.77
kerosene	0.36 – 0.38
diesel No 2	< 0.2

Nowadays, regular petrol is practically phased out in favour of unleaded fuel.

Using a density of 750 kg/m^3 for petrol (BUA, 1998) and of 867 kg/m^3 for ethylbenzene (BUA, 1997), one can derive the respective volume fractions as 1.6 – 4.1 vol % for unleaded petrol. Concurringly, Fishbein (1985) has given a value of 4 vol % in reformate. Another study found 0.8 – 4.6 vol % ethylbenzene in common German engine fuels (DGMK, 1994).

Exhaust hydrocarbon emissions from vehicles are expected to be a mixture of unburned and partially burned fuel species. Ethylbenzene has been observed in exhaust gases of combustion engines. Various sources quote the content of ethylbenzene in these gases between 0.7-2 wt % for gasoline and between 0.55-0.7 wt % for diesel. A value of 2.3 wt % is given for vehicles thereby not differentiating between gasoline and diesel (cited in Crookes and Howe, 1991).

Annual consumption of petrol was about 120 million tons in the EU between 1990-1994 (see EU, 2001). According to data by IEA (2003) annual petrol consumption in the EU decreased slightly during the last years to about 111 million tons in 2001. Using an ethylbenzene content of ~ 2 wt %, given by DGMK (1994) and confirmed by CONCAWE (CEFIC, 2004), a quantity of **2.2 x 10^6 t/a** ethylbenzene can be roughly estimated to be present in petrol in the EU.

Ethylbenzene can be discharged during handling and combustion of gasoline (automobiles and aeroplanes). These petrol related emissions, e.g. from crude oil production, transport, exhaust gases, are estimated in Chapter 3.1.2.4.1 and taken into account for the calculation of the regional background concentrations.

2.2.3.2 Other uses of "mixed xylenes"

The remainder of the "mixed xylenes" is mainly used as solvent in spray paints, primers, paint removers, thinners, wood stains, varnishes and other finishes, and cleaners for automotive and household uses (OECD, 2002). A further quantity is applied for the production of the individual isomers of xylene.

CEPE (2004) gave more details on the uses of paints containing ethylbenzene. The majority of these paints are used as industrial paint in the following sectors: automotive, vehicle refinishes, marine, can coating, wood furniture, electrical insulating, printing inks. Only a minor part is applied in decorative/DIY area. Whereas brushing and roller coating are the main application techniques in the decorative sector, spraying, curtain coating, dipping, coil coating are further techniques used in industry. Most of the industrial paints are (aromatic) solvent-based. Over 60 % of the total paints volume in the decorative sector is used as aqueous suspensions.

Recently, the Hydrocarbon Solvent Producers Association *HSPA* (2004) provided information on the quantities of “mixed xylenes” as solvent in Europe. That information is representative of > 90 % of the quantity of hydrocarbon solvents produced in Western Europe.

HSPA estimates the quantity of mixed xylenes used as solvent in Western Europe at 2.5 - 3.5 x 10^5 t/a. The content of ethylbenzene varies according to the production process. About 82 % of mixed xylenes originate from catalytic reformate containing typically 10 – 15 % ethylbenzene. Approximately 11 % is produced by gasoline pyrolysis resulting in a ethylbenzene content of 40 – 45 %. A further route is by toluene disproportionation; the ethylbenzene content is not known.

The upper estimate of the total amount of ethylbenzene in mixed xylenes used as solvent can be calculated as follows:

$$350000 \text{ t} \times (0.82 \times 0.15 + 0.18 \times 0.45) = 71400 \text{ t}$$

A quantity of **71000 t/a** ethylbenzene in about 350000 t/a mixed xylenes is used further in the risk assessment.

Summarising the unintential uses, an additional quantity of ethylbenzene of **2.27 x 10^6 t/a** is recognised. About 97 % (2.2 x 10^6 t/a) of this quantity is present in petrol; the remaining 3 % (7.1 x 10^4 t/a) are assumed to be used as solvents in various fields of application.

A total tonnage of **7.55 x 10^6 t/a** ethylbenzene is assumed to be present in the EU resulting from the quantity produced (5.28 x 10^6 t) and the quantity arising from unintential uses (2.27x 10^6 t).

2.2.4 Information from Product Registers

The SPIN (Substances in Preparations In the Nordic countries) database was searched for information on ethylbenzene in products on the national markets. The following data were found:

Table 2.4 Ethylbenzene in consumer products according to SPIN for 2001

country	number of preparations	tonnage
Norway	555	91,396
Finland	799	1,685
Denmark	1,589	366

Please note: The total amount of a substance in SPIN is the added quantity of the substance in all products, the export amount subtracted. That is to say that if a substance is registered first as the imported raw material and then as the final preparation, the quantity will be counted twice. Substances that are used for formulation of chemical products and that are imported, and most are in the Nordic countries, will thus be accounted for with maybe double the actual amount.

In addition, substances are registered in an interval tonnage range. The number obtained in SPIN and given in the table above represents the upper limit of that interval. Depending on how wide the interval is the given value might overestimate the true value.

Therefore, the given tonnage figures of Table 2.4 may not reflect the real situation.

Main industrial use categories are given as "Manufacture of coke, refined petroleum products and nuclear fuel" (Norway, 91266 t, 5 preparations), "Manufacture of chemicals and chemical products" (Finland, 1600 t, 44 preparations) and "Manufacture of fabricated metal products" (Denmark, 312 t, 600 preparations) as well as "Manufacture of other transport equipment" (Denmark, 192 t, 312 preparations). There was no more detailed information on the specifics of these industrial categories.

Specifying the use of these preparations, "Paints, lacquers and varnishes" (Norway: 375 preparations; Denmark: 914 preparations) and "Solvents" (Norway: 45 preparations; Denmark: 66 preparations) are identified as the main fields of application. Another significant technical use is as "Process regulator" (Norway: 80 preparations; Denmark: 123 preparations).

2.3 TRENDS

[click here to insert text]

2.4 LEGISLATIVE CONTROLS

3 ENVIRONMENT

3.1 ENVIRONMENTAL EXPOSURE

3.1.1 General discussion

Ethylbenzene is industrially produced and mainly used in the production of styrene. Another application is in the solvent sector (unintentional use). Ethylbenzene also occurs naturally in crude oil. Due to its presence in petrol and its volatility ethylbenzene is widely distributed in the atmosphere.

3.1.2 Environmental releases

Environmental releases of ethylbenzene occur during its production and processing to styrene. Solvent related emissions take place during formulation and use of the solvent (unintentional use). As a constituent of fuel ethylbenzene can be emitted during storage and refuelling whereby evaporative losses may happen, and as constituent of traffic exhaust. Furthermore, ethylbenzene can be released from various sources during combustion processes, e.g. from waste incinerators and power stations, however, these are not considered further.

3.1.2.1 Release from production

There are 9 companies at 16 sites in the EU which manufacture ~ 5.28 x 10^6 t/a.

Production and processing of ethylbenzene are reported for 11 sites. At another 5 sites production only takes place.

The quantity produced/processed at one site ranges from ~ 10,000 to ~ 1.0 x 10^6 t/a. Unless specific information was provided by industry the following default emission factors were used (Table 3.1).

Table 3.1 Generic release factors for production of ethylbenzene

		water		air		soil	
alkylation of benzene (IC3/UC33)	90 %	ESD 3	0.003	A1.2	0.001 (1c)	A1.2	0.0001 (1c)
fractionating of xylenes (IC9/UC33)	10 %	A1.1	0.003	A1.1	0.001 (1c)	A1.1	0.0001

3.1.2.2 Release from processing/industrial use

About 99.5 % (~ 5.25 x 10^6 t/a) of the total ethylbenzene are processed to styrene which is subsequently polymerised.

Default release estimation has been carried out for sites without specific information using default emission factors summarised in Table 3.2.

Table 3.2 Generic release factors for processing of ethylbenzene

		water		**air**		**soil**	
production of styrene (IC3/UC33)	99.5 %	ESD 3	0.007	A3.3	0.0001 (1c)	A3.3	0.0001
production of other chemicals (IC3/UC33)	0.5 %	A3.3	0.007	A3.3	0.0001 (1c)	A3.3	0.0001

Summarising all specific information given by Industry up to now (i.e. 2004) shows that 6 of the 16 sites considered apply dry techniques (e.g. fixed bed catalyst) for production and/or processing. Four of these 6 sites use a dry production process but at the same time a wet processing technique. One company has two plants at one site, one wet-operating plant and one dry-operating plant. Only one company employs a completely dry process resulting in zero emissions to waste water.

One producer supplied the information that waste water from production as well as processing is steam stripped before going into the wwtp. In this process ethylbenzene concentrations are reduced from about 0.2 g/l (solubility limit) to 0.1 mg/l. The steam loaded with ethylbenzene is redirected into the working processes. Therefore, no emissions to the atmosphere are expected by the stripping procedure.

3.1.2.3 Release from disposal

Ethylbenzene is volatile. Therefore, ethylbenzene is found mainly in the atmosphere.

Various producers state that exhaust gases and solid waste from production and processing are incinerated. Expected products of the complete combustion are H_2O and CO_2. No further information is available. However, no relevant emissions of ethylbenzene are expected from the incineration plants. Please, refer to Chapter 2.2.3 for information on combustion.

3.1.2.4 Unintential releases of ethylbenzene

Ethylbenzene is a constituent of "mixed xylenes" which are used in petrol and as solvent. Due to the high vapour pressure the atmosphere is the main target compartment for ethylbenzene.

It is not possible to exactly quantify ethylbenzene emissions caused by unintential uses. The only known information on recent petrol consumption is the statistics supplied by IEA (2003). However, emissions will vary under different conditions. No exposure data are available concerning the application as solvent.

On the other hand, the discharge of ethylbenzene by these sources is substantial and significant. Therefore, releases for all identified sources are estimated and used for the calculation of the regional background concentrations.

3.1.2.4.1 Petrol-related emissions

Basis of this chapter is the assumption made in 2.2.3.1 that the annual consumption of petrol in the EU is about 111 million tons. The steps considered relevant in the production and use of gasoline are listed in Table 3.3. Only emissions to the gas phase are considered since the atmosphere is by far the most relevant compartment.

Emissions from traffic exhaust were calculated using measured concentrations and an emission factor of waste gas (see Table 3.3). The concentrations were measured on engines not fitted with a catalytic converter. Catalytic converters are able to reduce emissions to 12 % (BUA, 1997). Exact information about the proportion of cars equipped with converters is only available for Germany. Here, 96 % of all vehicles are emission reduced cars (KBA, 2002). For Europe this number is assumed to be slightly smaller, i.e. 90 %.

Emission factors are taken from BUA (1997) and BUA (1998).

Table 3.3 Estimates of petrol-related emissions to gas phase

step	**parameter**	**value**	**emission [t/a]**
crude oil production	HC[1] emission factor content ethylbenzene in HC gas phase	(0.1 kg HC) / (t crude oil) [2] [3] 0.38 % [4]	42
petrol refining	HC[1] emission factor content ethylbenzene in HC gas phase	(0.3 kg HC) / (t petrol) [2] 0.38 % [4]	127
transport and storage	HC[1] emission factor content ethylbenzene in HC gas phase	(3.11 kg HC) / (t petrol) [4] 0.38 % [4]	1,312
refuelling	HC[1] emission factor content ethylbenzene in HC gas phase	(15 kg HC) / (t petrol) [4] 0.38 % [4]	6,327
traffic exhaust	waste gas emission	(11,800 m^3 waste gas) / (t petrol) [4]	
	ethylbenzene concentration in exhaust (no catalytic converter)	12.3 – 49.0 mg m^{-3} [4]	
		cars with converter (90 % of cars, reduction of emission to 12 %)	1,740 – 6,931
		cars without converter (10 % of cars)	1,611 – 6,418
		total	3,351 – 13,349
		total (max)	**21,157**

[1] Hydrocarbon

[2] BUA (1998)

[3] As first approach it is set: tonnage (crude oil) = tonnage (petrol), i.e. calculations based on 111 x 10^6 t .

[4] BUA (1997)

3.1.2.4.2 Other sources

A quantity of 7.1 x 10^4 t/a ethylbenzene is assumed to be contained in about 3.5 x 10^5 t of "mixed xylene solvents". Diffuse entry of ethylbenzene is expected resulting from formulation and use of the solvents. In Table 3.4 the relevant release factors are shown.

Table 3.4 Release factors for formulation and use of mixed xylene solvents (solvent-based)

		water		**air**		**soil**	
formulation	IC3/UC48	A2.1	0.003	A2.1	0.005 (1c)	A2.1	0.0001
technical use	IC14/UC48	A3.15	0.02	A3.15	0.9	A3.15	0.001

3.1.2.5 Summary of releases

Intentional releases result from all identified and significant life cycle stages of ethylbenzene: production and processing as chemical intermediate. Unintentional releases occur by means of production and use of petrol as well as formulation and use of mixed xylene solvents.

Summaries of all regional and continental releases can be found in Table 3.15 and Table 3.16.

3.1.3 Environmental fate

3.1.3.1 Degradation in the environment

3.1.3.1.1 Atmospheric degradation

Direct photolysis is not expected to be an important removal process since ethylbenzene does not significantly absorb light at wavelengths > 290 nm.

Reaction with OH radicals is by far a more significant degradation pathway. Atkinson (1989) studied the reaction of ethylbenzene and OH radicals in air at 25 °C. A rate constant of 7.1 x 10^{-12} cm^3 $molecules^{-1}$ s^{-1} was obtained which corresponds to a half life of 2.3 d under atmospheric conditions (i.e. OH-radical concentration of 5 x 10^5 molec cm^{-3}). Ohta and Ohyama (1985) derived a rate constant of 6.8 x 10^{-12} cm^3 $molecules^{-1}$ s^{-1} at room temperature resulting in an atmospheric half life of 2.4 d. Another study reported a rate constant of 8.2 x 10^{-12} cm^3 $molecules^{-1}$ s^{-1} at 25 °C for the lower troposphere corresponding to $t_{1/2}$= 2.0 d (Ravishankara et al., 1978). A further value of 8.0 x 10^{-12} cm^3 $molecules^{-1}$ s^{-1} at 300 K agrees well (SINGH et al., 1981).

Atmospheric oxidation was also modelled by the Atmospheric Oxidation Program AOPWin v. 1.90 for comparative purposes. The model is based on structure-activity relationship (SAR) methods. It estimates the rate constant for the atmospheric gas-phase reaction between photochemically produced hydroxyl radicals and organic chemicals. The overall OH rate constant was derived as 5.9×10^{-12} cm^3 $molecules^{-1}$ s^{-1} giving a half life of 2.7 d (OH-radical concentration of 5×10^5 molec cm^{-3}).

The half life of 2.3 d is used in the further risk assessment. This value is the most recent one and is within the range of the other values.

3.1.3.1.2 Aquatic degradation (incl. sediment)

Abiotic

Ethylbenzene is not expected to hydrolyse under typical environmental conditions.

Aerobic biodegradation

Many tests on the biological degradation of ethylbenzene are available. As ethylbenzene has a high volatility only closed tests are appropriate to determine the biodegradation. The most relevant test results for the risk assessment are presented below.

In a respirometric test on ready biodegradation according to EEC method performed with domestic activated sludge from a laboratory sewage treatment plant as inoculum, a biodegradation of 50 % after 28 days was obtained. The concentration of ethylbenzene was 87 mg/l. Biodegradation was measured as BOD. A repetition of the test resulted in a degradation of the test substance of > 60 % after 33 days for 4 of 6 test vessels. From the available degradation curve it can be concluded that the pass level was already reached after 28 d for these 4 parallels. However, for 2 test vessels the degradation was only about 25 % and 55 % respectively after 28 and 33 days. As the degradation in the parallel vessels differs by more than 20 %, the test has to be regarded as not valid according to the OECD guideline. (BASF AG, 1988).

As ethylbenzene is toxic to microorganisms at concentrations around 100 mg/l (cf. 3.2.1.1.4) and the test was performed at a concentration of 87 mg/l, the variable results obtained may be caused by toxic effects on the inoculum.

In a MITI I test performed with ethylbenzene in 3 replicates, in one replicate 100 % degradation was achieved while in the other 2 replicates 0 % degradation was found (CERI). These findings may also be explained by toxicity to microorganisms as the test substance concentration in the MITI I test was 100 mg/l.

In a recently performed CO_2-headspace test according to ISO 14593 a mean biodegradation of 79 % (measured as TIC/ThIC) was found after 28 days (BASF AG, 2003). At the end of the 10d window about 68 % biodegradation was obtained. The ethylbenzene concentration was 22 mg/l, equivalent to 20 mg/l TOC. As inoculum activated sludge from a laboratory wastewater treatment plant treating municipal sewage was used with a concentration of 4 mg/l. Aniline as reference substance was degraded by 88 % within 14 days. From this study it can clearly be concluded that ethylbenzene is readily biodegradable fulfilling the 10d window criterion.

In a MITI-II test (OECD 302C) a biodegradation of 81-126 % after 14 days was reached (CITI, 1992). From this study ethylbenzene can be classified as inherently biodegradable.

In addition, several biodegradation studies are available that have not been performed according to standardised methods. The most relevant studies for assessment purposes are described below.

The 5d BOD of ethylbenzene was determined by Babeu and Vaishnav (1987) using acclimated mixed microbial cultures. The ethylbenzene concentration was in the range of 0.4 to 3.2 ppm. A BOD_5/ThOD ratio of 0.29 was determined.

The 35d BOD of ethylbenzene was tested by ZoBell and Prokop (1966). An oxygen-saturated seawater medium was used that was inoculated with specific enrichment cultures of hydrocarbon-oxidizing bacteria. The concentration of ethylbenzene was about 2 mg/l. A biodegradation of 54 % was found.

Weber et al. (1987) studied the removal of ethylbenzene in a completely mixed batch reactor and a completely mixed flow reactor. A synthetic waste water with a background TOC of 100 mg/l was used in the experiments. Adapted activated sludge from a municipal wwtp served as inoculum. In the complete mixed batch reactor a removal of ethylbenzene of 82 % was reached. In the complete mixed flow reactor an influent concentration of ethylbenzene of between 50 and 150 µg/l (not exactly given) was reduced by > 99 %. 22 % of the influent concentration was removed by volatilisation and 78 % by primary degradation. Typical operating conditions of the flow reactor were a hydraulic retention time of 5.5 h, a solids residence time of 6 d and a MLSS concentration of 3500 mg/l.

The elimination of ethylbenzene in 6 different wastewater treatment systems was studied by Hannah et al. (1986). A 1:1 mixture of raw wastewater with secondary effluent from a wwtp was used as feed. This wastewater was spiked with 21 priority substances, among them ethylbenzene, providing a concentration of 100 µg/l for each substance. Among the examined wastewater treatment systems were a conventional activate sludge system and two lagoon systems (aerated and facultative) as representatives for a biological wastewater treatment. In addition, physical elimination by filtration and flocculation was studied. For ethylbenzene, the highest removal rates of 96 % and 93 % were obtained with the activated sludge system and the facultative lagoon, followed by the aerated lagoon (70 %).

In an industrial sewage treatment plant ethylbenzene was removed from an initial concentration of 29 µg/l by 78 %. The plant treats wastes from an organic chemicals manufacturing site by neutralisation and settling, followed by a combined powdered carbon-biological process. Ethylbenzene concentration was measured by GC/MS (Hutton and Du Pont, 1980).

As ethylbenzene is readily biodegradable, a degradation rate constant of 1 h^{-1} is used for the degradation of ethylbenzene in wwtp.

No tests are available that simulate the biodegradation of ethylbenzene in surface waters. Therefore, the rate constant and half-life for biodegradation in surface waters has to be derived based on the results from the available screening tests. For readily biodegradable substances a rate constant of $4.7 \cdot 10^{-2}$ d^{-1} that is equivalent to a half-life of 15 d is proposed by the TGD.

3.1.3.1.3 Degradation in soil and sediment

No tests are available that can be used for an assessment of the biodegradation of ethylbenzene in soil. Therefore, the rate constant and half-life for biodegradation in soil has to be based on the results from the available screening tests. For readily biodegradable substances with a Kpsoil < 100 $l \cdot kg^{-1}$ the TGD proposes a half-life of 30 d that corresponds to a rate constant of $2.31 \cdot 10^{-2}$ d^{-1}.

For sediments a half-life of 300 d, equivalent to a rate constant of $2.31 \cdot 10^{-3}$ d^{-1} can be derived according to the TGD.

3.1.3.1.4 Summary of environmental degradation

Direct photolysis or hydrolysis are not expected. Under atmospheric conditions ethylbenzene has a half live of 2.3 d (rate constant of 7.1×10^{-12} cm^3 $molecules^{-1}$ s^{-1}) due to reaction with the OH radical ($Conc_{[OH]}$ of 5×10^5 molec cm^{-3}).

Ethylbenzene has been classified as readily biodegradable in surface water and wwtp. The following table shows the derived rate constants and half lives in different compartments.

Table 3.5 Rate constants and half lives due to biodegradation of ethylbenzene

	Rate constant	**Half live**
Surface water	4.7×10^{-2} d^{-1}	15 d
wwtp	1 h^{-1}	-
Soil	2.31×10^{-2} d^{-1}	30 d
Sediment	2.31×10^{-3} d^{-1}	300 d

3.1.3.2 Distribution

The equilibrium distribution in the environment was quantified by EQC Model Level I (v. 1.0) based on chemical-physical properties. Using the properties given in Chapter 1 the following distribution in different compartments was derived (Table 3.6).

Table 3.6 Distribution in the environment, Mackay Level I

	%
Air	99.45
Water	0.45
Soil	0.05
Sediment	0.05

3.1.3.2.1 Adsorption

The organic carbon-water partitioning coefficient Koc was derived according to TGD ("predominantly hydrophobics") using a log Kow of 3.13. Further partitioning coefficients can be found in Table 3.7 (see Appendix I for details).

Table 3.7 Partition coefficients between different media

	unit	value
K_{oc}		431.8
Kp_{susp}	$l\ kg^{-1}$	43.1
Kp_{sed}	$l\ kg^{-1}$	21.6
Kp_{soil}	$l\ kg^{-1}$	8.6
$K_{soil\text{-}water}$	$m^3\ m^{-3}$	13.2
$K_{susp\text{-}water}$	$m^3\ m^{-3}$	11.7
$K_{sed\text{-}water}$	$m^3\ m^{-3}$	22.4

The order of magnitude of Koc (log Koc = 2.64) indicates a moderate mobility in soil.

A measured log $K_{sed\text{-}water}$ of 1.01 (Foc_{sed} = 4 %) corresponds to a $K_{sed\text{-}water}$ of 10.2 m^3/m^3 (Vowles, 1987). Only the solute phase was analysed. Loss of compound can not be excluded, e.g. by volatilisation. A log Koc of 2.47 was experimentally derived by Szabo (1992) whereby analysis was based on above cited log $K_{sed\text{-}water}$ of 1.01.

Partitioning coefficients as shown in the table above are used in the risk assessment.

3.1.3.2.2 Volatilisation

Ethylbenzene has a water solubility of 160 mg/l and a relatively high vapour pressure (930 Pa). A Henry's Law constant (H) of 617 Pa $m^3\ mol^{-1}$ can be computed from these values indicating rapid volatilisation. The dimensionless K_{air_water} of 0.26 was derived from this Henry's Law constant (see Appendix I).

3.1.3.2.3 Distribution in wastewater treatment plants

Using a Koc of 432, a Henry constant of 617 Pa m^3 mol^{-1} and a rate constant of 1 h^{-1}, the following distribution of ethylbenzene in waste water treatment plants was calculated with Simple Treat 3.0.

Table 3.8 Summary of distribution in STP

	% of total
air	46.7
water	5.4
sludge	3.7
degraded	44.2
total removal	94.6

3.1.3.3 Accumulation and metabolism

The log Kow of 3.13 indicates a potential for bioaccumulation. According to the TGD a BCF of 91 can be estimated from this value.

No bioaccumulation studies performed with pure ethylbenzene are available. In several studies the water-soluble fraction (WSF) of crude oil that contains ethylbenzene was tested.

Roubal et al. (1978) investigated the bioconcentration of ethylbenzene from the WSF of crude oil by Coho salmon (*Oncorhynchus kitutsch*) and starry flounder (*Platichthys stellatus*). The fish were exposed for 6 weeks (salmon) and 2 weeks (flounder) in a flow-through system to a mean WSF concentration of 0.9 mg/l containing a mean ethylbenzene concentration of 0.005 mg/l. At the end of the exposure periods, both species were transferred to clean sea water for 2 weeks to study the depuration. Bioconcentration factors for C2-substituted benzenes (related to dry weight) were 1.1, 2.4, 2 and 1 after 2, 3, 5 and 6 weeks of exposure for Coho salmon (muscle tissue). For the starry flounder the bioconcentration factors for C2-substituted benzenes in muscle tissues were determined to be 20 and 4 after 1 and 2 weeks of exposure. Depuration of the accumulated ethylbenzene to concentrations below the detection limit (0.05 mg/kg) occurred within 1 week for salmon and within 2 weeks for the flounder.

Manila clams (*Tapes semidecussata*) were exposed for 8 days in a flow-through system to the water-soluble fraction of crude oil containing a mixture of 6 monoaromatics (Nunes and Benville, 1979). The amount of aromatics in water was measured three times a day. The mean ethylbenzene concentration was 0.08 mg/l. Every 48 h a sub-sample of 10 test organisms was pooled and analyzed for aromatic content by GC. After 2 days of exposure the ethylbenzene concentration in the tissue (related to wet weight) was 0.34 mg/kg and after 8 days 0.37 mg/kg. After transfer of the clams into clean water, depuration of the ethylbenzene to concentrations below the detection limit (0.13 mg/kg) occurred within 7 days.

In a poorly documented study Ogata et al. (1984) determined a log BCF of 1.19 (BCF = 15) for ethylbenzene in goldfish. From the description of the study it is not clear whether the fish were exposed to pure ethylbenzene or to a mixture of alkyl benzenes. No information is given on the exposure duration or whether steady state conditions had been achieved. Therefore, the study is not regarded as valid and the result is not used for the risk assessment.

The validity of the available bioconcentration studies is limited as for all tests there is no information whether steady state was reached. In addition, the test organisms were not exposed to pure ethylbenzene but to a mixture of oil components. However, the available study results can be used as an indication that the bioaccumulation potential of ethylbenzene may be lower than predicted from the log Kow. The predicted BCF of 91 is used further in the risk assessment.

3.1.4 Aquatic compartment (incl. sediment)

3.1.4.1 Calculation of predicted environmental concentrations (PEC_{local})

All calculated PEC_{local} can be seen in Table 3.9. Site-specific dilution factors are used if known. However, the maximum dilution factor is 1000 for site-specific assessments according to the new TGD. If no specific information is available, the Emission Scenario Document of the new TGD (Part IV, Chapter 7) is used (IC3, dilution factor: 40).

Five sites (P3, P4, P5, PP5, PP7) are located at the sea. Dilution factor of 100 is used for sites situated at coastal zones. Please refer to Chapter 3.3.4.2 for results of marine assessment.

Table 3.9 Data used in local aquatic exposure assessment

		site-specific information[5]	**release factor to waste water**[6] **[kg/t]**	**Clocal $_{eff}$ (= PEC $_{stp}$)**[7] **[mg/l]**	**Clocal $_{water}$ [µg/l]**	**PEClocal $_{water}$**[8] **[µg/l]**
P1	production	effluent concentration, emission days	0.02	0.05	1.25	1.31
P2	production	emission factor, river flow rate, emission days	0	0	0	0.06
P3	production	waste water discharge rate, waste water concentration, emission days, direct discharge to sea	1 x 10^{-3}	-	0.075	0.081
P4	production	waste water discharge rate, waste water concentration, emission days, direct discharge to sea	< 1 x 10^{-5}	-	0.019	0.025
P5	production	emission days, effluent concentration	3 x 10^{-3}	1 x 10^{-3}	0.010	0.016
PP1	production and processing	effluent concentration, dilution	2 x 10^{-5}	2 x 10^{-4}	1.83 x 10^{-3}	0.066
PP2	production and processing	release for production, effluent concentration	0.05	14.0	14.0	14.1
PP3	production and processing	effluent discharge rate, municipal wwtp, emission days	1.5 x 10^{-3}	0.050	4.91	4.97
PP4	production and processing	effluent concentration, dilution, emission days	2 x 10^{-3}	1.0	9.99	10.06

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[5] If there was no site-specific information, calculations were done by rapporteur according to new TGD.

[6] Refers to maximum volume handled at that site (independent of process/es involved)

[7] Not given if known that there is no WWTP (either by specific information that there is no WWTP, or default assumption of no WWTP for known marine sites).

[8] PEC$_{regional}$ for marine sites as described in Chapter 3.3.4.2.

PP5	processing	effluent discharge rate, emission days, direct discharge to sea	0.02	-	1.063	1.07
PP6	production and processing	effluent concentration, dilution, emission days	1.4×10^{-3}	0.01	0.031	0.095
PP7	production and processing	effluent concentration, effluent discharge rate	1×10^{-3}	0.062	0.620	0.630
PP8	production and processing	river flow rate, emission days, effluent concentration, dilution	0.09	0.02	0.122	0.19
PP9	production and processing	effluent concentration	5×10^{-4}	0.005	0.125	0.19
PP10	production and processing	WWTP influent concentration, dilution	3×10^{-4}	5×10^{-4}	0.023	0.09
PP11	production and processing	effluent concentration, elimination in WWTP, effluent discharge rate	4×10^{-3}	0.23	5.75	5.81
	other processing (generic)	-	7.0	0.665	16.6	16.7

3.1.4.1.1 Calculation of PEC_{local} for production, or production and processing

There are 11 sites where production and processing takes place ("PP"), sole production takes place at 5 sites ("P"). Table 3.9 lists the calculated PECs and the respective data used in the calculation.

$PEC_{regional}$ as listed in Table 3.17 was taken into account in the calculation of the local PECs.

Based on site-specific information a highest value of PEC_{local}= 1.31 µg l^{-1} for production is calculated.

Using the highest reported tonnage of 1×10^6 t/a the maximum value for production and processing (generically calculated) can be obtained:

PEC_{local}= 4.5×10^3 µg l^{-1}	(T = 1×10^6 t/a (prod + proc), f_{prod} = 0.003, f_{proc} = 0.007, $T_{emission}$ = 300 d/a (prod + proc), $elimination_{STP}$: 94.6 %, dilution factor: 40).

Site-specific data for production and processing show a maximum PEC_{local} of

PEC_{local}= 14.1 µg l^{-1}

which is more than two orders of magnitude below the generic value.

3.1.4.1.2 Calculation of PEC_{local} for other processing

Ethylbenzene is used as chemical intermediate. Styrene production (99.5 %) was evaluated site-specifically (see 3.1.4.1.1). A small amount of ethylbenzene processed (0.5 %) could not be allocated to a specific site and was generically calculated giving a

PEC_{local}= 16.7 µg l^{-1}	(T = 26 400 t/a, f = 0.007 (A 3.3), $T_{emission}$ = 300 d/a, f_{ms} = 0.2 (B 3.2), $elimination_{STP}$: 94.6 %, dilution factor: 40).

Results are shown in Table 3.9.

3.1.4.1.3 Calculation of PEC_{local} for disposal

No calculation was performed (see 3.1.2.3).

3.1.4.2 Measured data

Monitoring data are reported in the literature, particularly from government and public institutions.

3.1.4.2.1 Water

The following table summarises the measured concentrations between 1985 and 1994. Details can be found in the Appendix II.

Table 3.10 Measured ethylbenzene concentrations in water compartments (1985-1994)

Water compartment	Concentration range [µg/l]	Typical value [µg/l]	Remarks
Surface water	0.004 - 5	0.01	Measured in rivers: Rhine, Lippe, Emscher (D) and Brazo, Lower Tennessee (USA)
Sea water	<0.005 - 15	0.02	Measured in North Sea (D) and Gulf of Mexico; wide range of concentrations due to measurements at sites with and without direct anthropogenic influence
Rain	0.007 - 0.44	~ 0.03	Measured at various sites in CH, D and USA; concentrations depending on season
Snow	0.13 - 2.7	1.1	Measured in CH
Ground water	0.01 - 3320		Measured in D, NL, UK, I, CAN and USA; partly at highly polluted sites, e.g. beneath former paint factory or former harzardous waste site
Drinking water	<0.05 - 30	1 - 2	Measured in USA, CAN, D

More recent measurements in surface waters are available for Germany, The Netherlands and France.

Ethylbenzene was measured at 132 different points throughout Germany including large and small rivers (1 – 25 measurements per year and per point). The 90th percentile of the maximum measured concentration of all values was < 1 µg/l between 1999 – 2001 (UBA (D), 2003a; UBA (D), 2003b).

Ethylbenzene was monitored in The Netherlands (RIVM). Concentrations monitored at 7 surface water sites for the years 1998 – 2004 (5-27 measurements per year per site) were consistently below the analytical detection limit of 0.01 µg/l. Older data of the same sites from 1987-1994 shows that concentrations in those years were (with the exception of 1987) also below the detection limit, which was 0.1 µg/l in those years.

There are 3 measured concentrations in French surface waters (all 0.1 µg/l) for 2000 and 2002, however, no more detailed information is available regarding the sites (INERIS, 2004). In 2002, 88 measurements were below the detection limit (0.1 µg/l).

The Environment Agency (2004) provided monitoring data for various regions within the UK dating from 1990-2003. Although specific locations are identified (by name and number code), the regions are neither further described (e.g. reason for monitoring) nor exactly spatially defined. For 3 regions (NEast, NWest, Midlands) the data comprise about 7000 samples each over that period. Between 100 – 1000 samples each were provided by the other regions. The 90 percentile values are shown in the following table.

Table 3.11 Measured ethylbenzene concentrations in the UK in [µg/l] (90th percentile value) between different time periods

Region	1993 - 2003	2001 - 2003
Anglian	≤ 0.7	≤ 0.5
Midlands	≤ 10.0	≤ 10.0
N East	≤ 18.5	≤ 2.0
N West	≤ 10.0	≤ 10.0
Southern	≤ 10.0	≤ 1.92
S West	≤ 0.10	≤ 0.11
Thames	≤ 0.50	≤ 0.10
Wales	≤ 10 600.0	≤ 100.0

The data vary widely. Spot checks revealed that some points of measurements are in the direct vicinity of industrial sites which might be one reason for the large differences between the regions. In general, one can notice a decreasing trend in ethylbenzene concentration measured over the last years.

Due to the heterogeneity of monitoring data it is difficult to draw specific conclusions. Typical concentrations of ethylbenzene found in surface, sea and rain water are at or below 0.1 µg/l. The calculated $PEC_{regional}$ (surface water) of 0.06 µg/l falls in that range too.

3.1.4.2.2 Sediment

France provided monitoring data of ethylbenzene in sediment from 2000 to 2002 (INERIS, 2004). The 90th percentile of all values is 4.0 µg/kg (63 values; in addition, 100 values were below the detection limit in 2002). No further information regarding the specifics of the sites or results (e.g. wet or dry weight) is known.

There are two further measurements regarding ethylbenzene in sediment: 4.0 µg/kg from the lower Tennessee River (Goodley and Gordon, 1976) and 5.0 mg/kg from the USEPA STORET database (median, dry weight) (Staples et al., 1985). No further information about location or conditions are known and it is also not known if the value of 4.0 µg/kg is based on wet or dry weight, therefore, these values can not be assessed.

3.1.4.2.3 Sewage sludge

The Austrian EPA analysed sludge from municipal WWTP (UBA (A), 1995) within a project to investigate sewage sludge for organic, inorganic and biological parameters. There was only one out of 17 samples showing ethylbenzene < 4.29 µg/l (wet weight), in all other samples ethylbenzene could not be detected (detection limit: 1.20 µg/l).

There is a further Austrian study of a pilot unit of the main Vienna WWTP (UBA (A), 2000). The samples were taken over 4 days (24 h) in May/June 1999, and subsequently mixed to 4 day samples. Only a few selected chemicals/chemical classes were quantitatively determined. Other substances, like ethylbenzene, were screened for, and their concentrations roughly estimated. Concentrations of ethylbenzene in sewage sludge were between < 0.05 and 0.1 mg/kg (dry weight). Ethylbenzene could not be detected in the wastewater (detection limit < 0.1 µg/l). Based on that the authors assume that ethylbenzene is formed in the WWTP as metabolite of other compounds.

The VOC concentrations of 12 digested sludges obtained from rural, urban and industrial wastewater treatment works in northwest England were investigated (Wilson et al., 1994). The percentage of industrial influent on the total influent flow varied between 1.4 to 45.6 %. Ethylbenzene was detected between 0.2 mg/kg dw (4.2 µg/l wet volume) and 9.0 mg/kg dw (338 µg/l wet volume). There was no apparent relationship between ethylbenzene concentration and percent of industrial influent, population served (capacity between 18 000 – 490 000 inhabitants) or solids content of sludge (1.7 – 6.5 %). Since values vary widely without specific information on the sites or origin of wastewater, these data can only be considered as indicative.

An American conference paper refers to measurements on municipal sludges done by EPA in 1980 (Naylor and Loehr, 1982). Combined sludges (i.e. a mixture of sludges generated by two or more wastewater treatment processes) of 13 treatment plants across the United States were analysed for priority pollutants. Ethylbenzene was detected in 12 of these sludges in concentrations between 1.0 – 51 mg/kg dw (median: 5.5 mg/kg dw), corresponding to 45 – 2100 µg/l wet volume (median: 248 µg/l wet volume).

None of the monitoring data available can be taken as representative since the studies are not described detailed enough. The American paper refers to measurements in the USA from over 20 years ago. The Austrian studies were done for screening purposes only. Therefore, the measured data can provide valuable additional information. However, the sludge concentration used further in the risk assessment is based on default calculations according to TGD (cf. 3.1.5).

3.1.4.3 Calculation of Predicted Environmental Concentration for Sewage Treatment Plants (PEC_{stp})

Since the PEC for micro-organisms in the STP (PEC_{stp}) equals the concentration in the effluent, the PEC_{stp} can be found in Table 3.9. The maximum value of effluent concentration is 14.0 mg l^{-1}, however there is a non-biological WWTP in place at that specific site. Therefore, the highest PEC_{stp} relevant for micro-organisms is 1.0 mg l^{-1}.

3.1.4.4 Calculation of Predicted Environmental Concentration for Sediment (PEC_{stp})

Using the highest aquatic exposure of PEC_{local_water} = 14.1 µg l^{-1} based on specific data (production and processing), K_{susp_water} = 11.69 m^3/m^3 and RHO_{susp} = 1150 kg/m^3 results in a

$$PEC_{local\_sed} = \frac{K_{susp\_water}}{RHO_{susp}} \cdot PEC_{local\_water}$$

PEC_{local_sed} = 142.9 µg kg^{-1} (wet weight).

3.1.5 Terrestrial compartment

Ethylbenzene is expected to rapidly evaporate and therefore to occur mainly in the vapour phase (see Chapter 3.1.3.2). However, the log Kow = 3.13 (Koc = 432) indicates a moderate adsorptivity. According to the SimpleTreat 3.0 model about 3.7 % of the total ethylbenzene are directed to sludge in the STP.

It is generally assumed that only sludge from municipal STPs is applied to soil. It is known of just one producer (PP3) to discharge effluents into a municipal STP. The expected sludge concentration is

C_{sludge}(PP3) = 107 mg/kg_{dw}.

This value is higher than all available measured data. The highest available value monitored is 51 mg/kg_{dw} (Naylor and Loehr, 1982). More recently obtained data show a range of 0.05 up to 9 mg/kg_{dw} (cf. 3.1.4.2.3). However, all available monitoring data have to be considered as not representative, since they are either only spot checks without detailed documentation, or over 20 years old. Therefore, the calculated C_{sludge} of 107 mg/kg_{dw} is used further in the risk assessment.

3.1.5.1 Calculation of PEC_{local}

Local soil scenarios are calculated as the sum of exposure through application of sludge and deposition. C_{sludge} of 107 mg/kg_{dw} results from production and processing with subsequent discharge of the effluents into a municipal WWTP.

A $PECregional_{nat\ soil}$ = 1.23 x 10^{-5} mg/kg_{wwt} was obtained as regional concentration in natural soil (see Table 3.17).

The results of the calculation for site PP3 are shown in the following table. For comparison, the results of the calculations for PP1 (highest deposition flux) are also shown which only gets input via deposition (no sludge application).

Table 3.12 Data used in local terrestrial exposure assessment

	Sludge appli-cation	DEPtotal $_{ann}$ [mg/(m^2 d)]	PEClocal $_{soil}$* [mg/kg]	PEClocal $_{agr\ soil}$* [mg/kg]	PEClocal $_{grassl}$* [mg/kg]	PEClocal $_{soil\_porew}$ [mg/l]	PEClocal $_{agr\ soil\_porew}$ [mg/l]	PEClocal $_{grassl\_porew}$ [mg/l]
PP3	yes	0.017	0.066	0.013	0.004	0.008	0.002	< 0.001
PP1	no	0.932	0.039	0.039	0.047	0.005	0.005	0.006

*Please refer to TGD, Chapter 2.3.8.5, Table 11 for characteristics of soil and respective endpoints.

Although the deposition rate assumed for PP1 is over 50 times higher than for PP3, the resulting PEClocal$_{soil}$(PP1) and PEClocal$_{soil}$(PP3) are of the same order of magnitude.

A model calculation for PP1 using the deposition flux of DEPtotal$_{ann}$ of 0.932 mg/(m^2 d) as well as sludge application (C$_{sludge}$ of 107 mg/kg$_{dw}$) results in a PEClocal$_{soil}$ of 0.104 mg/kg pointing to the fact that both exposure routes (i.e. sludge application and deposition) may be significant for local soil concentration of ethylbenzene. It should be kept in mind that the DEPtotal $_{ann}$ used were derived from generic calculations.

3.1.5.2 Measured data

Monitoring data of ethylbenzene in soil are very scarce and can therefore not be considered representative. 76 mg/kg was measured at a contaminated site of a former asphalt production unit in Deventer/NL (VANDERHOEK et al., 1989). Measurements in the immediate vicinity of 8 petrol stations near Hamburg/Germany found ethylbenzene in concentrations between < 0.1 mg/kg (limit of detection) and 120 mg/kg (Stachel, 1993). For these values it is not known if they are based on wet or dry weight.

3.1.6 Atmosphere

3.1.6.1 Calculation of PEC$_{local}$

All calculated PEC$_{local}$ (annual average) as well as the total release to air and the average annual deposition rate can be seen in Table 3.13. Background concentrations were used as given in Table 3.17.

Table 3.13 Data used in local atmospheric exposure assessment

		site-specific release information	direct release to air [t/a]	Clocal $_{air\_ann}$ [mg/m^3]	PEClocal $_{air\_ann}$ [mg/m^3]	total release to air (direct and from wwtp) [t/a]	DEPtotal $_{ann}$ [mg/(m^2 d)]
P1	production	release	2	1.5×10^{-3}	2.0×10^{-3}	3.6	0.003
P2	production	release, monitoring data	9	6.6×10^{-3}	7.0×10^{-3}	9	0.007
P3	production	release	3.6	0.003	3.2×10^{-3}	3.6	0.003
P4	production	release	1.2	9.1×10^{-4}	1.4×10^{-3}	1.2	0.001
P5	production	-	9.5	7.2×10^{-3}	7.7×10^{-3}	9.5	0.008
PP1	production and processing	-	1 134	0.864	0.864	1 134	0.932
PP2	production and processing	release	43.4	0.033	0.034	63.0	0.052
PP3	production and processing	release	20	0.015	0.016	21	0.017
PP4	production and processing	release	3.2	2.4×10^{-3}	2.9×10^{-3}	4.4	0.004
PP5	processing	release, monitoring data	5.1	3.9×10^{-3}	4.4×10^{-3}	6	0.005
PP6	production and processing	release	0.17	6.4×10^{-4}	1.1×10^{-3}	1.0	8.3×10^{-4}
PP7	production and processing	-	432	0.329	0.330	432	0.355
PP8	production and processing	release	8.7	0.025	0.026	42	0.034
PP9	production and processing	release	4.4	3.4×10^{-3}	3.8×10^{-3}	4.5	0.004
PP10	production and processing	-	436	0.332	0.333	436	0.359
PP11	production and processing	release	424	0.323	0.323	424	0.349
	other processing		2.6	0.013	0.014	89	0.015

3.1.6.1.1 Calculation of PEC_{local} for production, or production and processing

Generic scenario gives a maximum

$PEClocal_{air\_ann} = 3.55$ mg m^{-3}

for production and processing using T = 1 x 10^6 t/a (prod + proc), $f_{prod} = 0.001$ (A 1.2, MC 1c), $f_{proc} = 0.0001$ (A 3.3. MC 1c), $T_{emission} = 300$ d/a (prod + proc).

Using site-specific information results in a highest

$PEClocal_{air\_ann} = 0.864$ mg m^{-3}

for the same life cycle step.

For production only, a maximum $PEClocal_{air\_ann}$ of 0.008 mg m^{-3} was obtained using site-specific information.

3.1.6.1.2 Calculation of PEC_{local} for other processing

Using generic emission factors a $PEClocal_{air\_ann}$ of 0.014 mg m^{-3} was obtained for the processing of ethylbenzene not including styrene (Table 3.13). Input data used were $T_{ethylbenzene} = 26\,400$ t/a, f = 0.0001 (A 3.3, MC 1c), $T_{emission} = 300$ d/a, $f_{ms} = 0.2$ (B 3.2).

3.1.6.1.3 Calculation of PEC_{local} for disposal

No calculation was performed (see 3.1.2.3).

3.1.6.2 Measured data

There are a number of measurements of ethylbenzene in the atmosphere dating from 1984 - 1995. Concentrations vary greatly depending on the location and conditions. Over the Pacific Ocean ethylbenzene was measured in the range of 5 to 10 ng/m^3. In remote or rural areas (e.g. the Black Forest) measurements showed concentrations in the range of 0.01 to 3 µg/m^3. In major cities in B, CH, D, NL, USA monitoring data are mainly between 1 µg/m^3 and 100 µg/m^3, with a maximum value of about 10 mg/m^3 measured in Zurich/Switzerland. Most values are between 1 µg/m^3 and 10 µg/m^3. Measurements at industrial sites or places with heavy traffic result in values between 3 µg/m^3 and 200 µg/m^3. For details please refer to Appendix II.

There are very few monitoring data provided specifically by industry for this risk assessment. At one production site ethylbenzene was measured in the range of 0 – 136 ng/m^3 (131 measurements). One sporadic measurement at a downwind location of a processing site was given as 6.6 ng/m^3 (no further information).

Ethylbenzene can be released during combustion processes, e.g. power stations and waste incinerators. Only very few measurements exist.

Jay and Sieglitz (1995) analysed the emission of a municipal German incineration plant. They identified about 250 individual compounds representing ca. 42 % of the total organic carbon (TOC) in the emissions. Ethylbenzene concentration was determined to be about 3 µg/m^3. However, the authors mention a probable error of 50 %.

Measurements at another municipal German incineration plant identified an ethylbenzene concentration of < 5 µg/m^3 (Dohmann et al., 1999).

Concentrations of ethylbenzene in the exhaust of a Japanese waste incineration plant are cited as 38 µg/m^3 and 85 µg/m^3 (BUA, 1997). The same reference gives the quantity of ethylbenzene released by incineration plants in Germany as about 0.06 % of the traffic-related releases.

3.1.7 PEClocal for unintentional uses

As described in Chapter 3.1.7 significant emissions of ethylbenzene could occur from unintentional use of ethylbenzene. Main known source are the "mixed xylenes" which are predominantly used as petrol additive. Petrol-related emissions are only considered for the background concentration.

However, a generic calculation to obtain a PEClocal is performed for formulation and technical use of mixed xylenes as solvent (see Chapter 3.1.2.4.2). The fraction of main source was derived from the appropriate B-Tables, based on the estimated quantity of 7.1 x 10^4 t/a ethylbenzene in about 3.5 x 10^5 t/a mixed xylene solvents.

The following table shows the results. Background concentrations were used as given in Table 3.17.

Soil scenario was only calculated for life cycle step "technical use" since formulation is supposed to take place at site with industrial wwtp. Input to soil is assumed to be by deposition (DEPtotal $_{ann}$ = 2.65 mg m^{-2} d^{-1}) and sludge application (Csludge = 1.24 x 10^4 mg kg^{-1}).

Table 3.14 PEClocal for unintentional use of "mixed xylenes" as solvents for water, air and soil

		PEC local $_{water}$ [µg/l]	**PEC local $_{air\_ann}$** [mg/m^3]	**PEC local $_{soil}$** [mg/kg]
formulation	IC3/UC48	766	0.109	-

technical use	IC14/UC48	639	2.43	7.67

These PEClocal are higher (soil, water) or in the upper range (atmosphere) of PEClocal derived in Chapters 3.1.4, 3.1.5 and 3.1.6 in case default values had to be used there. Most PEClocal for sites where specific data were available are clearly below the above values. However, one has to keep in mind that all values of the above table are derived by using default values and that these have to be considered as worst-case assumptions.

3.1.8 Secondary poisoning

The log Kow of 3.13 indicates a potential for bioaccumulation. According to the TGD a BCF of 91 can be estimated from this value. However, experimental data (see 3.1.3.3) indicate that bioaccumulation of ethylbenzene is lower than predicted. Therefore, an assessment of secondary poisoning is not necessary.

3.1.9 Calculation of $PEC_{regional}$ and $PEC_{continental}$

For the calculation of the background concentration intentional and unintentional releases of ethylbenzene are taken into account. Intentional releases result from the identified and significant life cycle stages of ethylbenzene: production and processing as chemical intermediate. Unintentional releases occur by means of production and use of petrol as well as formulation and use of mixed xylene solvents.

The assumption is made that all producers and processors possess a waste water treatment plant.

Petrol-related emissions are only considered for the air compartment. All effluents from the formulation of mixed xylene solvents are thought to be treated in a wwtp, however, a connection rate of 80 % is believed to be realistic for the life cycle step of use of these solvents.

Table 3.15 and Table 3.16 summarise the total regional and continental releases.

Table 3.15 Summary of regional releases of ethylbenzene

		release to wwtp [t/a]	**release to surface water** [t/a]	**direct release to air** [t/a]	**release to soil** [t/a]
intentional	production, processing	31	0	254	105
unintentional	petrol-related			2 116	
	formulation and use of mixed solvent	135	28	6 426	8

total regional		166	28	8 796	113

Table 3.16 Summary of continental releases of ethylbenzene

		release to wwtp [t/a]	release to surface water [t/a]	direct release to air [t/a]	release to soil [t/a]
intentional	production, processing	280	0	2 285	941
unintentional	petrol-related			19 041	
	formulation and use of mixed solvent	1 214	256	57 829	70
total continental		1 494	256	79 155	1 011

Regional and continental background concentrations of ethylbenzene in different compartments were calculated using the values of Table 3.15 and Table 3.16 and SimpleBox 2.0a. Results are shown in Table 3.17 (see Appendix III).

Table 3.17 Continental and regional background concentrations

	unit	regional	continental
PEC surface water	$mg\ l^{-1}$	6.40×10^{-5}	7.20×10^{-6}
PEC air	$mg\ m^{-3}$	4.62×10^{-4}	1.43×10^{-4}
PEC agr soil	$mg\ kg_{wwt}^{-1}$	7.40×10^{-5}	9.50×10^{-6}
PEC porewater agr soil	$mg\ l^{-1}$	9.56×10^{-6}	1.23×10^{-6}
PEC nat soil	$mg\ kg_{wwt}^{-1}$	1.23×10^{-5}	3.81×10^{-6}
PEC sediment	$mg\ kg_{wwt}^{-1}$	5.62×10^{-4}	7.03×10^{-5}

3.2 EFFECTS ASSESSMENT: HAZARD IDENTIFICATION AND DOSE (CONCENTRATION) - RESPONSE (EFFECT ASSESSMENT)

3.2.1 Aquatic compartment (incl. sediment)

3.2.1.1 Toxicity test results

For ethylbenzene many ecotoxicity tests are reported. Due to the volatility of the substance only studies using flow-through or closed systems with analytical measurement of ethylbenzene concentrations are suitable for effect assessment purposes. Other available acute studies using static testing methods without supporting analysis were therefore not used in this assessment.

The most relevant results of acute toxicity tests with aquatic organisms are summarized in Table 3.18 and are described in more detail below.

Table 3.18 Most relevant results of acute toxicity tests with aquatic organisms

Test organism/ source	**duration**	**test design/ remarks**	**analytical data**	**effect concentration [mg/l]**	**effect**
Vertebrates, short-term toxicity					
Menidia menidia (Boeri, 1987a)	96 h	flow-through saltwater	y	96 h-LC_{50} = 5.1	mortality
Pimephales promelas (Geiger et al., 1986)	96 h	flow–through freshwater	y	96 h-LC_{50} = 12.1	mortality
Oncorhynchus mykiss (Galassi et al., 1988)	96 h	semi-static, closed bottles OECD 203 freshwater	y	96 h-LC_{50} = 4.2	mortality
Morone saxatilis (Benville and Korn, 1977)	96 h	static, open system more than 99% of test substance was lost within 24 h saltwater	y	96 h-LC_{50} = 4.3 a)	mortality
Poecilia reticulata (Galassi et al., 1988)	96 h	semi-static, closed bottles OECD 203 freshwater	y	96 h-LC_{50} = 9.6	mortality
Invertebrates, short-term and long-term toxicity					
Mysidopsis bahia (Boeri, 1988)	96 h	flow-through saltwater	y	96 h-LC_{50} = 2.6	mortality
Daphnia magna (Vigano, 1993)	24 h 48 h	static, EPA method F closed system freshwater	y	24 h-LC_{50} = 2.3-2.9 48 h-LC_{50} = 1.8-2.4	immobilization
Ceriodaphnia dubia (Niederlehner et al., 1998)	7 d	semi-static, EPA Whole Effluent Testing Program method, modified to minimize volatilization freshwater	y	7 d-LC_{50} = 3.6 7 d-IC_{50} = 3.3 (repro) 7 d-LOEC = 1.7 (repro) 7 d-NOEC = 1.0 (repro) 48 h-LC_{50} = 3.2	mortality / reproduction
Daphnia magna (Abernethy et al., 1986; Bobra et al., 1983)	48 h	static, closed system freshwater	n	48 h-LC_{50} = 2.1 b)	mortality
Artemia salina (Abernethy et al., 1986)	24 h	static, closed system saltwater	n	24 h-LC_{50} = 15.4 b)	mortality
Daphnia magna (MacLean and Doe, 1989)	48 h	static, closed system freshwater	y	48 h-EC_{50} = 2.9	immobilization

Test organism/ source	duration	test design/ remarks	analytical data	effect concentration [mg/l]	effect
Artemia salina (MacLean and Doe, 1989)	48 h	static, closed system saltwater	y	48 h-EC_{50} = 9.2	immobilization
Crago franciscorum (Benville and Korn, 1977)	24 h 96 h	static, open system more than 99% of test substance was lost within 24 h saltwater	y	24 h-EC_{50} = 2.2 [a] 96 h-EC_{50} = 0.49 [a]	y
Daphnia magna (Galassi et al., 1988)	24 h	OECD 202 effect: immobilization freshwater	y	24 h-IC_{50} = 2.2	immobilization
Plants					
Selenastrum capricornutum (Boeri, 1987b)	96 h	TSCA 797.1050 freshwater	y	72 h-E_RC_{50} = 5.9 72 h-NOEC = 3.4 96 h-E_RC_{50} = 5.0 96 h-E_RC_{10} = 3.4	growth rate
Skeletonema costatum (Boeri, 1987c)	96 h	TSCA 792.1050, static saltwater	y	72 h-E_RC_{50} = 7.7[b] 72 h-NOEC = 4.5 [b]	growth rate
Selenastrum capricornutum (Galassi et al., 1988)	72 h	growth inhibition test freshwater	y	72 h-E_RC_{50} = 4.6	growth rate

[a] test result is not valid [b] exponential growth in the control only over 72 h

3.2.1.1.1 Fish

The short-term toxicity of ethylbenzene to the fathead minnow (*Pimephales promelas*) was examined by Geiger et al. (1986) using a flow-through water test supported by chemical analysis. Fish were exposed at about 26°C for 96 h in dechlorinated laboratory water or unfiltered lake water (pH 7.4, oxygen content 7.0 mg/l, water hardness 45.6 mg/l $CaCO_3$). Different concentrations of test solutions were applied by diluting (factor 0.5) a stock solution of the test substance. The toxicant concentrations causing 50% mortality of the fish with corresponding 95% confidence intervals were calculated using the corrected average of the analysed tank concentrations. For ethylbenzene a 96 h-LC_{50} of 12.1 mg/l (95% confidence limits 11.5-12.7 mg/l) was found.

Galassi et al. (1988)) studied the acute toxicity of ethylbenzene in fish with *Oncorhynchus mykiss* (rainbow trout) and *Poecilia reticulata* (guppy) as test organisms. Toxicity tests were carried out according to the OECD Guideline 203 "Fish acute toxicity tests" (1981). Due to the volatility of the test substance tests were performed in closed bottles. At 48 hours from the beginning of the test, test solutions were renewed. Based on mean measured concentrations a 96 h-LC_{50} of 4.2 mg/l for *Oncorhynchus mykiss* and a 96 h-LC_{50} of 9.6 mg/l for *Poecilia reticulata* was obtained from this study.

Benville and Korn (1977) investigated the toxicity of ethylbenzene to the striped bass *Morone saxatilis*. Fish were exposed in a static system for 96 h with five test concentrations (nominal concentration range from 1.0 to 20 mg/l). A saturated solution of ethylbenzene was prepared and diluted to the desired concentration with natural seawater (salinity 25‰, temperature 16°C). The study was designed as a single dose test where the concentration was decreasing over time. Based on analytical results it was observed that more than 99% of the initial concentration in the test system was lost within 24 hours. As no attempt was made to supplement the toxicant and it is not known how the mean exposure concentration over the whole test duration was calculated, the test result is regarded as not valid.

A further acute toxicity bioassay was conducted by Boeri (1987a) using the Atlantic silverside *Menidia menidia* as test organism. The test was performed under flow-through conditions with five test concentrations ranging nominally from 21 to 100 mg/l and a dilution water control. Chemical analysis of ethylbenzene in the test vessels was conducted on samples collected at 0, 48 and 96 hours after the start of the test. Suitable precautions were taken to prevent losses of test substance by volatilization in the test samples. As dilution water natural seawater (salinity 20-21‰, temperature 21-22°C, dissolved oxygen 6.9-9.2 mg/l, pH 7.7-8.2) was used. Twenty fish per treatment divided in two groups (average length 12 mm, average weight 0.008 g, age not stated) were exposed. Referring to mean, measured concentrations a 96 h-LC_{50} of 5.1 mg/l (95% confidence limits 4.4-5.7 mg/l) was found.

3.2.1.1.2 Aquatic invertebrates

The 96 hr acute toxicity of ethylbenzene to the mysid *Mysidopsis bahia* was determined by Boeri (1988). The test was conducted under flow-through conditions with five test concentrations of ethylbenzene ranging nominally from 1.0 to 9.1 mg/l and a dilution water control. As dilution water filtered natural seawater (salinity 20‰, pH 7.8-8.0, $CaCO_3$ 117 mg/l, temperature 25 +/- 1°C) was used. Twenty mysids were randomly distributed among two replicates of each concentration level. Test vessels consisted of loosely covered glass aquaria that contained 9 l of media and mysids were fed live *Artemia salina* during the test. The number of live mysids and the occurrence of abnormal behavior were determined daily. Aeration was not employed during the test and the photoperiod was adjusted to 14 h light and 10 h dark. Based on mean measured concentrations a 96 h-LC_{50} of 2.6 mg/l (95% confidence limits 2.0-3.3 mg/l) was derived.

Vigano (1993) investigated the ecotoxic effect of ethylbenzene on juvenile *Daphnia magna* fed on different food rations. Animals were tested in closed bottles that were completely filled with test solutions. Concentration of dissolved oxygen, measured at the end of the tests (48 h), was always higher than 5 mg/l (approx. 60% saturation). The test medium had a hardness of 150 mg/l as $CaCO_3$, alkalinity 120 mg/l as $CaCO_3$, Ca/Mg = 4, Na/K = 1, water temperature 20°C. Cultures were maintained under a photoperiod of 16 h light and 8 h dark. Toxic effects were recorded as percentage of immobility at 24 and 48 h of exposure. Test results were based on measured concentrations. The toxicity test results at 48 h of exposure revealed only minor effects of feeding levels. A 24 h-EC_{50} of 2.3-2.9 mg/l and a 48 h-EC_{50} of 1.8-2.4 mg/l respectively was obtained from this study.

The response of the daphnid *Ceriodaphnia dubia* to ethylbenzene was determined by Niederlehner et al. (1998) using the standard short-term and chronic test method developed for U.S. EPA's Whole Effluent Testing Program (U.S. EPA 1994) The test design was modified to minimize volatilization of test chemicals. Organisms were tested in completely filled and tightly closed bottles. Tests were conducted in artificial moderately hard water (pH 7.6, hardness 68.3, alkalinity 88.0, dissolved oxygen above 7.0 ppm). Light was provided at a photoperiod of 16 h light and 8 h dark. Solutions were renewed daily. Survival, behaviour, and reproduction were observed at the time of daily renewal. Acute toxicological results were based on the geometric mean of two measured concentrations for each treatment level measured at the beginning of the test. Chronic toxicological results were based on the geometric mean of four measured concentrations of each treatment level measured during the duration of the experiment. 84.4% of initial test concentration was present at the end of the study. The toxicity studies in *Ceriodaphnia dubia* found with a 48 h-LC_{50} of 3.2 mg/l, a 7 d-LC_{50} of 3.6 mg/l and a 7 d-IC_{50} of 3.3 mg/l (reproduction) almost identical values for the acute and the repeated exposure toxicity. As long-term NOEC a 7 d-NOEC of 1.0 mg/l (reproduction) was derived.

A further acute toxicity test was conducted by Abernethy et al. (1986) with two planktonic crustaceans (freshwater *Daphnia magna* and saltwater *Artemia salina*) as test organisms. A saturated aqueous solution of the test substance was prepared and diluted to provide at least five exposure concentrations. As dilution water distilled water and saltwater (salinity 30‰) respectively was used. To minimize volatilization loss of the toxicant from water, test chambers were filled completely and sealed. Bioassays were conducted in the dark at approx. 23°C for *Daphnia* and at approx. 20°C for *Artemia* tests. Toxicant solutions were not aerated during the exposure period, the lowest oxygen concentration measured after 48 h was 5 mg/l in *Daphnia* tests. As the effective concentrations were not measured, results of this study should be used with care. Referring to nominal concentrations a 48 h-LC_{50} of 2.1 mg/l for *Daphnia magna* and a 24 h-LC_{50} of 15.4 mg/l for *Artemia salina* was obtained.

An acute immobilzation study with *Daphnia magna* in reconstituted freshwater and *Artemia salina* in synthetic seawater (salinity 30‰) was performed by Maclean and Doe (1989). As test substance the water soluble fraction of ethylbenzene was used. Test chambers were capped immediately with no air space. Tests with *Artemia salina* were conducted in the dark at a temperature of approx. 20°C, tests with *Daphnia magna* were carried out with a photoperiod of 16 h light and 8 h dark at temperature of approx. 20°C. Initially and at test termination selected test solutions were analysed using fluorescence spectroscopy. Test solutions were also measured for temperature, dissolved oxygen and pH. For *Daphnia magna* a 48 h-EC_{50} of 2.9 mg/l and for *Artemia salina* a 48 h-EC_{50} of 9.2 mg/l was derived.

Galassi et al. (1988) studied the acute toxicity of ethylbenzene in *Daphnia magna*. Toxicity tests were carried out according to the OECD Guideline 202 “Immobilization”. The determination of 24-h IC_{50} (immobilization concentration for 50% of the organisms) on Daphnia was performed in closed bottles, completely filled with the test solution. A 48 h-IC_{50} of 2.2 mg/l based on the mean values of the analytically detected concentrations was reported.

Benville and Korn (1977) studied the toxicity of ethylbenzene to the bay shrimp *Crago franciscorum*. Mature shrimp were exposed for 96 h in a static system with five test concentrations (nominal concentration range from 1.0 to 20 mg/l). A saturated solution of ethylbenzene was prepared and diluted to the desired concentration with natural seawater (salinity 25‰, temperature 16°C). The study was designed as a single dose test where the concentration was decreasing over time. Based on analytical results it was observed that more than 99% of the initial concentration in the test system was lost within 24 hours. As no attempt was made to supplement the toxicant and it is not known how the mean exposure concentration over the whole test duration was calculated, the test result is regarded as not valid.

3.2.1.1.3 Algae

The acute toxicity of ethylbenzene to the freshwater algae *Selenenastrum capricornutum* and to the diatom *Skeletonema costatum* was determined by Boeri (1987b; 1987c). Tests were conducted with five test concentrations of ethylbenzene ranging nominally from 15 to 100 mg/l and a dilution water control. As test water deionized water (pH 4.2, $CaCO_3 < 5.0$ mg/l, temperature approx. 24°C) and natural seawater (pH 8.0, salinity 30‰, temperature approx. 20°C) respectively was used. To minimize the loss of test substance by volatilization test vessels consisted of 40 ml glass vials filled to capacity and were sealed with Teflon caps. Test vessels were replicated 16 times, allowing three vials to be sacrificed for algal counts at 24, 48, 72 and 96 hours after the start of the test and four vials to be taken for chemical analysis at 0, 48 and 96 hours after the start of the test. Analytical determination of test material was performed on media from one replicate test vial at the initiation and termination of the test. All calculations were performed using mean, measured concentrations. A 96 h-E_RC_{50} of 5.0 mg/l (95% confidence limits 4.6-5.5 mg/l) and a 96 h-E_RC_{10} of 3.4 mg/l was derived for *Selenastrum capricornutum*. Since the algae in the study with *Skeletonema costatum* were only during the first 72 hours in the exponential growth phase, the effects assessment for *Skeletonema costatum* is based on this period leading to a 72 h-E_RC_{50} of 7.7 mg/l (95% confidence limits 6.79-8.79 mg/l) and a 72 h-NOEC of 4.5 mg/l.

Galassi et al. (1988) studied the acute toxicity of ethylbenzene in *Selenastrum capricornutum*. Toxicity tests were carried out according to the OECD Guideline 201 “Alga, Growth Inhibition Test”. For the determination of 72 h-EC_{50} (concentration resulting in 50% growth inhibition) on *Selenastrum* the test vessels were modified in order to maintain constant concentration and to allow sampling of the culture medium without opening the vessel. Algal growth was evaluated by a Coulter Counter. A 72 h-E_RC_{50} of 4.6 mg/l based on the mean values of the analytically detected concentrations was reported.

3.2.1.1.4 Microorganisms

Several data sets are reported for microorganisms including studies with mixed or single-species inoculum of aerobic and anaerobic bacteria. Additionally, results from protozoa are available. From the data reported, the most relevant are described in more detail below.

Blum and Speece (1991) investigated the toxicity of several chemicals to aerobic heterotrophs and *Nitrosomonas*. Assays were carried out in sealed serum bottles under similar experimental conditions:

Seed bacteria for the aerobic heterotroph culture were obtained from the mixed liquor of an activated sludge wastewater treatment plant. Diffused aeration provided complete mixing and aeration in the reactor. The reactor was fed a complex carbon source (COD 3800 mg/l). The hydraulic and the solids retention time was 5 days. The nitrifier populations were estimated to be only 1 % of the total bacteria population. Inhibition of oxygen uptake was used as criterion for the toxic inhibition of the aerobic heterotrophs. Data were collected at 15, 27, 38 and 49 hours after the start of the test.

The seed bacteria for the nitrifying enrichment culture was obtained from the mixed liquor of an activated sludge plant treating meat-packing, rendering, and hide-curing wastewater. Diffused aeration provided complete mixing and aeration in the reactor. The culture was fed two times per day approximately 1000 mg/l ammonia-nitrogen. The hydraulic and the solids retention time was 25 days. As the criterion for the toxic inhibition of *Nitrosomonas* the inhibition of ammonia consumption was used.

Table 3.19 Toxicity in aerobic heterotrophs *and Nitrosomonas (*Blume and Speece, 1991*)*

Species	exposure period	Temp. [°C]	effect concentration	Initial atmosphere	effect
Aerobic heterotrophs	15 h	25 or 35	15 h-IC_{50} = 130 mg/l	pH =7 N2 : O2 = 1 : 1	Inhibition of oxygen consumption
Nitrosomonas	24 h	25	24 h-IC_{50} = 96 mg/l	pH =7 N2 : O2 = 1.6 : 1	Inhibition of ammonia consumption

In a respiration inhibition test according to OECD Guideline 209 (test was modified to minimize the loss of volatile organic compunds) Volskay and Grady (1990) observed after 30 minutes of incubation a 30%-decrease in oxygen consumption. The concentration of ethylbenzene was at the limit of solubility in the medium (approximately 150 mg/l). The activated sludge source used for the experiment was maintained in continuous flow reactor (solids retention time 2 days, temperature 10°C) receiving a complex synthetic feed designed to mimic the soluble content of domestic wastewater. Because the culture was grown primarily for other purposes, the feed also contained different aromatics. In a respiration inhibition kinetic analysis (RIKA) with butyric acid as substrate the same authors recorded after 3 hours of exposure 100% inhibition for the same initial concentration.

Bringmann and Kühn (1977) studied the effects of ethylbenzene on bacteria in a cell multiplication inhibition study. For *Pseudomonas putida* a toxicity threshold of 12 mg/l (exposure period 16 hours) was obtained. As other more reliable test results are available for ethylbenzene this result is not used for the assessment.

Table 3.20 summarizes the test results for different protozoa which were obtained from cell multiplication inhibition studies by Bringmann and Kühn (1981). As the test vessels were sealed only with metal caps and the effective concentrations of ethylbenzene were not measured, the reported toxicity threshold values should be used with care.

Table 3.20 Toxicity in protozoa (Bringmann and Kühn ,1981)

Species	exposure period	pH	Temp. [°C]	effect concentration
Chilomonas paramaecium (saprozoic flagellates)	48 h	6.9	20	48 h-TGK (EC_5) > 56
Uronema parduzci (holozoic, bacterial-eating ciliates)	20 h	6.9	25	20 h-TGK (EC_5) > 110
Entosiphon sulcatum (holozoic, bacterial-eating flagellates)	72 h	6.9	25	72 h-TGK (EC_5) = 140

In an oxygen consumption test with mixed bacterial populations Krebs (1991) determined a 24 h-EC_{10} of 21 mg/l and a 24 h-EC_{50} of 53 mg/l. The oxygen consumption test is a method, where the intoxication of the biochemical degradation of organic substances by heterotrophic bacteria occurring in surface waters is measured via a reduced oxygen depletion in sealed incubation bottles. As this method is designed to assess the harmful effects of waste waters on the self purification capacity of surface waters, which are not representative for an activated sludge system, this test result is regarded as not suitable for the determination of a $PNEC_{microorganism}$.

3.2.1.2 Calculation of Predicted No Effect Concentration (PNEC)

3.2.1.2.1 Determination of PNECaqua

For ethylbenzene short-term results are available for organisms representing three trophic levels including freshwater and saltwater species. The relevant LC_{50}-/EC_{50}-values are in the narrow range of 1.8 mg/l (daphnids) to 4.6 mg/l (algae) showing a similar sensivity of the three trophic levels. The most sensitive organism appears to be the aquatic invertebrate *Daphnia magna* with a 48 h-EC_{50} of 1.8 mg/l.

As two long-term NOECs from two trophic levels are available (aquatic invertebrates and algae) according to TGD an assessment factor of 50 should be used. The most sensitive species in long-term studies was the saltwater invertebrate *Ceriodaphnia dubia* with a 7 d-NOEC of 1.0 mg/l.

However, it was pointed out by Member States that ethylbenzene is a neutral organic substance well-known to act by baseline toxicity. Consequently the TC NES agreed to use an assessment factor of 10 in consistency with the approach taken for other neutral organic chemicals. Applying an assessment factor of 10 to the long-term result of aquatic invertebrates leads to

$$\mathbf{PNEC_{aqua} = 1.0\ mg/l / 10 = 100\ \mu g/l}$$

3.2.1.2.2 Determination of $PNEC_{microorganisms}$

According to the different endpoints and sensitivities of the used test systems, the TGD recommends the following assessment factors (AF):

Activated sludge (respiration inhibition)	15 h-EC_{50} =	130 mg/l	AF = 100	⇒ PNEC = 1.3 mg/l
Nitrosomonas	15 h-EC_{50} =	96 mg/l	AF = 10	⇒ PNEC = 9.6 mg/l

The most sensitive microorganism to ethylbenzene was *Nitrosomonas* representing the nitrification step in a sewage treatment plant (STP).

Although the PNEC derived from the activated sludge test is lower than the PNEC derived from the lowest effect value for *Nitrosomonas*, it is proposed to use the latter for the risk assessment according to TGD. Therefore,

$$\mathbf{PNEC_{microorganisms} = 9.6\ mg/l}$$

3.2.1.3 Toxicity test results for sediment organisms

As no experimental results with benthic organisms are available the $PNEC_{sed}$ can be provisionally calculated using the equilibrium partitioning method. According to TGD this method uses the $PNEC_{aqua}$ for aquatic organisms (= 100 µg/l) and the Ksusp_water of 11.7 m^3/m^3 as inputs and leads to

$$PNEC_{sed} = \frac{K_{susp\_water}}{RHO_{susp}} \cdot PNEC_{water} \cdot 1000$$

$PNEC_{sed}$ = 1017 µg/kg $_{wwt}$

3.2.2 Terrestrial compartment

3.2.2.1 Toxicity test results

3.2.2.1.1 Earthworm

In an earthworm contact test with four earthworm species (*Eisenia fetida*, *Allolobophora tuberculada*, *Eudrilus eugeniae* and *erionyx excavatus*) as test organisms Callahan et al. (1994) found a LC_{50} of 4.93 µg kg^{-1} body weight after two days of exposure. As the report does not specify which species was used for ethylbenzene, this test result is not assignable.

A further study of 48 hours duration using filter paper media was conducted in an indoor laboratory with laboratory obtained *Eisenia fetida* (earthworm). In this study Neuhauser et al. (1985) found a 48 h-LC_{50} of 47 µg cm^{-2} contact area (95% confidence level 42-53 µg cm^{-2}).

3.2.2.2 Calculation of Predicted No Effect Concentration ($PNEC_{soil}$)

The only available test results for the terrestrial compartment were originated from contact tests with soil dwelling organisms. A $PNEC_{soil}$ cannot be deduced from these data.

If there are no data on effects to terrestrial organisms available, for an indicative risk assessment, the $PNEC_{soil}$ can be provisionally calculated using the equilibrium partitioning method. Applying this method and using K_{soil_water} of 13.2 m^3/m^3 leads to

$$PNEC_{soil} = \frac{K_{soil\_water}}{RHO_{soil}} \cdot PNEC_{water} \cdot 1000$$

$PNEC_{soil,\ calculated}$ = 776 µg/kg (wet weight)

3.2.3 Atmosphere

3.2.3.1 Biotic effects

Terrestrial plants

On exposing leaves of the runner bean (*Phaseolus multiflorus*) and parsnip (*Pastinaca sativa*) to ethylbenzene at a range of vapour concentrations for 1 h it was found that the concentrations causing no damage and those completely killing the leaves were close. The author subsequently determined an EC_{50} of 27 and 48 g/m³ respectively (Ivens, 1952).

Determination of $PNEC_{air}$

The only available experimental data on terrestrial plants are obtained from fumigation studies with *Phaseolus multiflorus* and *Pasticana sativa*.

Data base is considered to be not sufficient for the derivation of the $PNEC_{air}$ for ethylbenzene.

3.2.3.2 Tropospheric ozone formation

The formation of tropospheric ozone involves complicated chemical reactions between NO_x and VOC driven by the solar radiation. In order for these reactions to occur in substantial quantities, meteorological conditions must prevail that prevents dispersion of NO_x and hydrocarbons. After a night time accumulation NO_x reacts with sunlight to produce NO and highly reactive atomic oxygen. The atomic oxygen may react with many compounds in the air, i.e. O_2 to produce O_3 or VOC to produce free radicals. The time scale of ozone production is such that ozone concentrations may build up over several days under suitable weather conditions, and that this pollutant and its precursors can be transported over considerable distances (European Commission DG XI, 1998).

There is as yet no consensus on the quantitative yield of these reactions, making modelling of these processes difficult. In addition to the VOC speciation and concentrations, VOC/NO_x ratio, solar radiation and meteorological conditions vary from city to city within the EU. Since the environmental conditions differ considerably, a certain concentration of VOC may lead to very different ozone concentrations within the EU. For example European Commission DGXI (European Commission DG XI, 1998) used a simplified EMEP model calculations and showed how a change in the VOC concentration may affect the ozone formation to a small extent in some parts of Europe (NO_x limited region), while in other parts of Europe a change in the VOC concentration will lead to a considerable change in the ozone formation (high NO_x regions). Thus there is no simple relationship between the VOC and NO_x concentrations and the resulting tropospheric ozone creation. The ozone concentrations may at some places of Europe even be higher at the same VOC concentration and at lower NO_x concentrations than may be the case at other places. Likewise the time trends of the tropospheric ozone concentration for Europe in general cannot not be forecasted by predicting the future concentrations of VOC and NO_x.

Nevertheless, the member countries in UNECE have agreed to use a Photochemical Ozone Creation Potential (POCP) factor system where the individual VOC's potential to create ozone is given as a relative equivalence factor expressed as g ethylene / g VOC (gas) (Hauschild and Wenzel, 1998). Here their relative importance has been evaluated against ethylene, which is given a value of 100. Two sets of factors exist corresponding to a low and high NO_x situation.

Hauschild and Wenzel (1998) proposed POCP equivalence factors for ethylbenzene of 0.5 g C_2H_4/g ethylbenzene gas in a low NO_x situation and 0.6 g C_2H_4/g ethylbenzene gas in a high NO_x situation.

To evaluate the relative importance of ethylbenzene for the creation of troposheric ozone using the POCP factor system the VOC composition within the region of concern has to be known. For a simple evaluation of the relative importance of the isolated commercial product ethylbenzene for the creation of ozone the VOC composition from industrial sources as well as the VOC composition from other sources e.g. traffic emissions have to be known. For a more in depth evaluation also the solar radiation and the NO_x concentrations have to be taken into account. These will of course vary considerably in Europe, between regions and between individual sites within the region as will also the VOC composition which depends on composition of the regional / local industrial sector and the traffic.

In the following an attempt to evaluate the relative contribution of non-isolated ethylbenzene (traffic emissions) and isolated ethylbenzene to the ozone creation potential has been performed.

3.2.3.2.1 Creation of tropospheric ozone due to non-isolated ethylbenzene in car exhaust based on one monitoring event

In Table 3.21 the mean road site concentrations of individual NMVOCs (non-methane volatile organic compounds) at a site in Copenhagen during 5 d in December 1997 is shown. Using the POCP equivalence factors it is possible to estimate the relative contribution of non-isolated ethylbenzene to the potential overall tropospheric ozone creation for such a NMVOC composition. It has to be emphasised that NMVOC composition from this site in Copenhagen is only used as an example, and that it is unlikely in this specific case that considerable ozone concentrations will build up within the region of Copenhagen as a consequence of these ethylbenzene concentrations due to low solar radiation and the prevailing wind conditions.

Table 3.21 Monitoring results of different NMVOCs at Jagtvej, Copenhagen December 1-5 1997 (Christensen (1999), and the relative contribution to potential ozone creation. Table from the EU Toluene RAR, Final Report March 2001

Substance	Mean	Range	S.D.	Median	POCP g C2H4/g gas[9]		Relative O3 creation[10]	
	ppbv	ppbv	ppbv	ppbv	low NOx	High NOx	low NOx	high NOx
Pentane	**2.4**	**0.4-5.7**	**1.2**	**2.5**	**0.3**	**0.4**	**2.12E-03**	**2.83E-03**
trans-2-Pentene	**0.2**	**0.01-0.5**	**0.1**	**0.2**	**0.4**	**0.9**	**2.29E-04**	**5.16E-04**
2-Methyl-2-butene	**0.4**	**0.02-0.9**	**0.2**	**0.3**	**0.5**	**0.8**	**5.73E-04**	**9.17E-04**
cis-2-Pentene	**0.1**	**0.01-0.3**	**0.1**	**0.1**	**0.4**[11]	**0.9**	**1.15E-04**	**2.58E-04**
2,2-Dimethylbutane	**0.9**	**0.04-2.3**	**0.5**	**0.9**	**0.3**	**0.3**	**9.51E-04**	**9.51E-04**
Cyclohexane	**0.5**	**0.04-1.1**	**0.3**	**0.5**	**0.25**	**0.25**	**4.30E-04**	**4.30E-04**
2,3-Dimethylbutane	**0.4**	**0.03-1.0**	**0.2**	**0.4**	**0.4**	**0.4**	**5.64E-04**	**5.64E-04**
2-Methylpentane	**2**	**0.2-5.2**	**1.1**	**2.1**	**0.5**	**0.5**	**3.52E-03**	**3.52E-03**
3-Methylpentane	**1.1**	**0.1-2.7**	**0.6**	**1**	**0.4**	**0.4**	**1.55E-03**	**1.55E-03**
n-Hexane	**0.8**	**0.1-2.3**	**0.5**	**0.8**	**0.5**	**0.4**	**1.41E-03**	**1.13E-03**
Isoprene	**0.2**	**0.01-0.6**	**0.1**	**0.2**	**0.6**	**0.8**	**3.34E-04**	**4.46E-04**
2-Methyl-1-Pentene	**0.04**	**0.01-0.1**	**0.02**	**0.02**	**0.5**[12]	**0.9**	**6.88E-05**	**1.24E-04**
cis-2-Hexene	**0.03**	**0.01-0.1**	**0.01**	**0.02**	**0.5**	**0.9**	**5.16E-05**	**9.29E-05**
2,4-Dimethylpentane	**0.2**	**0.01-0.7**	**0.1**	**0.2**	**0.4**[13]	**0.4**	**3.28E-04**	**3.28E-04**
Methyl-cyclohexane	**0.3**	**0.02-0.6**	**0.1**	**0.3**	**0.5**	**0.6**	**6.02E-04**	**7.22E-04**
2- and 3-Methylhexane	**1.4**	**0.1-3.7**	**0.8**	**1.3**	**0.5**	**0.5**	**2.87E-03**	**2.87E-03**
n-heptane	**0.7**	**0.1-1.9**	**0.4**	**0.6**	**0.5**	**0.5**	**1.43E-03**	**1.43E-03**
Benzene	**3.4**	**0.2-8.0**	**1.7**	**3.3**	**0.4**	**0.2**	**4.34E-03**	**2.17E-03**
2- and 3-Methylheptane	**0.4**	**0.01-1.0**	**0.2**	**0.3**	**0.5**	**0.5**	**9.34E-04**	**9.34E-04**
Toluene	**10.2**	**0.8-21.5**	**5.6**	**8.9**	**0.47**	**0.6**	**1.81E-02**	**2.31E-02**
Ethylbenzene	**2**	**0.1-4.9**	**1.1**	**1.9**	**0.5**	**0.6**	**4.34E-03**	**5.21E-03**
o-Xylene	**2.7**	**0.1-6.2**	**1.4**	**2.6**	**0.2**	**0.7**	**2.34E-03**	**8.20E-03**
m- and p-Xylene	**5.5**	**0.3-12.7**	**2.9**	**5.5**	**0.5**	**0.95**	**1.19E-02**	**2.27E-02**
Relative contribution of non-isolated ethylbenzene: %							**7.34**	**6.41**

The result of this calculation shows that if the VOC composition is as measured in the Copenhagen study non-isolated ethylbenzene potentially would exhibit approx. between 6.4 and 7.4 % of the total VOC contribution to ozone creation.

3.2.3.2.2 Creation of tropospheric ozone due to ethylbenzene based on estimated emissions

As described the creation of tropospheric ozone is dependent on the occurrence of VOC, NO_x, solar radiation and thus OH-radicals in a complicated relationship. The VOC composition will be highly variable and depend on the industrial sources, traffic emissions and natural sources. The contribution from isolated commercial ethylbenzene will depend on the composition of local and regional industry. Therefore, average calculations are likely to underestimate the magnitude of the problem within certain regions with high exposure potential.

The total NMVOC emitted in EU15 is shown in the table below.

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[9] POCP equivalence factors from Hauschild & Wenzel (1998) except for cyclohexane from EU RAR

[10] Calculated at Standard Temperature and Pressure (STP)

[11] Data for *trans*-2-Pentene used

[12] Average data for alkanes with double bonds used

[13] Average data for alkanes without double bonds used

Table 3.22 Emission of NMVOC in EU15 (EEA - European Environment Agency, 2001)[14]

NMVOC in EU15 (Kilotons)										
1980	1985	1990	1991	1992	1993	1994	1995	1996	1997	1998
16435	16248	16097	15521	14690	14323	14203	13736	13078	12715	12478

The mean total emission of NMVOC in 1998 is approx. 12 500 kt/a. This value is in the following table related to the known emissions of ethylbenzene (cf. 3.1.9).

Table 3.23 Fraction of ethylbenzene emissions to gas phase of total NMVOC emissions in EU15

	Emission [t/a]	% of 12 500 kt/a
Isolated (production and processing)	2559	0.02
Non-isolated (traffic and mixed solvent)	85412	0.68
Total emissions for EU	87971	0.70

The proportion of isolated ethylbenzene relative to total NMVOC is approx. 0.02 %. If non-isolated emissions are included in this estimate, the portion of ethylbenzene rises to about 0.7 % of the total NMVOC emissions.

The POCP equivalence factor for the total NMVOC is not known because the composition of individual NMVOC species is not available. Ethylbenzene may have a slightly higher photochemical ozone creation potential than the average NMVOC and thus contribute slightly more to the ozone creation than indicated by the proportion of isolated ethylbenzene relative to total NMVOC.

It has to be emphasised that the local and regional NMVOC composition may have a higher concentration of ethylbenzene than indicated by the average calculations due to differences in local NMVOC sources.

To conclude isolated ethylbenzene contributes in the order of 0.02 % to the total NMVOC emission. Thus isolated ethylbenzene in general only contributes to a small extent to the total SMOG problem, however, for a single substance among hundreds of different VOCs the contribution may be significant.

3.2.4 Secondary poisoning

As the available bioaccumulation studies indicate that ethylbenzene has only a low bioaccumulation potential, it is not necessary to perform a risk assessment for secondary poisoning.

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[14] More up-to-date value not available at that source.

3.3 RISK CHARACTERISATION [15]

3.3.1 Aquatic compartment (incl. sediment)

3.3.1.1 Surface water

Using the derived PNECaqua of 100 µg/l, the following PEC/PNEC ratios are obtained for surface water. Please refer to Chapter 3.3.4 for sites located at the sea.

Table 3.24 PEC/PNEC ratios for aquatic compartment (surface water)

		site-specific information	**PEClocal $_{water}$ [µg/l]**	**PEClocal $_{water}$/PNEC$_{aqua}$**
P1	production	effluent concentration, emission days	1.31	0.013
P2	production	emission factor, river flow rate, emission days	0.06	6×10^{-4}
PP1	production and processing	effluent concentration, dilution	0.07	7×10^{-4}
PP2	production and processing	release for production, effluent concentration	14.1	0.14
PP3	production and processing	effluent discharge rate, municipal wwtp, emission days	5.0	0.05
PP4	production and processing	effluent concentration, dilution, emission days	10.1	0.10
PP6	production and processing	effluent concentration, dilution, emission days	0.09	9×10^{-4}
PP8	production and processing	river flow rate, emission days, effluent concentration	0.19	2×10^{-3}
PP9	production and processing	effluent concentration	0.19	2×10^{-3}
PP10	production and processing	WWTP influent concentration, dilution	0.09	9×10^{-4}
PP11	production and processing	effluent concentration, elimination –in WWTP, effluent discharge rate	5.81	0.06
	other processing (generic)	-	16.7	0.17

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[15] Conclusion (i) There is a need for further information and/or testing.
Conclusion (ii) There is at present no need for further information and/or testing and no need for risk reduction measures beyond those which are being applied already.
Conclusion (iii) There is a need for limiting the risks; risk reduction measures which are already being applied shall be taken into account.

PEC/PNEC < 1 could be derived for all known sites at which production, or production and processing of ethylbenzene take place. A PEC/PNEC < 1 was also derived for the generically calculated life cycle step “other processing”.

Conclusions to the risk assessment for the aquatic compartment (surface water):

Conclusion (ii) There is at present no need for further information and/or testing and no need for risk reduction measures beyond those which are being applied already.

Conclusion (ii) applies to all sites where production, or production and processing take place.

3.3.1.2 Sediment

No experimental results with benthic organisms are available, hence only a provisional $PNEC_{sed}$ was calculated using the equilibrium partitioning method. No risk characterisation was performed. $PEC/PNEC_{sed}$ is covered by $PEC/PNEC_{aqua}$.

3.3.1.3 Waste water treatment plants

Using the derived $PNEC_{microorgansims}$ of 9.6 mg/l, the following PEC/PNEC ratios are obtained. Sites with non-biological or without any WWTP are not listed in this table.

Table 3.25 PEC/PNEC ratios for microorganisms

		site-specific information	$Clocal_{eff}$ (= PEC_{stp}) [mg/l]	$PEC_{stp}/PNEC_{microorganisms}$
P1	production	effluent concentration, emission days	0.05	5×10^{-3}
P2	production	emission factor, river flow rate, emission days	0	0
P5	production and processing	emission days, effluent concentration	1×10^{-3}	1×10^{-4}
PP1	production and processing	effluent concentration, dilution	2×10^{-4}	2×10^{-5}
PP3	production and processing	effluent discharge rate, municipal wwtp, emission days	0.050	5×10^{-3}

PP4	production and processing	effluent concentration, dilution, emission days	1.0	0.10
PP6	production and processing	effluent concentration, dilution, emission days	0.01	1×10^{-3}
PP7	production and processing	effluent discharge rate, effluent concentration	0.062	6×10^{-3}
PP8	production and processing	river flow rate, emission days, effluent concentration	0.02	2×10^{-3}
PP9	production and processing	effluent concentration	0.005	5×10^{-4}
PP10	production and processing	WWTP influent concentration, dilution	5×10^{-4}	5×10^{-5}
PP11	production and processing	effluent concentration, elimination in WWTP, effluent discharge rate	0.23	0.02
	other processing (generic)	-	0.665	0.07

All PEC/PNEC ratios are below 1, and so it is unlikely that ethylbenzene poses a risk to microorganisms in the WWTP.

Conclusions to the risk assessment for the waste water treatment plants:

Conclusion (ii) There is at present no need for further information and/or testing and no need for risk reduction measures beyond those which are being applied already.

Conclusion (ii) applies to all sites where production, or production and processing take place.

3.3.2 Terrestrial compartment

Releases of ethylbenzene into the terrestrial compartment are to be expected as a result of deposition and sludge application. C_{sludge} used was calculated from production and processing at PP3 the only site known to discharge effluents to a municipal WWTP. A $PEClocal_{soil}$ of 0.066 mg/kg was obtained for site PP3. Comparison with the calculated $PNEC_{soil}$ of 776 µg/kg results in a PEC/PNEC of 0.08.

For comparison, the $PEClocal_{soil}$ at site PP1 was calculated. Input takes place only via deposition (maximum deposition rate at that site). The derived $PEClocal_{soil}$ of 0.039 mg/kg is below $PEClocal_{soil}$ (PP3). There is no indication of a risk.

A further calculation for site PP1 using the deposition rate of $DEP_{total\ ann}$ (PP1) = 0.932 mg/(m^2 d) and the sludge concentration calculated for PP3 of C_{sludge} of 107 mg/kg_{dw}, resulted in a $PEClocal_{soil}$ of 0.104 mg/kg which again leads to PEC/PNEC < 1.

Conclusions to the risk assessment for the terrestrial compartment:

Conclusion (ii) There is at present no need for further information and/or testing and no need for risk reduction measures beyond those which are being applied already.

Conclusion (ii) applies to production and processing of ethylbenzene.

3.3.3 Atmosphere

On account of the atmospheric half-life ($t_{1/2}$ = approx. 2.3 days), abiotic effects on the atmosphere, such as global warming and ozone depletion in the stratosphere, are not to be expected in the case of ethylbenzene.

Direct releases into the atmosphere occur during production and processing of pure ethylbenzene (about 2 540 t/a for Europe). Indirect releases come from stripping processes in waste water treatment plants. According to the SimpleTreat calculations 46.7 % of the releases to WWTP are accounted to air (about 311 t/a). Thus, WWTP are a not negligible source of ethylbenzene.

The calculated $Clocal_{air\_ann}$ ranging from < 0.001 mg/m^3 to 0.9 mg/m^3. The 90th percentile of all sites for the production and/or processing of pure ethylbenzene is 0.330 mg/m^3 and the mean $Clocal_{air\_ann}$ is 0.116 mg/m^3.

As derived in Chapter 3.2.3.1, the effect data are very scanty and insufficient for the derivation of a distinct PNEC. However, they allow the statement that ethylbenzene seems not to be of concern for plants with regard to exposure via the atmosphere except at very high concentrations (g/m^3). Therefore, only an indicative risk characterization for the atmospheric compartment is conducted using selected measured or calculated environmental concentrations. As highest ethylbenzene concentrations in air the PEC_{local} (100 m distance from point source) of 0.9 mg/m^3 is chosen. This value is a factor of 30 000 below the concentration range at which effects on plants were observed. In view of these ratios it should be concluded that in the present immission situation no harmful effects on outdoor vegetation resulting from exposure to ethylbenzene in air are to be expected.

Result

(ii) There is at present no need for further information and/or testing.

It is known that ethylbenzene contributes to tropospheric VOC and contributes to the tropospheric formation of ozone. The photochemical formation of ozone and other compounds depends on emission of all VOCs and other compounds in a complex interaction with other factors.

Changes in VOC emissions lead to changes in ozone formation. The efficiency of VOC emission reductions in reducing ground level ozone concentrations may vary from place to place and depends on the occurrence of NO_x, the solar radiation and the prevailing wind conditions. Thus the effects on ozone creation of emissions arising from the production and use of the isolated commercial product ethylbenzene may differ substantially between different regions in the EU.

The industrial use of the commercial product ethylbenzene contributes significantly to the overall emission of ethylbenzene, however, emission of ethylbenzene in exhaust gases expelled from motor vehicles seem to be the largest single source.

Based on a rough estimation utilising available information, the current risk assessment indicates that emission of ethylbenzene from the use and production of the commercial product ethylbenzene may be in the order of 0.02 % of total NMVOC emissions. Locally and regionally this proportion may vary substantially due to differences between regions in the VOC emission pattern from industrial sectors using ethylbenzene. Even a simple evaluation of the photochemical ozone creation potential of the emission of isolated ethylbenzene is difficult to perform, when the emission pattern of individual NMVOCs is not available.

Effects of ozone exposure are documented on plants, animals and humans. Reporting on monitoring results are most frequently done in relation to exceedance of thresholds for information or warning of the human population, but this reporting may also give indication on the magnitude of environmental effects, because effect concentrations seem to be in the same order of magnitude for both vegetation and humans. The threshold values set by the European Union to protect human health and the vegetation are frequently exceeded (cf. e.g. De Leeuw et al, 1996)

In 1995 90% of the EU population (both urban and rural) experienced an exceedance of the current EU threshold for health protection (110 240 µg/m3, 8h average) for at least one day during the summer 1995. Over 80% experienced exposure above the threshold for more than 25 days. The highest concentrations (≥240 µg/m3) were recorded in Italy and Greece (De Leeuw et al., 1996; WHO, 1999).

In 1999 the threshold for information of the public in EU (180 $\mu g/m^3$, 1h average) were not exceeded in 4 member states while up to 70 % of the monitoring stations in other member states did exceed this threshold (Sluyter and Camu, 1999). On average 27 % of all monitoring stations in EU did exceed the threshold. The number of days that the threshold was exceeded ranged from 2 days in Luxembourg to 68 days in Italy (out of 153 days in the reporting season).

The severity of exceedance of the EU threshold for health protection (110 $\mu g/m^3$, 8 h average) has been estimated by WHO (WHO, 1999). The 1995 summer ozone incidence is estimated to have caused 1500-3700 deaths (0.1-0.2 % of all deaths) and further 300-1000 extra emergency hospital admissions due to respiratory diseases. “It is likely that the total number of health impacts is higher than the estimated impact of the days with high levels only. This is suggested by epidemiological studies where the effects can be seen also below the 110 $\mu g/m^3$ level.” (WHO, 1999).

If these figures are used to estimate the impact of emissions from the production and use of the commercial product ethylbenzene through formation of ozone then this emission may have probably caused 1 death in the summer of 1995 if a linear relationship exists between the emission of ethylbenzene, the emission of NMVOCs and the creation of ozone. Similarly, the vegetation and wildlife may be severely affected by ozone incidences and ethylbenzene is likely to contribute to these effects.

However, no simple relationship has been established between the proportion of ethylbenzene to total NMVOC emitted - and thus also between emissions arising from the use of the commercial product ethylbenzene - and the creation of tropospheric ozone.

Result

(iii) There is a need for limiting the risk; risk reduction measures which are being applied shall be taken into account.

Conclusions to the risk assessment for the atmosphere:

Conclusion (ii) There is at present no need for further information and/or testing and no need for risk reduction measures beyond those which are being applied already.

Conclusion (iii) There is a need for limiting the risks; risk reduction measures which are already being applied shall be taken into account.

Conclusion (ii) applies to biotic effects of ethylbenzene in the atmosphere.

Conclusion (iii) applies to the contribution of the commercial product ethylbenzene to the formation of ozone. In the context of the consideration of which risk reduction measures that would the most appropriate, it is recommended that under the relevant Air Quality Directives a specific in-depth evaluation be performed. Such an evaluation should focus on the contribution of isolated as well as non-isolated ethylbenzene to the complex issue of ozone and smog formation and the resulting impact on air quality.

3.3.4 Marine Assessment including PBT Assessment

3.3.4.1 PBT Assessment

The following table shows the PBT/vPvB criteria as defined in the TGD and the values relevant for ethylbenzene. The description of the relevant tests can be found in Chapter 3.1.3 (**P** and **B**) and in Chapter 3.2 (**T**).

Table 3.26 Data for ethylbenzene and PBT/vPvB criteria according to TGD

Criterion	PBT-criteria	vPvB-criteria	Ethylbenzene
P	Half-life > 60 d in marine water or > 40 d in freshwater or half-life > 180 d in marine sediment or > 120 d in freshwater sediment	Half-life > 60 d in marine- or freshwater or half-life > 180 d in marine or freshwater sediment	readily biodegradable in surface water (half-life: 15d)
B	BCF > 2000	BCF > 5000	BCF < 100
T	Chronic NOEC < 0.01 mg/l or CMR or endocrine disrupting effects	Not applicable	7d NOEC (daphnid): 1.0 mg/l

Ethylbenzene has to be considered as readily biodegradable. There are no tests on degradation of ethylbenzene in soil or sediment available.

A BCF of 92 was derived from log Kow of 3.13 according to TGD. Measured BCF in fish showed BCF ≤ 20, however the validity of the tests is limited.

The lowest long-term effect value of 1.0 mg/l was found for *Ceriodaphnia dubia*.

It can be concluded that ethylbenzene does not meet the PBT criteria.

3.3.4.2 Marine Assessment

There are no indications that ethylbenzene persists or accumulates in the environment. However, it is known that there are 5 sites located at the sea. PEClocal for these sites are estimated using the defaults described in the TGD for the marine assessment. If available, site-specific data are used.

There is information that two of the 5 marine sites operate a WWTP. All other sites discharge effluents directly to the sea. A standard dilution factor of 100 was used. In a first approach the marine regional background concentration was derived from the fresh water value by division by 10:

$$PEC_{regional}\ (seawater) = 6.4 \times 10^{-3}\ \mu g\ l^{-1}.$$

The value was added to the Clocal $_{water}$ to obtain the respective PEClocal $_{water}$ (see Table 3.9) for the marine sites.

The PNEC$_{marine}$ was derived by dividing the PNEC$_{aqua}$ by 10:

$$PNEC_{marine} = \frac{PNEC_{aqua}}{10} = \frac{100\ \mu g\ l^{-1}}{10} = \underline{10\ \mu g\ l^{-1}}$$

Using this PNEC$_{marine}$, the following PEC/PNEC ratios for marine environment can be derived.

Table 3.27 PEC/PNECseawater ratios for marine sites

		site-specific information	PEClocal $_{seawater}$	PEClocal$_{seawater}$/PNEC$_{marine}$

			[µg/l]	
P3	production	waste water discharge rate, waste water concentration, emission days, discharge to sea	0.081	8.1 x 10^{-3}
P4	production	waste water discharge rate, waste water concentration, emission days, discharge to sea	0.025	2.5 x 10^{-3}
P5	production and processing	emission days, effluent concentration	0.016	1.6 x 10^{-3}
PP5	processing	effluent discharge rate, emission days, discharge to sea	1.07	0.107
PP7	production and processing	effluent concentration, effluent discharge rate	0.63	0.063

The PEC/PNEC < 1 for all marine sites.

Conclusions to the risk assessment for the marine environment:

Conclusion (ii) There is at present no need for further information and/or testing and no need for risk reduction measures beyond those which are being applied already.

Conclusion (ii) applies to all identified marine sites. Ethylbenzene does not meet the PBT or vPvB criteria.

3.3.5 Unintentional uses

As described in Chapter 3.1.2.4 significant emissions of ethylbenzene could occur from unintentional use of ethylbenzene. Main known sources are the "mixed xylenes" which are predominantly used as petrol additive. Emissions are only considered for the background concentration.

A generic calculation to obtain PEClocal was performed for formulation and technical use of mixed xylenes as solvent (see Chapter 3.1.7). If a risk characterisation was to be performed a possible risk could be identified for surface water and soil.

There are only scarce data regarding the unintentional uses. Since unintentional uses are generally not covered by Council Regulation (EEC) 793/93 the Rapporteur does not have the possibility to improve the data base. Available information has been included in the risk assessment since it is considered valuable information. However, no quantitative risk characterisation has been performed.

There are indications that there may be a risk to surface water and soil arising from formulation and technical use of mixed xylenes as solvent containing ethylbenzene. It is recommended this to be further evaluated.

3.3.6 Secondary poisoning

No risk characterisation was performed since experimental data indicate that bioaccumulation of ethylbenzene is low.

4 HUMAN HEALTH

4.1.1.1 Humans exposed via the environment

According to Appendix VII of Chapter 2 of the TGD, the indirect exposure to humans via the environment through food, drinking water and air is estimated for a local and a regional approach. For the local concentrations the generic scenario for production and processing at site PP2 is used, representing the local worst case. This scenario is compared to an average intake due to exposure via the regional background concentration. In the Appendix IV the input data and results of the calculations are presented. The following table shows the input parameters selected.

Table 4.1 Input parameter for calculation of indirect exposure ("Production and processing at PP2")

$PEClocal_{water\_ann}$	0.0116	mg l^{-1}
$PEClocal_{air\_ann}$	0.034	mg m^{-3}
$PEClocal_{grassland}$	0.00261	mg kg^{-1}
$PEClocal_{agri\_soil\_porewater}$	2.80×10^{-4}	mg l^{-1}
$PEClocal_{grassland\_porewater}$	3.34×10^{-4}	mg l^{-1}
$PEClocal_{agri\_soil\_groundwater}$	2.80×10^{-4}	mg l^{-1}
$PECregional_{water}$	6.40×10^{-5}	mg l^{-1}
$PECregional_{air}$	4.62×10^{-4}	mg m^{-3}
$PECregional_{agri\_soil}$	7.40×10^{-5}	mg kg^{-1}
$PECregional_{agri\_soil\_porewater}$	9.56×10^{-6}	mg l^{-1}

The resulting total daily doses are:

$$\mathbf{DOSE_{tot\_local} = 9.247\ \mu g \cdot kg_{b.w.}^{-1} \cdot d^{-1}}$$

$$\mathbf{DOSE_{tot\_regional} = 0.111\ \mu g \cdot kg_{b.w.}^{-1} \cdot d^{-1}}$$

The calculated doses comprise the following routes

Table 4.2 Routes of exposure (percentage of total dose) for regional and local model

route	regional model, percentage of total dose (%)	point source model; percentage of total dose (%)
drinking water	0.83	1.79
air	89.41	78.79
stem	0.40	0.35
root	0.68	0.24
meat	<0.01	<0.01
milk	<0.01	<0.01
fish	8.67	18.82

The most significant route of exposure in the regional as well as in the local model is that via air.

However, it has to be noted, that the applied model calculations are of preliminary nature and have to be revised as soon as further information become available.

5 RESULTS

5.1 INTRODUCTION

5.2 ENVIRONMENT

Environment

Conclusion (ii) There is at present no need for further information and/or testing and no need for risk reduction measures beyond those which are being applied already.

Conclusion (iii) There is a need for limiting the risks; risk reduction measures which are already being applied shall be taken into account.

Conclusion (ii) applies to

all production sites as well as all production and processing sites to *Surface water*, *Waste water treatment plants* and the *Terrestrial compartment*. It also applies to biotic effects of ethylbenzene in the *Atmosphere*.

Conclusion (iii) applies to

Atmosphere (indirect effects of ethylbenzene)

Conclusion (iii) applies to the contribution of the commercial product ethylbenzene to the formation of ozone. In the context of the consideration of which risk reduction measures that would the most appropriate, it is recommended that under the relevant Air Quality Directives a specific in-depth evaluation be performed. Such an evaluation should focus on the contribution of isolated as well as non-isolated ethylbenzene to the complex issue of ozone and smog formation and the resulting impact on air quality.

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ABBREVIATIONS

[update the list to correspond to the substance RAR]

ADI	Acceptable Daily Intake
AF	Assessment Factor
ASTM	American Society for Testing and Materials
ATP	Adaptation to Technical Progress
AUC	Area Under The Curve
B	Bioaccumulation
BBA	Biologische Bundesanstalt für Land- und Forstwirtschaft
BCF	Bioconcentration Factor
BMC	Benchmark Concentration
BMD	Benchmark Dose
BMF	Biomagnification Factor
bw	body weight / *Bw*, *b.w.*
C	Corrosive (Symbols and indications of danger for dangerous substances and preparations according to Annex III of Directive 67/548/EEC)
CA	Chromosome Aberration
CA	Competent Authority
CAS	Chemical Abstract Services
CEC	Commission of the European Communities
CEN	European Standards Organisation / European Committee for Normalisation
CMR	Carcinogenic, Mutagenic and toxic to Reproduction
CNS	Central Nervous System
COD	Chemical Oxygen Demand
CSTEE	Scientific Committee for Toxicity, Ecotoxicity and the Environment (DG SANCO)
CT_{50}	Clearance Time, elimination or depuration expressed as half-life
d.wt	dry weight / dw
dfi	daily food intake
DG	Directorate General
DIN	Deutsche Industrie Norm (German norm)
DNA	DeoxyriboNucleic Acid
DOC	Dissolved Organic Carbon
DT50	Degradation half-life or period required for 50 percent dissipation / degradation
DT90	Period required for 50 percent dissipation / degradation
E	Explosive (Symbols and indications of danger for dangerous substances and preparations according to Annex III of Directive 67/548/EEC)
EASE	Estimation and Assessment of Substance Exposure Physico-chemical properties [Model]

EbC50	Effect Concentration measured as 50% reduction in biomass growth in algae tests
EC	European Communities
EC10	Effect Concentration measured as 10% effect
EC50	median Effect Concentration
ECB	European Chemicals Bureau
ECETOC	European Centre for Ecotoxicology and Toxicology of Chemicals
ECVAM	European Centre for the Validation of Alternative Methods
EDC	Endocrine Disrupting Chemical
EEC	European Economic Communities
EINECS	European Inventory of Existing Commercial Chemical Substances
ELINCS	European List of New Chemical Substances
EN	European Norm
EPA	Environmental Protection Agency (USA)
ErC50	Effect Concentration measured as 50% reduction in growth rate in algae tests
ESD	Emission Scenario Document
EU	European Union
EUSES	European Union System for the Evaluation of Substances [software tool in support of the Technical Guidance Document on risk assessment]
F(+)	(Highly) flammable (Symbols and indications of danger for dangerous substances and preparations according to Annex III of Directive 67/548/EEC)
FAO	Food and Agriculture Organisation of the United Nations
FELS	Fish Early Life Stage
GLP	Good Laboratory Practice
HEDSET	EC/OECD Harmonised Electronic Data Set (for data collection of existing substances)
HELCOM	Helsinki Commission -Baltic Marine Environment Protection Commission
HPLC	High Pressure Liquid Chromatography
HPVC	High Production Volume Chemical (> 1000 t/a)
IARC	International Agency for Research on Cancer
IC	Industrial Category
IC50	median Immobilisation Concentration or median Inhibitory Concentration
ILO	International Labour Organisation
IPCS	International Programme on Chemical Safety
ISO	International Organisation for Standardisation
IUCLID	International Uniform Chemical Information Database (existing substances)
IUPAC	International Union for Pure and Applied Chemistry
JEFCA	Joint FAO/WHO Expert Committee on Food Additives
JMPR	Joint FAO/WHO Meeting on Pesticide Residues
Koc	organic carbon normalised distribution coefficient

Kow	octanol/water partition coefficient
Kp	solids-water partition coefficient
L(E)C50	median Lethal (Effect) Concentration
LAEL	Lowest Adverse Effect Level
LC50	median Lethal Concentration
LD50	median Lethal Dose
LEV	Local Exhaust Ventilation
LLNA	Local Lymph Node Assay
LOAEL	Lowest Observed Adverse Effect Level
LOEC	Lowest Observed Effect Concentration
LOED	Lowest Observed Effect Dose
LOEL	Lowest Observed Effect Level
MAC	Maximum Allowable Concentration
MATC	Maximum Acceptable Toxic Concentration
MC	Main Category
MITI	Ministry of International Trade and Industry, Japan
MOE	Margin of Exposure
MOS	Margin of Safety
MW	Molecular Weight
N	Dangerous for the environment (Symbols and indications of danger for dangerous substances and preparations according to Annex III of Directive 67/548/EEC
NAEL	No Adverse Effect Level
NOAEL	No Observed Adverse Effect Level
NOEL	No Observed Effect Level
NOEC	No Observed Effect Concentration
NTP	National Toxicology Program (USA)
O	Oxidizing (Symbols and indications of danger for dangerous substances and preparations according to Annex III of Directive 67/548/EEC)
OECD	Organisation for Economic Cooperation and Development
OEL	Occupational Exposure Limit
OJ	Official Journal
OSPAR	Oslo and Paris Convention for the protection of the marine environment of the Northeast Atlantic
P	Persistent
PBT	Persistent, Bioaccumulative and Toxic
PBPK	Physiologically Based PharmacoKinetic modelling
PBTK	Physiologically Based ToxicoKinetic modelling
PEC	Predicted Environmental Concentration

pH	logarithm (to the base 10) (of the hydrogen ion concentration {H^+}
pKa	logarithm (to the base 10) of the acid dissociation constant
pKb	logarithm (to the base 10) of the base dissociation constant
PNEC	Predicted No Effect Concentration
POP	Persistent Organic Pollutant
PPE	Personal Protective Equipment
QSAR	(Quantitative) Structure-Activity Relationship
R phrases	Risk phrases according to Annex III of Directive 67/548/EEC
RAR	Risk Assessment Report
RC	Risk Characterisation
RfC	Reference Concentration
RfD	Reference Dose
RNA	RiboNucleic Acid
RPE	Respiratory Protective Equipment
RWC	Reasonable Worst Case
S phrases	Safety phrases according to Annex III of Directive 67/548/EEC
SAR	Structure-Activity Relationships
SBR	Standardised birth ratio
SCE	Sister Chromatic Exchange
SDS	Safety Data Sheet
SETAC	Society of Environmental Toxicology And Chemistry
SNIF	Summary Notification Interchange Format (new substances)
SSD	Species Sensitivity Distribution
STP	Sewage Treatment Plant
T(+)	(Very) Toxic (Symbols and indications of danger for dangerous substances and preparations according to Annex III of Directive 67/548/EEC)
TDI	Tolerable Daily Intake
TG	Test Guideline
TGD	Technical Guidance Document
TNsG	Technical Notes for Guidance (for Biocides)
TNO	The Netherlands Organisation for Applied Scientific Research
UC	Use Category
UDS	Unscheduled DNA Synthesis
UN	United Nations
UNEP	United Nations Environment Programme
US EPA	Environmental Protection Agency, USA
UV	Ultraviolet Region of Spectrum
UVCB	Unknown or Variable composition, Complex reaction products of Biological material

vB	very Bioaccumulative
vP	very Persistent
vPvB	very Persistent and very Bioaccumulative
v/v	volume per volume ratio
w/w	weight per weight ratio
WHO	World Health Organization
WWTP	Waste Water Treatment Plant
Xn	Harmful (Symbols and indications of danger for dangerous substances and preparations according to Annex III of Directive 67/548/EEC)
Xi	Irritant (Symbols and indications of danger for dangerous substances and preparations according to Annex III of Directive 67/548/EEC)

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The report provides the comprehensive risk assessment of the substance Ethylbenzene. It has been prepared by Germany in the frame of Council Regulation (EEC) No. 793/93 on the evaluation and control of the risks of existing substances, following the principles for assessment of the risks to man and the environment, laid down in Commission Regulation (EC) No. 1488/94.

The evaluation considers the emissions and the resulting exposure to the environment and the human populations in all life cycle steps. Following the exposure assessment, the environmental risk characterisation for each protection goal in the aquatic, terrestrial and atmospheric compartment has been determined.

The environmental risk assessment concludes that there is no concern for the aquatic environment (including sediment) and the terrestrial environment due to the production and processing of ethylbenzene. There is also no concern for the atmosphere due to biotic effects of ethylbenzene. Concern is identified for the atmosphere due to the contribution to the formation of ozone of ethylbenzene. It is recommended that further evaluation is performed under the relevant Air Quality Directives.

The human health part is not included in this report.