European Union Risk Assessment Report

2-ETHOXYETHYL ACETATE

CAS-No.: 111-15-9

EINECS-No.: 203-839-2

RISK ASSESSMENT

15.02.2008

FINAL APPROVED VERSION

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Information on the rapporteur

Contact point:

Bundesanstalt für Arbeitsschutz und Arbeitsmedizin (BAuA)
Chemikalien, Anmeldung und Zulassung
Federal Institute for Occupational Safety and Health
Division Chemicals, Notification and Authorisation
Friedrich-Henkel-Weg 1-25
44149 Dortmund

fax: +49-(0)231-9071-2679
e-mail: chemg@baua.bund.de

Foreword

We are pleased to present this Risk Assessment Report which is the result of in-depth work carried out by experts in one Member State, working in co-operation with their counterparts in the other Member States, the Commission Services, Industry and public interest groups.

The Risk Assessment was 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 Health and Environmental Risks (SCHER) which gives its opinion to the European Commission on the quality of the risk assessment.

If a Risk Assessment Report concludes that measures to reduce the risks of exposure to the substances are needed, beyond any measures which may already be in place, the next step in the process is for the "Rapporteur" to develop a proposal for a strategy to limit those risks.

The Risk Assessment Report is also presented to the Organisation for Economic Co-operation and Development as a contribution to the Chapter 19, Agenda 21 goals for evaluating chemicals, agreed at the United Nations Conference on Environment and Development, held in Rio de Janeiro in 1992 and confirmed in the Johannesburg Declaration on Sustainable Development at the World Summit on Sustainable Development, held in Johannesburg, South Africa in 2002.

This Risk Assessment improves our knowledge about the risks to human health and the environment from exposure to chemicals. We hope you will agree that the results of this in-depth study and intensive co-operation will make a worthwhile contribution to the Community objective of reducing the overall risks from exposure to chemicals.

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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]

Note - Human Health Section

With the approval of all Member States and the ECB the Human Health Section of the RAR of 2-Ethoxyethyl acetate was not carried out and thus the risk assessment report is not finalised.

The reason for this decision is mentioned in the following:

Due to considerable changes in uses during recent years, the production was ceased by all producers in the EU in 2002. There is actually no producer or importer of this substance in the EU. The lead company Dow Europe was the last producer of 2- Ethoxyethyl acetate and discontinued all sales by 01.08.2002. It is not expected that any production or import of the substance will start again in the future.

The substance is classified in Annex I of 67/548 EEC with T, Repro Cat. 2, R10, Xn, R20, R21, R22, R60 and R61. Due to a preliminary human health effect assessment no changes in classification and labelling are expected.

Since the exposure situation does not exist anymore a risk characterisation regarding workers and consumers would lead to conclusion ii. there is at present no need for risk reduction measures beyond those which are being applied already“. For that reason a risk management strategy will not be necessary.

The environmental risk assessment was however performed at a much earlier stage, and in order not to loose these assessment results, the current risk assessment report covering the environmental part is published. The assessment is entirely based on old import figures and on information of a former producer on the use pattern.

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0 OVERALL CONCLUSIONS/RESULTS OF THE RISK ASSESSMENT

CAS No.	111-15-9
EINECS No.	203-839-2
IUPAC Name	2-Ethoxyethyl acetate

Overall results of the risk assessment:

() i) There is need for further information and/or testing

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

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

Summary of conclusions:

Environment

ii)

Based on the scenarios “Paints, lacquers and varnishes industry/solvents” (IC/UC 14/48) and “Chemical industry: chemicals used in synthesis/intermediates” (IC/UC 3/33) no risk was identified to surface water. Conclusion (ii) also applies to waste water treatment plants for all scenarios and to the terrestrial compartment.

Concerning the scenario “Chemical Industry: basic chemicals/solvents” (IC/UC 2/48) a risk to the aquatic environment was identified. Using default values from the TGD the risk was identified for both the 1,000 t and the 5,000 t import per year.

However, **at present** there is no need for further information and/or testing nor for risk reduction measures beyond those which are being applied already because at present there is no production within the EU, nor is there any import into the EU and presumably therefore no use. **Based on this information conclusion (ii) is drawn.**

The risk assessment is based solely on historical data and can currently be considered of historical value only. Thus the identified risk should be regarded as hypothetical.

If production, importation and/or use in the EU are restarted the conclusion would need to be reassessed and any manufacturer or importer would then be asked to provide current import figures and site specific exposure data.

Human Health

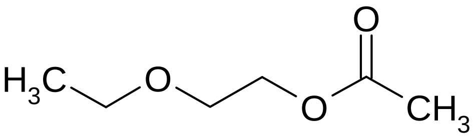
The Human Health Section of 2- Ethoxyethyl acetate was not carried out (see note on page 2).

1 GENERAL SUBSTANCE INFORMATION

Identification of the substance

CAS-No.:	111-15-9
EINECS No.	203-839-2
IUPAC Name	2-ethoxyethyl acetate
Synonyms:	ethylglycol acetate, ethylene glycol mono ethyl ether acetate, 2-EEA, acetic acid, 2-ethoxyethyl ester, ethoxyethanol acetate, EGA, Cellosolve Acetate, Ethoxol Acetate, Oxitol Acetate

Molecular weight:	132.1 g/mol
Empirical formula:	$C_6H_{12}O_3$
Structural formula:	



Purity/impurities, additives

Purity:	≥ 99 % w/w
Impurities:	< 0.5 % w/w ethyleneglycol diacetate
	< 0.5 % w/w 2-ethoxyethanol
	< 0.1 % w/w 2-ethoxyethanolformate
	< 0.1 % w/w water
	< 0.05 % w/w ethyleneglycol monoacetate
	< 0.01 % w/w 2-(2-ethoxyethoxy)ethyl acetate
Additives:	0.008-0.012 % 2,6-di-tert-butyl-p-cresol (BP-Chemical, UK) function: inhibition of peroxide formation

Physico-chemical properties

2-Ethoxyethyl acetate (2-EEA) is a colourless liquid with a fruity smell at room temperature and normal pressure. Data on the physical and chemical properties are given in table 1.1.

Table 1.1: Physico-chemical properties

Melting point	< - 62 °C	Kirk-Othmer (1980)
Boiling point	156 °C	Merck-Index (1989)
Relative density	0.9730 at 20 °C	Kirk-Othmer (1980)
Vapour pressure	270 Pa at 20 °C	Kirk-Othmer (1980)
Surface tension	67.1 mN/m at 25 °C 1)	Union Carbide (1998)
Water solubility	229 g/l at 20 °C	Kirk-Othmer (1980)
Partition coefficient	Log Pow 0.24 (experimental) 2)	Hüls AG (1989)
Flash point	51 °C (closed cup)	Chemsafe (1996)
Flammability	flammable 3)	Chemsafe (1996)
Ignition temperature	380 °C (DIN 51794)	Chemsafe (1996)
Explosive properties	not explosive 4)	Chemsafe (1996)
Oxidizing properties	no oxidizing properties 5)	Chemsafe (1996)
Henry’s law constant	0.16 Pa * m^3 * mol^{-1} 6)	

1) Ring method

2) Determined by shaking method

3) Test A.10 not conducted (substance is a liquid)
Test A.12 and A.13 not conducted because of structural reasons

4) No test conducted because of structural reasons

5) No test conducted because of structural reasons

6) The Henry law constant is based on the Water solubility-Vapour Pressure Method. Johanson Dynesius present an experimental Henry law constant as 0.36 Pa m^3/mol (Johanson Dynesius: Liquid-air partition coefficients of six commonly used glycol ethers. Br J Ind Med 45(8): 561-564). The value of 0.16 Pa m^3/mol corresponds with a calculated value from the EPI database (0.15 Pa m^3/mol) based on water solubility and vapour pressure data and is therefore used for the risk assessment.

Classification

- Classification according to Annex I of directive 67/548/EEC (31st ATP):

  R 10 flammable

  Reprotox. Cat. 2,

  T toxic

  R 60 may impair fertility

  R 61 may cause harm to unborn child

  Xn Harmful R 20 harmful by inhalation

  R 21 harmful in contact with skin

  R 22 harmful if swallowed ;

- Proposal of the rapporteur (only environmental part)

  According to the data presented below and the criteria of Directive 67/548/EEC 2-ethoxyethyl acetate has not to be classified as dangerous for the environment.

2 GENERAL INFORMATION ON EXPOSURE

Production and Import

2-Ethoxyethyl acetate (hereafter referred to as 2-EEA) belongs to the group of glycol ethers which are mainly used as solvents. 2-EEA is produced by standard esterification techniques using 2-Ethoxyethanol, the acid anhydride or chloride and an acid catalyst. The production process for 2-Ethoxyethanol involves the reaction of ethanol with ethylene oxide (Kirk-Othmer, 1980).

No production of 2-EEA takes place within the EU at present. The last European production site ceased production in 1996. According to IND estimated sales in the year 2000 were less than 5,000 tonnes. In August 2002 the last importer announced that it discontinued all sales of 2-EEA. With this withdrawal from the market it was predicted "*that the amount of product onto the EU market may rapidly drop even below 1,000 tonnes per year in the near future*". The European market with respect to the produced/imported amount of 2-EEA is completely different form the market 10 years ago. In the early 1990´s 11,000 – 25,000 t 2-EEA per year were produced in and imported into the EU. Six producers/importers were listed in the IUCLID from 1996. However, at present there is no production of 2-EEA in the EU and, according to the latest information, 2-EEA is currently not imported to the EU. Hence, no current import figures of 2-EEA are available. The reason for this development seems to be the chemicals labelling with R60/R61 and its ongoing substitution with less hazardous substances.

The last information available is that in the year 2000 about 5,000 t 2-EEA were onto the EU market. Although no import/production takes place at present in the EU the amount estimated to be at the European market might be somewhere under 5,000 t/a, maybe even below 1,000 t/a. As the Rapporteur has no current import figures all exposure scenarios where both calculated with 1,000 t/a and with 5,000 t/a in order to get an idea of the possible risk 2-EEA might pose to the environment. The Rapporteur can not estimate the potential for other companies to supply the substance in order to meet the potential gap in the market.

Use

According to former industry information 2-EEA was mainly used as a solvent in the chemical industry and for the formulation of paints, lacquers and varnishes for industrial use. 2-EEA was also used as an intermediate in the chemical industry (see table 2.1). This information is presumably based on historic information and seems to have no relevance at present. No information is available on the current use pattern and no information is available as to which products 2-EAA is further processed to. According to Ashford's Dictionary of Industrial Chemicals the sole intermediate use of the substance was to produce 2-ethoxyethyl cyanoacrylate, which is subsequently used in low-odour cyanoacrylate adhesives. The same source indicated a commercial route to manufacture 2-ethoxyethyl cyanoacrylate based on 2-ethoxyethyl acetate/cyanogen chloride/formaldehyde (dehydrochlorination/aldol condensation/thermal depolymerisation). However, this information could not be verified in practice.

In the past 2-EEA was used in wide dispersive applications such as paints for private use, in surface treatment of metals and in construction, wood- and furniture industry. In the Swedish Product Register from 1994 nine consumer products were mentioned. In the Danish Product Register from 1996 896 products with a total quantity of 758 tonnes were listed. The product types listed are paints, lacquers and varnishes, thinners, cleaning and binding agents as well as hardeners. The industry groups are metal, wood- and furniture and construction industry as well as private households. In the IUCLID database from 1996 wide dispersive applications are mentioned such as the use of 2-EEA in washing and cleaning agents, disinfectants and as solvent. The IPCS EHC document 115 from 1990 mentions a range of potential uses for 2-EEA, including paints, lacquers, the production of food-contact plastics, resin solvents, surface coatings and inks for silk-screen printing, as solvents for dyes in textile and leather finishing and as general solvent in a wide variety of home and industrial cleaners.

The Rapporteur has no indication that the applications described above are still in use. No production in and no import into the EU takes place. Neither detailed information on the use pattern nor detailed monitoring data are available.

In 1998 a voluntary programme of industry, represented by the Oxygenated Solvents Producers Association (OSPA), was implemented in order to monitor the end use applications of glycol ether solvents, among them 2-EEA. Since then the distributors and customers of this chemical have to ensure that 2-EEA is not used in consumer goods, household products, cosmetics and other applications where exposure is poorly controlled. If they do not comply with this rule the supplier will discontinue sales.
Regarding 2-EEA in printing inks there is an Exclusion List for Printing Inks and Related Products produced by the European Council of the Paint, Printing Ink and Artists' Colours Industry (CEPE 2001). 2-EEA is on the substances list for substances which are excluded from raw materials for the manufacture of printing inks and related products supplied to printers. This exclusion list is based on health and safety matters in the production and marketing of printing inks and associated products employing Good Manufacturing Practices.
In the German Washing and Cleansing Agents Database about 12 t 2-EEA were registered in the year 2002. All products listed in this database are intended for industrial use, not for private use, and this amount of 2-EEA is therefore considered to be covered by the use patterns provided below (use of 2-EEA as solvent in the chemical and paint, lacquers and varnishes industries; IC2/UC48 and IC14/UC48). The Rapporteur has no information that 2-EEA is currently used as solvent in cleaning agents/disinfectants and cosmetics for personal/domestic use within Europe. In the past several products for the private sector containing 2-EEA were listed in the German Washing and Cleansing Agents Database. But these products are not longer produced and/or marketed.

Table 2.1 shows the industrial and use categories of 2-EEA for the European Market.

Table 2.1 Industrial and use categories of 2-EEA

Main category (MC)	Industrial category (IC)	Use category (UC)	Mass balance [%]	1,000 t import [t/a]	5,000 t import [t/a]
Non-dispersive use (**3**)	Chemical industry (**3**)	Intermediate (**33**)	**< 15**	**150**	**750**
Non-dispersive use (**3**)	Chemical industry (**2**)	Solvent (**48**)	**< 10**	**100**	**500**
Wide dispersive use (**4**)	Paint, lacquers and varnishes industry (**14**)	Solvent (**48**)	**~ 75**	**750**	**3,750**

A summary of the content of 2-EEA in different products in the Nordic Countries is presented in the SPIN Database from June 2003 as shown in table 2.2. The most frequent product types are paints, lacquers and varnishes as well as solvents and to a lesser extend reprographic agents. Only one product is reported to be a cleaning and washing agent and there are nine preparations (5.7 tonnes) listed as disinfectants.

Table 2.2: Total use of 2-EEA in the Nordic Countries

Country	Year	No. of preparations	Tonnes	Consumer preparations
Finland	2001	19	81.8	
Norway	2001	27	25.0	
Denmark	2001	34	22.0	
Sweden	2000	26	21.0	x

3 ENVIRONMENT

3.1 ENVIRONMENTAL EXPOSURE

3.1.1 General discussion

Release into the environment

Releases of 2-EEA into the environment are to be expected during processing as well as formulation and industrial use of solvents. Specific release data were not submitted by Industry and all calculations are based on default values of the TGD.

There is an Emission Scenario Document on the use of chemicals in the coatings industry published by UK and France but there are not enough information available on the further use of 2-EEA to use this ESD.

Direct releases to agricultural or natural soil can not be assessed from the current use pattern as no specific data are available on the further use of 2-EEA, e.g. as an intermediate. Potentially one of the assumed applications may lead to direct release to soil.

2-EEA has not been reported to occur as a natural substance.

The entire exposure assessment is based on old import figures and on information of a former producer on the use pattern. No information is available of how much 2-EEA might be onto the European Market and whether the use pattern has any relevance at present. According to the latest information there has been no production and import of the substance into the EU since 2002. This was confirmed by the ECB LPVC register.

The exposure assessment was calculated with 1,000 t/a and 5,000 t/a in order to get an idea of the possible risk that 2-EEA might pose to the environment (see Chapter 2 Production and Import).

No production and no import takes place at present and 2-EEA is not a PBT-candidate as it is readily biodegradable. Hence, no PBT-assessment and no marine assessment were conducted.

Degradation

Biodegradation

The biodegradation of 2-EEA has been determined according to three OECD standard tests. 2-EEA can be considered as readily biodegradable.

In the Modified OECD Screening Test (OECD 301 E) (Hüls, 1995a), performed in 1979, 2-EEA (1,000 mg/l) was added to a mineral medium which was aerated and inoculated at 20 °C. The used inoculum was taken from a municipal waste water treatment plant treating predominantly domestic waste water. 2-EEA was degraded by 98 % (measured as DOC) within a period of 14 days. The pass level for ready biodegradability of 70 % within the 10 day window was achieved. The OECD 301E test is not ideal for substances with a significant volatility as the flasks are aerated. Some DOC removal might have resulted from volatilisation rather than biodegradation. However, due to the substance's very high water solubility the removal due to volatilisation is not considered significant.

In a Zahn-Wellens Test (OECD 302 B) (Hüls, 1995b), 2-EEA (500 mg/l) was added to the mineral medium. The same inoculum as in the above mentioned OECD-screening test was used. The study was conducted at 20 – 22 °C in a static system. 2-EEA was degraded by 100 % within a period of 9 days (measured as DOC), the pass level for inherent biodegradation was achieved.

In a Coupled Units test system according to OECD 303A (Hüls, 1995c) a removal of 98 % was determined by DOC analysis after 14 days. The initial 2-EEA concentration was 10 mg/l related to DOC, the test was conducted over 44 days, the mean retention time was 6 hours. Although the substance has a high vapour pressure it is unlikely that a significant amount of 2-EEA evaporated in the test system because of its very high water solubility. Furthermore 2-EEA is considered to have a low potential for adsorption to organic matter (see "Distribution"). Hence the elimination in the above described tests can be considered due to biodegradation.

There are also biodegradation tests available which were conducted according to APHA methods (American Public Health Association, Price et al. 1974, Bridié et al. 1979b). Due to missing information the results of these tests lead only to the qualitative conclusion that 2-EEA is rapidly biodegradable. However, these results are consistent with the described OECD-standard-tests.

No biodegradation studies were conducted in sediment, soil and surface water.

Conclusion:

According to the biodegradation standard tests it can be concluded that 2-EEA is readily biodegradable. The following rate constants for biodegradation of 2-EEA are considered in accordance with the TGD:

Table 3.1: Biodegradation rate constants for different compartments

Compartment	**degradation constant**	**Half life**
Waste water treatment plant	$kbio_{WWTP} = 1\ h^{-1}$	0.7 h
Aquatic environment	$kbio_{SW} = 0.047\ d^{-1}$	15 d
Soil	$kbio_{Soil} = 0.023\ d^{-1}$	30 d
Sediment	$kbio_{SED} = 0.0023\ d^{-1}$	300 d

(see Appendix A1-1)

Photodegradation

An estimation of the half life for the atmospheric reaction of 2-EEA with hydroxyl radicals with the programme AOP 1.87 results in a half-life of 25.6 h (24-h day, $5*10^5$ OH/cm^3). This leads to a k_{deg_air} of 0.65 d^{-1}. There are three measured half-lives available from 18.1 h to 29.6 h depending on the concentration of OH-radicals of $5*10^5$ to $1*10^6$ molecules*cm^{-3}. The calculated value is in the range of the measured values and is used in all further calculations.

Hydrolysis and Photolysis

Experimental results on the hydrolysis behaviour of 2-EEA are not available. Considering the chemical structure hydrolysis is not to be expected. Also no direct photolysis in water takes place as there is no relevant absorption above a wavelength of 290 nm.

However, the substance is an ester and this linkage could be susceptible to hydrolysis. The USEPA EPIWIN (v3.11) gave a hydrolysis half-life of 305 days at pH 7 and of 30.5 days at pH 8. The predicted rate of hydrolysis is thus slower than that assumed in the assessment for biodegradation.

Distribution

With a Henry's law constant of 0.16 Pa*m³*mol^{-1} 2-EEA is considered as moderately volatile (classification of 'moderate volatility' is defined by being >0.03 and <100 Pa*m³*mol^{-1}, Thomas, 1982).

Since there are no experimental results on the adsorption of 2-EEA to soil available the estimation of the adsorption coefficients to soil, sediment, suspended matter and sewage sludge is performed according to the TGD, using a log K_{ow} of 0.24. A K_{OC} of 13.9 l/kg was calculated (see Appendix A1-1 for the calculation).

Table 3.2: Partition Coefficients for different media

Compartment	Partition coefficients	
Soil-water	Kp_{soil} = 0.279 l/kg	$K_{soil-water}$ = 0.619
Sediment-water	Kp_{sed} = 0.698 l/kg	$K_{sed-water}$ = 1.149
Suspended matter-water	Kp_{susp} = 1.396 l/kg	$K_{susp-water}$ = 1.249
Sewage sludge-water	Kp_{sludge} = 5.164 l/kg	

(see Appendix A1-1 for calculation)

Using the fugacity model of Mackay (EQC-model, level 1), the theoretical distribution of 2-EEA at equilibrium can be estimated.

Table 3.3: Equilibrium distribution according to fugacity model of Mackay (EQC-model 1.0, level 1)

Compartment	**%**
Air	5.2
Water	94.8
Soil	0.01
Sediment	0.01

According to this model the hydrosphere is the target compartment for the substance in the environment. However, the IPCS EHC document 115 indicates that *"atmospheric emissions resulting from the use of glycol ethers as evaporative solvents result in the greatest environmental exposure."*

As 2-EEA has a high vapour pressure as well as a high water solubility it seems likely that which environmental compartment 2-EEA enters predominantly depends on how the substance is used. If 2-EEA is used in aqueous applications the hydrosphere is likely to be the target compartment, whereas 2-EEA used as an evaporative solvent results in the highest atmospheric emissions.

Elimination in waste water treatment plants

Based on physico-chemical properties (log H = -0.81; log Pow = 0.24), as well as the biodegradation rate of 1 h^{-1} in the wwtp, the elimination due to biodegradation and distribution of 2-EEA in a wwtp can be estimated with the model SimpleTreat 3.0 (debugged version, Feb. 07/1997, see Appendix A1-1 for calculation).

Table 3.4: Elimination in wwtps

Compartment	**% 2-EEA**
Air	0.1
Water	12.6
Sludge	0
degraded	87.3
total removal	87.4

Accumulation

Tests on bioaccumulation are not available for 2-EEA. The measured log P_{OW} of 0.24 does not indicate a potential for bioaccumulation. Based on this value a **BCF of 0.32 $l*kg^{-1}$** can be calculated for fish (*Pimephales promelas*) according to the EU TGD. The BCF was calculated according to the following equation for substances with logKow < 6:

log BCF = 0.85 logKow – 0.70 (TGD part III, chapter 4, table 6).

Due to the calculated K_{OC} of 13.9 l/kg 2-EEA is unlikely to accumulate in organic matter in soils. Based on the Kp_{soil} of 0.279 l/kg 2-EEA is expected to be highly mobile in soil and may leach to the groundwater.

3.1.2 Aquatic compartment (incl. sediment)

At present 2-EEA is neither produced in nor imported into the EU. The last known figures are 5,000 tonnes import into the EU in the year 2000. At present the amount of 2-EEA which is onto the European market is somewhere under 5,000 t/a, maybe even below 1,000 t/a. There are no information available on current import figures. Because of this lack of data and in order to get an idea of the risk that 2-EEA may pose to the environment all exposure scenarios where calculated both with 1,000 and 5,000 t import/a.

Releases to waste water occur during processing, formulation and industrial use of solvents consisting of 2-EEA. No site specific data were provided by IND on the number of processing sites, processed quantities at each site, information on releases into the hydrosphere and dilution factors. Therefore all calculations are based on the A- and B-tables of the TGD.

Results of the calculations of the $Clocal_{water}$ are listed in table 3.5 (see also Appendices 2-1 to 2-8 for calculation).

3.1.2.1 Determination of the $Clocal_{water}$ / generic approach: processing

2-EEA is used in the chemical industry as an intermediate. It is not known which substances are produced. No information on the number of processing sites is given and hence no site specific exposure data are available. All calculations are based on A- and B-tables of the TGD.

3.1.2.2 Determination of the $Clocal_{water}$ / generic approach: use as a solvent

According to industry information, 2-EEA is presently used as a solvent only for industrial use in the chemical as well as in the paint/lacquer/varnishes industry.

For the release estimations based on formulation and industrial use of 2-EEA as a solvent in the paints, lacquers and varnishes industry (IC14/UC48) a mass content of 10 % 2-EEA in products is used for the derivation of the fraction of main source. This assumption is based on limited information available on the content of 2-EEA in industrial cleansing agents listed in the German Washing and Cleansing Agents Database. According to information given there the content of 2-EEA in industrial cleansing agents is in the range of 1 to 30 %. Over 85 % of the listed products contain 2-EEA with a mass content of ≤ 10 %. However, there is no information whether this data are representative and up to date.

This assumption leads to an amount of 7,500 t/a (1,000 t import) and 37,500 t/a (5,000 t import/a) of formulation, respectively.

Although there is only limited information available there is a possibility that there is a large number of industrial paint applicators and hence the 10 % rule is used for the application IC/UC 14/48 “industrial use of solvents”. This reduces the relevant tonnages for this life cycle to 75 and 375 t/a, respectively. For the release factor to waste water in this application the water based factor of 0.1 is used. This seems justified because of the very high water solubility of 2-EEA.

Concerning the formulation (IC14/UC48) the 10 % rule is not applied because there is no indication on even distribution over Europe. Furthermore, the low tonnage of the product would not support this rule.

The results of the calculations of the $\text{Clocal}_{\text{water}}$ are summarised in the following table (see Appendix 2 for calculation). The $\text{PEC}_{\text{local}}$ includes the $\text{PEC}_{\text{regional\_water}}$ of 0.03 µg/l (1,000 t import per year) and 0.15 µg/l (5,000 t import per year), respectively.

Table 3.5: Summary of results for 1,000 **(5,000 t/a)** tonnes import per year

Types of use	**Solvents in paints/lacquers/varnishes - industrial formulation and use**		**solvent in chemical industry**	**Intermediate in chemical industry**
Tonnage [t/a]	750 **(3,750)**	75 **(375)**	100 **(500)**	150 **(750)**
Main category	non-dispersive use (Ic)	wide dispersive use	non-dispersive use (Ic)	non-dispersive use (Ic)
Industrial category Use category	14 48 (solvents)	14 48 (solvents)	2 48 (solvent)	3 33 (intermediate)
Life cycle step	**formulation**	**industrial use**	**industrial use**	**processing**
Number of days	300 **(300)** B-table 2.10	300 **(300)** B-table 3.13	20 **(50)** B-table 3.2	30 **(75)** B-table 3.2
Fraction of main source	0.8 **(0.6)** B-table 2.3	0.15 **(0.15)** B-table 3.13	0.5 **(0.4)** B-table 3.2	0.5 **(0.4)** B-table 3.2
Release factor to water	0.02 **(0.003)** A-table 2.1	0.1 **(0.1)** A-table 3.15 water based	0.8 **(0.8)** A-table 3.2	0.02 **(0.02)** A-table3.3
Total emission to waste water [t/a]	15 **(11.25)**	7.5 **(37.5)**	80 **(400)**	3 **(15)**
Size of STP [m^3/d]	2,000	2,000	2,000	10,000
Dilution in receiv. water	10	10	10	40
$Clocal_{effl.}$ [mg/l]	2.52 **(1.42)**	0.24 **(1.18)**	126 **(202)**	0.63 **(1.01)**
$Clocal_{water}$ [mg/l]	0.25 **(0.14)**	0.02 **(0.12)**	12.6 **(20.2)**	0.02 **(0.03)**
$PEC_{local\_surfacewater}$ [mg/l]	0.25 **(0.14)**	0.02 **(0.12)**	12.6 **(20.2)**	0.02 **(0.03)**

3.1.2.3 Data on occurrence in the hydrosphere

2-EEA was detected qualitatively in ground water samples collected beneath leaking underground storage tanks of a paint factory in Milan, Italy (Botta et al. 1984). These samples were taken in a depth of 30 m beneath a 10 cm layer of clay in sandy soil.

2-EEA was further detected in one of eight weakly polluted small rivers and brooks in Southwest Germany (Rickenbach East). But no further data on concentrations etc. are available (Juettner, 1992).

No more measured data regarding the occurrence of 2- EEA in the hydrosphere are available.

3.1.2.4 Sediment

Data on the occurrence of 2-EEA in the sediment are not available. According to 2-EEA´s physico-chemical properties there is no indication for a potential to accumulate in organic matter.

3.1.3 Atmosphere

In spite of the relatively high vapour pressure of 2-EEA (270 Pa) the substance has a strong tendency to remain in the water compartment because of its very high water solubility (229 g/l) which results in a Henry´s law constant of 0.16 Pa*m^3*mol^{-1}. The result of the fugacity model of Mackay, according to which 94.8 % of the substance enters the water compartment and only 5.2 % the atmosphere, supports this assumption (see table3.3).

The release factors (TGD default values) to air are in the range of 0.01 (IC/UC 3/33 and 14/48, formulation) to 0.8 (water based) and 0.9 (solvent based) (IC/UC 14/48). As no information are available on the kind of use of 2-EEA in solvents the calculation for this scenario are based on the emission factor for solvent based formulations (worst case).

Table 3.6: Air emissions for import of 1000 t/a (5,000 t/a)

Types of use	**Solvent in paints/lacquers/varnishes** **Industrial formulation and use**		**solvent in chemical industry**	**Intermediate in chemical industry**
Tonnage [t/a]	750 **(3,750)**	75 **(375)**	100 **(500)**	150 **(750)**
Main category	non-dispersive use (Ic)	wide dispersive use	non-dispersive use (Ic)	non-dispersive use (Ic)
IC/UC	14/48	14/48	2/48	3/33
Life cycle step	formulation	industrial use	industrial use	processing
Release factor to air	0.01 A-table 2.1	0.9 (solvent based) A-table 3.15	0.1 A-table 3.2	0.01 A-table3.3
Total emission to air [t/a]	7.5 **(37.5)**	67.5 **(337.5)**	10 **(50)**	1.5 **(7.5)**

The calculated annual average 2-EEA concentrations in air are presented in table 3.7 (for calculations see appendices 3-1 to 3-8).

Table 3.7: Local PECs in air

Scenario **IC/UC**	**PEClocal (mg/m^3)** **(1000 t/a)**	**PEClocal (mg/m^3)** **(5000 t/a)**
14/48 formulation	$4.6*10^{-3}$	0.02
14/48 industrial use	$7.7*10^{-3}$	0.04
2/48	$3.8*10^{-3}$	0.02
3/33	$5.7*10^{-4}$	$2.3*10^{-3}$

3.1.4 Terrestrial compartment

The release of 2-EEA to soil occurs through atmospheric deposition after local releases to the atmosphere at the sites. The input through sludge application on agricultural soil is considered negligible. 2-EEA does not partition to sewage sludge in the waste water treatment plant (wwtp). The log Kow of 0.24 also indicates a low potential for adsorption to organic matter.

Using the worst case deposition rate of $DEPtotal_{ann}$ of $0.011\ mg \cdot m^2 \cdot d^{-1}$ (1,000 t/a) and $0.055\ mg*m^2*d^{-1}$ (5,000 t/a), respectively, calculated for scenario IC/UC 14/48, industrial use, the maximum equilibrium soil concentration in the vicinity of a production/processing plant can be calculated according to the procedure proposed in the TGD. The calculations are presented in Appendices 3-9 and 3-10 (the resulting concentrations in natural soil and in agricultural soil are equal).

1,000 t/a: $PEClocal_{soil} = 1.2 \cdot 10^{-3}\ mg/kg_{ww}$

5,000 t/a: $PEClocal_{soil} = 5.9 \cdot 10^{-3}\ mg/kg_{ww}$

1,000 t/a: $PEClocal_{soil\text{-}porew} = 3.2\ \mu g/l$

5,000 t/a: $PEClocal_{soil\text{-}porew} = 16\ \mu g/l$

3.1.5 Non compartment specific exposure relevant to the food chain

With a log Kow of 0.24 and a BCF_{fish} of 0.32 l/kg 2-EEA has only a low bioaccumulation potential. Hence, no risk characterization for secondary poisoning has to be conducted.

3.1.6 Other non industrial emissions of 2-EEA

There is no information regarding non industrial emissions of 2-EEA.

3.1.7 Regional concentrations

The total emission of 2-EAA to waste water is 106 t/a based on 1,000 t import/a and 464 t/a based on an import of 5,000 t/a. Considering the low tonnage and the lack of information regarding industrial wwtps it is assumed that 80 % of the waste water is treated in municipal wwtps and that 20 % enters directly surface waters.

All releases are considered in the determination of a regional background concentration. The local emissions from all scenarios are summarised and distributed to the regional and continental area in a ratio of 10 % to 90 %. The calculations for the regional PECs are performed with Simple Box 2.0 (see Appendix 4).

Table 3.8 shows the calculated regional PECs for water, air and soil.

Table 3.8: Regional PECs for water, air and soil

Compartment	**PEC regional (1000 t/a)**	**PEC regional (5000 t/a)**
Water	0.03 µg/l	0.15 µg/l
Air	$3.3*10^{-4}$ µg/m^3	$1.7*10^{-3}$ µg/m^3
Soil	$2.1*10^{-3}$ µg/kg$_{ww}$	0.01 µg/kg$_{ww}$

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

3.2.1 Aquatic compartment (incl. sediment)

Fish

The 2-EEA short-term toxicity studies to fish are summarised in the following table.

Table 3.9 : Acute toxicity data to fish

Species	**Endpoint**	**Effect concentration [mg/l]**	**Test system**	**Method**	**Reference**
Carassius auratus	24 h LC50	160	static	APHA 1971, No. 231	Bridié et al., 1979a
Lepomis macrochirus	96 h LC50	52.0	static	EPA 1975	Bailey et al., 1985
Leuciscus idus	48 h LC50	141	static	DIN 38412	Juhnke & Lüdemann, 1978
Leuciscus idus	48 h LC50	107	static	DIN 38412	Juhnke & Lüdemann, 1978
Pimephales promelas	96 h LC50	42.2	flow-through	*)	Holcombe et al.,1984
Ictalurus punctatus	96 h LC50	44.8	flow-through	*)	Holcombe et al.,1984
Lepomis macrochirus	96 h LC50	41.0	flow-through	*)	Bailey et al., 1985

*) all flow-through tests were conducted according to EPA, 1975.

In acute toxicity tests to fresh water species values in the range from 41 mg/l (*Lepomis macrochirus*) to 160 mg/l (*Carassius auratus*) were obtained. Several 96-hour LC50 values for freshwater fish species are in the range of 41-52 mg/l, with the lowest reported value of 41 mg/l for *L. machrochirus* based on measured concentrations in a flow-through test. In this test a minimum of four test concentrations plus a control group in duplicated was used. Water and toxicant flows were checked daily and adjusted when necessary. The pH and dissolved oxygen and toxicant concentrations of the test solutions were also determined at the beginning and end of the test. Mortality was recorded every 24 hours.

No tests on chronic toxicity to fish are available.

Aquatic invertebrates

Table 3.10 shows the available valid test results for 2-EEA obtained in short-term tests with aquatic invertebrates.

Table 3.10 : Acute toxicity data to invertebrates

Species	**Endpoint**	**Effect concentration [mg/l]**	**Test system**	**Procedure according to**	**Reference**
Daphnia magna	24 h EC50	354	no information Fresh water	DIN 38412, part 11	Hüls AG, 1987b
Artemia salina	24 h LC50	4,000	Static Salt water	no standard test	Price et al., 1974
Hydra attenuata (adults & embryos)	92 h MEC*	584	no information Fresh water	no standard test	Johnson et al.1984
Aplexa hypnorum (adult)	96 h LC50	65.2	flow-through Fresh water	EPA-660/3-75-009	Holcombe et al., 1984

*MEC = minimum toxic effect concentration

The test with the freshwater snail *Aplexa hypnorum* was conducted in order to compare sensitivity differences between the fish also used in this test (*Ictalurus punctatus*, see table 3.9) and other freshwater species. The snail was little less sensitive in this test than the fish, however, the two results are in the same order of magnitude. *Aplexa hypnorum* is the most sensitive aquatic invertebrate tested (fresh water). The marine species *Artemia salina* is at least one order of magnitude less sensitive than the freshwater species.

There is one test on chronic toxicity to *Daphnia magna* available with the endpoint reproduction rate (Hüls AG 1988b). The test was conducted according to an UBA proposal from 1984 and resulted in a 21 d NOEC of 30 mg/l. The EC50 in this test was > 100 mg/l (100 mg/l show 30 % inhibition of reproduction). The test is poorly documented and only few information are available. However, this UBA proposal is mostly equivalent to the OECD guideline 202 "*Daphnia* sp., Acute Immobilisation Test and Reproduction Test" from 1984 and the test result seems plausible.

Algae

The following table shows the toxicity of 2-EEA to the alga *Scenedesmus subspicatus*. The results are given as nominal concentrations.

Table 3.11: Acute toxicity data to *Scenedesmus subspicatus*

Criterion	**Duration** [h]	**Result** [mg/l]	**Test procedure**	**Reference**
Assimilation inhibition	24	EC_0 > 10,000	DIN 38412, L 12	Hüls AG, 1987a
Growth inhibition	72	EC_{10} ~ 1,000	UBA-GL, 1984	Hüls AG, 1988a

Concerning the algae there is only one test on growth inhibition available. A 72 h-EC10 of about 1,000 mg/l was found for the alga *Scenedesmus subspicatus* in this test conducted according to an UBA-test proposal from 1984 (Hüls AG 1988a).

Microorganisms

One toxicity test to bacteria has been carried out. In a growth inhibition test according to Bringmann and Kühn (Hüls, 1995d) an EC10 of 435 mg/l was determined. The test organism *Pseudomonas putida* was incubated in the presence of different concentrations during 18 hours at 25 °C. The growth inhibition was determined by turbidity measurements.

The concentration of 2-EEA in the biodegradation tests described in chapter 3.1.1 was 1000 mg/l (OECD 301 E) and 500 mg/l (OECD 302 B), respectively. In these tests high degradation rates were achieved which show that no inhibition of the activated sludge took place at this concentrations. Hence, the EC10 (*Pseudomonas putida*) of 435 mg/l is supported by these test results.

PNEC$_{water}$-calculations

In addition to short-term effect data for algae, invertebrates and fish, a long-term value (21d NOEC of 30 mg/l) for the inhibition of reproduction in Daphnia magna as well as a 72h EC10 for *Scenedesmus subspicatus* (growth inhibition) are available. As the most sensitive species is fish and no long term data on fish are available an assessment factor of 100 according to TGD is used for the derivation of the PNEC.

The PNEC calculation is based on the NOEC (daphnia magna) of 30 mg/l. The application of the safety factor 100 leads to a

PNEC$_{water}$ = 0.30 mg/l

PNEC$_{sediment}$

A PNEC for sediment was not calculated as 2-EEA does not adsorb to organic matter (log Kow = 0.24 and Koc = 13.9 l/kg) and there are no tests with benthic organisms available.

PNEC$_{microorganisms}$

The derivation of the PNEC$_{microorganisms}$ is based on the EC10 of 435 mg/l for *Pseudomonas putida.* According TGD an assessment factor of 1 is used for calculating the PNEC.

PNEC$_{wwtp}$ = 435 mg/l

3.2.2 Atmosphere

No ecotoxicological data are available for this environmental compartment.

Due to the low tonnage and the atmospheric half-life ($t_{1/2}$ = 25.6 h) abiotic effects on the atmosphere, such as contribution to global warming and ozone depletion are not to be expected in connection with 2-EEA.

3.2.3 Terrestrial compartment

PNEC$_{soil}$-calculations

As there are no studies with terrestrial species available the equilibrium partition method according to TGD was used to calculate a PNEC$_{soil}$.

PNEC$_{soil}$ = 0.11 mg/kg

3.3 RISK CHARACTERISATION

3.3.1 Aquatic compartment (incl. sediment)

Waste water treatment plants

The PEC/PNEC ratios are below 1 for all scenarios. The currently available data do not indicate any risk to microorganisms of waste water treatment plants. Regarding the $PNEC_{micro-organisms}$ of 435 mg/l the following PEC/PNEC ratios can be calculated:

Table 3.12: PEC/PNEC ratios for wwtps

Scenario IC/UC	**PEC [mg/l] 1,000 t/a**	**PEC/PNEC ratio**	**PEC [mg/l] 5,000 t/a**	**PEC/PNEC ratio**
14/48 formulation	2.52	< 0.01	1.42	< 0.01
14/48 industrial use	0.24	< 0.01	1.18	< 0.01
2/48	126	0.29	202	0.46
3/33	0.63	< 0.01	1.01	< 0.01

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

Surface water

From the $PNEC_{water}$ of 0.30 mg/l the following PEC/PNEC ratios are calculated:

Table 3.13: PEC/PNEC ratios for surface water

Scenario IC/UC	**PEC [mg/l] 1,000 t/a import**	**PEC/PNEC ratio**	**PEC [mg/l] 5,000 t/a import**	**PEC/PNEC ratio**
14/48 formulation	0.25	0.83	0.14	0.47
14/48 industrial use	0.02	0.07	0.12	0.40
2/48	12.6	**42**	20.2	**67**
3/33	0.02	0.07	0.03	0.1

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.

Based on the scenarios “Paints, lacquers and varnishes industry/solvents” (IC/UC 14/48) and “Chemical industry: chemicals used in synthesis/intermediates” (IC/UC 3/33) no risk has been identified to surface water.

Concerning the scenario “Chemical Industry: basic chemicals/solvents” (IC/UC 2/48) a risk to the aquatic environment was identified. Using default values from the TGD the risk was identified for both the 1,000 t and the 5,000 t import per year.

However, **at present** there is no need for further information and/or testing nor for risk reduction measures beyond those which are being applied already because at present there is no production within the EU, nor is there any import into the EU and presumably therefore no use. **Based on this information conclusion (ii) is drawn.**

The risk assessment is based solely on historical data and can currently be considered of historical value only. Thus the identified risk should be regarded as hypothetical.

If production, importation and/or use in the EU is restarted the conclusion would need to be reassessed and any manufacturer or importer would then be asked to provide current import figures and site specific exposure data.

3.3.2 Atmosphere

Due to the atmospheric half-life ($t_{1/2}$ = 25.6 h), abiotic effects on the atmosphere, such as global warming and ozone depletion, are not to be expected in connection with 2-EEA. The highest calculated air concentration are $7.7*10^{-3}$ mg/m^3 (1000 t/a) and 0.04 mg/m^3 (5000 t/a), respectively, for industrial use as solvent in paint and varnishes industry. Since no data are available on the ecotoxicological effect of the substance in connection with the atmosphere, it is not possible to perform a quantitative assessment of this environmental compartment. On the basis of the available information on the substance, further testing seems not necessary.

3.3.3 Terrestrial compartment

The PECs for the terrestrial compartment are $1.2 \cdot 10^{-3}$ mg/kg_{ww} (1,000 t/a) and $5.9 \cdot 10^{-3}$ mg/kg_{ww} (5,000 t/a). Given the PNECsoil of 0.11 mg/kg the PEC/PNEC ratios for this compartment are both < 0.1.

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

3.3.4 Non compartment specific effects relevant to the food chain (secondary poisoning)

Since there is no indication that 2-EEA possesses a bioaccumulation potential, a risk characterisation for exposure via the food chain is not considered necessary.

4 HUMAN HEALTH

The Human Health Section of 2- Ethoxyethyl acetate was not carried out (see note on page 2).

4.1 HUMAN HEALTH (TOXICITY)

4.1.1 Exposure assessment

4.1.1.1 General discussion

4.1.1.2 Occupational exposure

4.1.1.3 Consumer exposure

4.1.1.4 Indirect exposure via the environment

In accordance with the TGD the indirect exposure via the environment is calculated using data for oral intake via food, drinking water and air.

For calculation the most significant point sources regarding the atmosphere (IC14/UC48, Industrial Use) as well as the scenario which lead to the highest emission to waste water (IC2/UC48) is considered. The results of these calculations with the corresponding input values are summarised in Appendices 4-1 to 4-4.

Scenario IC14/UC48, Industrial Use

The resultant daily doses for the substance are as follows (see also table 4.1):

- 1,000 t/a $DOSE_{total\_local} = 0.004$ mg*kg body weight^{-1} day^{-1}
- 5,000 t/a $DOSE_{total\_local} = 0.02$ mg*kg body weight^{-1} day^{-1}

Table 4.1: Results of calculation of the indirect exposure for 1,000 t **(5,000 t/a)** import per year

Intake route	**% of total uptake**	
	Local	**regional**
drinking water	13.2 **(13.4)**	83.8 **(82.1)**
fish	0.24 **(0.25)**	1.54 **(1.51)**
plant stem	46.8 **(46.7)**	7.36 **(8.20)**
plant root	0.40 **(0.40)**	1.17 **(1.30)**
meat	<0.01 **(<0.01)**	< 0.01 **(< 0.01)**
milk	0.01 **(0.01)**	0.01 **(0.01)**
air	39.3 **(39.2)**	6.15 **(6.86)**

Plant stem and air are the most important intake routes for 2-EEA in the local approach, whereas drinking water is the most important intake route for 2-EEA in the regional approach.

Scenario IC2/UC48

The resultant daily doses for the substance are as follows:

- 1,000 t/a DOSE$_{total\_local}$ = 0.02 mg*kg body weight^{-1} day^{-1}
- 5,000 t/a DOSE$_{total\_local}$ = 0.09 mg*kg body weight^{-1} day^{-1}

Table 4.2: Results of calculation of the indirect exposure for 1,000 t **(5,000 t/a)** import per year

Intake route	**% of total uptake**	
	Local	**regional**
drinking water	90.2 **(90.4)**	83.8 **(82,1)**
fish	1.65 **(1.66)**	1.54 **(1.51)**
plant stem	4.40 **(4.32)**	7.36 **(8.20)**
plant root	0.04 **(0.03)**	1.17 **(1.30)**
meat	<0.01 **(<0.01)**	< 0.01 **(< 0.01)**
milk	0.01 **(0.01)**	0.01 **(0.01)**
air	3.70 **(3.63)**	6.15 **(6.86)**

Drinking water is the most important intake route for 2-EEA in the local and the regional approach.

4.1.1.4 (Combined exposure)

4.1.2 Effects assessment: Hazard identification and Dose (concentration) - response (effect) assessment

4.1.2.1 Toxico-kinetics, metabolism and distribution

4.1.2.2 Acute toxicity

4.1.2.3 Irritation

4.1.2.4 Corrosivity

4.1.2.5 Sensitisation

4.1.1.6 Repeated dose toxicity

4.1.2.7 Mutagenicity

4.1.2.8 Carcinogenicity

4.1.2.9 Toxicity for reproduction

4.1.3 Risk characterisation

4.1.3.1 General aspects

4.1.3.2 Workers

4.1.3.3 Consumers

4.1.3.4 Man exposed indirectly via the environment

4.2 HUMAN HEALTH (PHYSICO-CHEMICAL PROPERTIES)

4.2.3 Risk characterisation

4.2.3.1 Workers

5 CONCLUSIONS / RESULTS

Environment

(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.

Based on the scenarios “Paints, lacquers and varnishes industry, solvents” (IC/UC 14/48) and “Chemical industry: chemicals used in synthesis/intermediates” (IC/UC 3/33) no risk was identified to surface water. Conclusion (ii) also applies to waste water treatment plants for all scenarios and to the terrestrial compartment.

Concerning the scenario “Chemical Industry: basic chemicals/solvents” (IC/UC 2/48) a risk to the aquatic environment was identified. Using default values from the TGD the risk was identified for both the 1,000 t and the 5,000 t import per year.

However, **at present** there is no need for further information and/or testing nor for risk reduction measures beyond those which are being applied already because at present there is no production within the EU, nor is there any import into the EU and presumably therefore no use. **Based on this information conclusion (ii) is drawn.**

The risk assessment is based solely on historical data and can currently be considered of historical value only. Thus the identified risk should be regarded as hypothetical.

If production, importation and/or use in the EU are restarted the conclusion would need to be reassessed and any manufacturer or importer would then be asked to provide current import figures and site specific exposure data.

Human Health

The Human Health Section of 2- Ethoxyethyl acetate was not carried out (see note on page 2).

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7 APPENDIX 1-1

Calculation of

- Distribution and Fate
- Simple Treat 3.0

Distribution and Fate

$d := \mathrm{Tag}$

Substance: 2-EEA CAS.Nr.: 111-15-9

melting point:	$MP := 211 \cdot K$
vapour pressure:	$VP := 270 \cdot Pa$
water solubility:	$SOL := 229000 \cdot mg \cdot l^{-1}$
part. coefficient octanol/water:	$LOGP_{OW} := 0.24$
moleculare weight:	$MOLW := 0.132 \cdot kg \cdot mol^{-1}$
gas constant:	$R := 8.3143 \cdot J \cdot (mol \cdot (K))^{-1}$
temperature:	$T := 293 \cdot K$
conc. of suspended matter in the river:	$SUSP_{water} := 15 \cdot mg \cdot l^{-1}$
density of the solid phase:	$RHO_{solid} := 2500 \cdot kg \cdot m^{-3}$
volume fraction water in susp. matter:	$Fwater_{susp} := 0.9$
volume fraction solids in susp.matter:	$Fsolid_{susp} := 0.1$
volume fraction of water in sediment:	$Fwater_{sed} := 0.8$
volume fraction of solids in sediment:	$Fsolid_{sed} := 0.2$
volume fraction of air in soil:	$Fair_{soil} := 0.2$
volume fraction of water in soil:	$Fwater_{soil} := 0.2$
volume fraction of solids in soil:	$Fsolid_{soil} := 0.6$
aerobic fraction of the sediment comp.:	$Faer_{sed} := 0.1$
product of CONjunge and $SURF_{air}$:	$product := 10^{-4} \cdot Pa$

distribution air/water: Henry-constant

$$HENRY := \frac{VP \cdot MOLW}{SOL} \qquad HENRY = 0.156 \circ Pa \cdot m^3 \cdot mol^{-1}$$

$$\log\left(\frac{HENRY}{Pa \cdot m^3 \cdot mol^{-1}}\right) = -0.808$$

$$K_{air\_water} := \frac{HENRY}{R \cdot T} \qquad K_{air\_water} = 6.389 \bullet 10^{-5}$$

solid/water-partition ceefficient Kp $_{comp}$ and total compartment/water-partition coefficient K$_{comp\_water}$

$a := 0.52$ (a,b from TGD part III, chapter 4, table 4, Nonhydrophobics)

$b := 1.02$

$K_{OC} := 10^{a \cdot LOGP_{OW} + b} \cdot l \cdot kg^{-1}$ $K_{OC} = 13.957 \circ l \cdot kg^{-1}$

Suspended matter

$Kp_{susp} := 0.1 \cdot K_{OC}$ $Kp_{susp} = 1.396 \circ l \cdot kg^{-1}$

$K_{susp\_water} := Fwater_{susp} + Fsolid_{susp} \cdot Kp_{susp} \cdot RHO_{solid}$ $K_{susp\_water} = 1.249$

factor for the calculation of Clocal$_{water}$:

$faktor := 1 + Kp_{susp} \cdot SUSP_{water}$ $faktor = 1$

Sediment

$Kp_{sed} := 0.05 \cdot K_{OC}$ $Kp_{sed} = 0.698 \circ l \cdot kg^{-1}$

$K_{sed\_water} := Fwater_{sed} + Fsolid_{sed} \cdot Kp_{sed} \cdot RHO_{solid}$ $K_{sed\_water} = 1.149$

Soil

$Kp_{soil} := 0.02 \cdot K_{OC}$ $Kp_{soil} = 0.279 \circ l \cdot kg^{-1}$

$K_{soil\_water} := Fair_{soil} \cdot K_{air\_water} + Fwater_{soil} + Fsolid_{soil} \cdot Kp_{soil} \cdot RHO_{solid}$

$K_{soil\_water} = 0.619$

Sludge

$K_{p\_sludge} := 0.37 \cdot K_{OC}$ $K_{p\_sludge} = 5.164 \circ l \cdot kg^{-1}$

Elimination in STPs

rate constant in STP: $k = 1\ h^{-1}$

elimination P = f (k, logpow, logH) = 87.4 %

fraction directed to surface water $Fstp_{water} = 12.6\ \%$

biodegradation in different compartments

surface water

$kbio_{water} := 4.7 \cdot 10^{-2} \cdot d^{-1}$ (TGD part II, chapter 3, table 7)

soil

$DT50bio_{soil} := 30 \cdot d$ (TGD part II, chapter 3, table 8)

$kbio_{soil} := \frac{\ln(2)}{DT50bio_{soil}}$ $kbio_{soil} = 0.023 \circ d^{-1}$

sediment

$kbio_{sed} := \frac{\ln(2)}{DT50bio_{soil}} \cdot Faer_{sed}$ $kbio_{sed} = 2.31 \bullet 10^{-3} \circ d^{-1}$

degradation in surface waters

$khydr_{water} := 1.1 \cdot 10^{-3} \cdot d^{-1}$

$kphoto_{water} := 1 \cdot 10^{-99} \cdot d^{-1}$

$kdeg_{water} := khydr_{water} + kphoto_{water} + kbio_{water}$

$kdeg_{water} = 0.048 \circ d^{-1}$

Atmosphere

calculation of CONjunge * SURFaer for the OPS-model

$VPL := \frac{VP}{\exp\left[6.79 \cdot \left(1 - \frac{MP}{285 \cdot K}\right)\right]}$

$VP := wenn(MP > 285 \cdot K, VPL, VP)$

$VP = 270 \circ Pa$

$Fass_{aer} := \frac{product}{VP + product}$

$Fass_{aer} = 3.704 \bullet 10^{-7}$

degradation in the atmosphere

$kdeg_{air} = 2.71 * 10^{-2}\ h^{-1} = 0.65\ d^{-1}$ (see RAR)

```
            output of SimpleTreat 3.0 (debugged version, 7 Feb 97)                     today is    27. Feb 06
                          report of  2EEA
including primary sedimentation
    Elimination in the primary settler
                volatilization              0,0
                via primary sludge          0,0
                                   ____________
                total                       0,0 %
                                                          without primary sedimentation
    Elimination in the aerator                                Elimination in the aerator
                stripping                   0,0                            stripping                   0,0
                biodegradation             87,3                            biodegradation             91,5
                                   ____________                                               ____________
                total                      87,3 %                          total                      91,5 %

 Elimination in the solids liquid separator               Elimination in the solids liquid separator
                volatilization              0,0                            volatilization              0,0
                via surplus sludge          0,0                            via surplus sludge          0,0
                                   ____________                                               ____________
                total                       0,0 %                          total                       0,0 %

  Total elimination from waste water       87,4 %           Total elimination from waste water       91,5 %
     Total emission via effluent           12,6 %------V       Total emission via effluent           12,6 %------V
                                                12,63 % dissolved                                        12,64 % dissolved
                                                 0,00 % associated                                        0,00 % associated
                                   ____________                                               ____________
                balance                   100,0 %                          balance                   104,2 %

     Summary of distribution                                   Summary of distribution
                to air                      0,1                            to air                      0,0
                to water                   12,6                            to water                   12,6
                via primary sludge          0,0                            via surplus sludge          0,0
                via surplus sludge          0,0                            degraded                   91,5
                degraded                   87,3                                               ____________
                                   ____________                            total                     104,2 %
                total                     100,0 %

        Concentrations                                            Concentrations
                in air                 1,30E-08 g m-3                      in air                 6,79E-09 g m-3
                in combined sludge     2,08E-01 mg kg-1                    in surplus sludge      4,13E-02 mg kg-1
                  |___________  in primary sludge:  2,61E-01 mg kg-1       in effluent (total)    6,32E-02 mg l-1
                  |___________  in surplus sludge:  4,08E-02 mg kg-1         |___________       dissolved     6,32E-02 mg l-1
                in effluent (total)     0,06317 mg l-1                       |___________      associated     1,24E-06 mg l-1
                  |___________        dissolved  6,32E-02 mg l-1           in solids effluent     4,13E-02 mg kg-1
                  |___________       associated  1,23E-06 mg l-1
                in solids effluent     4,08E-02 mg kg-1

    Operation of the plant equipped with a primary settler        Operation of the plant without primary settler
  Sludge loading rate =          0,15 kg BOD (kg dw)-1 d-1        Sludge loading rate =          0,15 kg BOD (kg dw)-1 d-1
                  HRT =           6,9 h                                          HRT =          10,8 h
                  SRT =          9,20 d                                          SRT =          9,20 d
       Aeration mode =   surface aeration                             Aeration mode =   surface aeration
      Primary sludge =       6,00E+02 kg dry weight d-1               Surplus sludge =       3,31E+02 kg dry weight d-1
      Surplus sludge =       1,90E+02 kg dry weight d-1             Total wastewater =       2,00E+03 m3 d-1
        Total sludge =       7,90E+02 kg dry weight d-1
    Total wastewater =       2,00E+03 m3 d-1
```

8 APPENDIX 2-1

PEC local_water

Scenario IC/UC 14/48

Formulation – 1,000 t/a

Estimation of Clocal$_{water}$ of chemicals used as a solvent in paint during formulation (IC = 14) **status: TGD,A+B table, IC - 14**

$\mu g := 10^{-9} \cdot kg$

$d := 86400 \cdot s$

$a := 365 \cdot d$

chemical : 2-EEA CAS-Nr.: 111-15-9

Total annual tonnage of chemical: $TONNAGE := 750 \cdot tonne \cdot a^{-1}$

Release factor (A 2.1): $f_{emission} := 0.02$

Fraction of main source (B 2.10): $Fmainsource := 0.8$

Waste water flow of wwtp: $EFFLUENT_{stp} := 2000 \cdot m^3 \cdot d^{-1}$

Duration of emission (B 2.10): $Temission := 300 \cdot d \cdot a^{-1}$

Fraction of emission directed to water:
(SimpleTreat; k:1 h^{-1}; logPow:0.24 ; logH:-0.81) $Fstp_{water} := 12.6 \cdot \%$

Dilution factor (TGD): $DILUTION := 10$

Factor (1+Kp * SUSPwater): $FACTOR := 1$

***Emission per day*:**

$$Elocal_{water} := \frac{TONNAGE \cdot Fmainsource \cdot f_{emission}}{Temission} \qquad Elocal_{water} = 40 \circ kg \cdot d^{-1}$$

Influent concentration:

$$Clocal_{inf} := \frac{Elocal_{water}}{EFFLUENT_{stp}} \qquad Clocal_{inf} = 20 \circ mg \cdot l^{-1}$$

Effluent concentration:

$$Clocal_{eff} := Clocal_{inf} \cdot Fstp_{water} \qquad Clocal_{eff} = 2.52 \circ mg \cdot l^{-1}$$

Concentration in surface water:

$$Clocal_{water} := \frac{Clocal_{eff}}{FACTOR \cdot DILUTION} \qquad Clocal_{water} = 252 \circ \mu g \cdot l^{-1}$$

Total release for the regional model (without elimination in STPs):

$$RELEASE := TONNAGE \cdot f_{emission} \qquad RELEASE = 15 \circ tonne \cdot a^{-1}$$

Annual average local concentration in water:

$$Clocal_{water\_ann} := Clocal_{water} \cdot \frac{Temission}{365 \cdot d \cdot a^{-1}} \qquad Clocal_{water\_ann} = 207.1 \circ \mu g \cdot l^{-1}$$

9 APPENDIX 2-2

PEC local_water

Scenario IC/UC 14/48

Industrial Use – 1,000 t/a

Estimation of Clocal$_{water}$ of chemicals used as a solvent in paint during industrial processing (IC = 14) status: TGD,A+B table, IC - 14

$\mu g := 10^{-9}\cdot kg$

$d := 86400\cdot s$

$a := 365\cdot d$

chemical : 2-EEA CAS-Nr.: 111-15-9

Total annual tonnage of chemical:	$TONNAGE := 75\cdot tonne\cdot a^{-1}$
Release factor (A 3.15):	$f_{emission} := 0.1$
Fraction of main source (B 3.13):	$Fmainsource := 0.15$
Waste water flow of wwtp:	$EFFLUENT_{stp} := 2000\cdot m^{3}\cdot d^{-1}$
Duration of emission (B 3.13):	$Temission := 300\cdot d\cdot a^{-1}$
Fraction of emission directed to water: (SimpleTreat; k:1 h^{-1}; logPow:0.24 ; logH:-0.81)	$Fstp_{water} := 12.6\cdot\%$
Dilution factor (TGD):	$DILUTION := 10$
Factor (1+Kp * SUSPwater):	$FACTOR := 1$

Emission per day:

$$Elocal_{water} := \frac{TONNAGE\cdot Fmainsource\cdot f_{emission}}{Temission} \qquad Elocal_{water} = 3.75 \circ kg\cdot d^{-1}$$

Influent concentration:

$$Clocal_{inf} := \frac{Elocal_{water}}{EFFLUENT_{stp}} \qquad Clocal_{inf} = 1.88 \circ mg\cdot l^{-1}$$

Effluent concentration:

$$Clocal_{eff} := Clocal_{inf}\cdot Fstp_{water} \qquad Clocal_{eff} = 0.24 \circ mg\cdot l^{-1}$$

Concentration in surface water:

$$Clocal_{water} := \frac{Clocal_{eff}}{FACTOR\cdot DILUTION} \qquad Clocal_{water} = 23.6 \circ \mu g\cdot l^{-1}$$

Total release for the regional model (without elimination in STPs):

$$RELEASE := TONNAGE\cdot f_{emission} \qquad RELEASE = 7.5 \circ tonne\cdot a^{-1}$$

Annual average local concentration in water:

$$Clocal_{water\_ann} := Clocal_{water}\cdot\frac{Temission}{365\cdot d\cdot a^{-1}} \qquad Clocal_{water\_ann} = 19.4 \circ \mu g\cdot l^{-1}$$

Appendix 2-3

PEC local_water

Scenario IC/UC 14/48

Formulation – 5,000 t/a

Estimation of Clocal$_{water}$ of chemicals used as a solvent in paint during formulation (IC = 14) status: TGD,A+B table, IC - 14

$\mu g := 10^{-9} \cdot kg$

$d := 86400 \cdot s$

$a := 365 \cdot d$

chemical : 2-EEA CAS-Nr.: 111-15-9

Total annual tonnage of chemical:	$TONNAGE := 3750 \cdot tonne \cdot a^{-1}$
Release factor (A 2.1):	$f_{emission} := 0.003$
Fraction of main source (B 2.10):	$Fmainsource := 0.6$
Waste water flow of wwtp:	$EFFLUENT_{stp} := 2000 \cdot m^{3} \cdot d^{-1}$
Duration of emission (B 2.10):	$Temission := 300 \cdot d \cdot a^{-1}$
Fraction of emission directed to water: (SimpleTreat; k:1 h^{-1}; logPow:0.24 ; logH:-0.81)	$Fstp_{water} := 12.6 \cdot \%$
Dilution factor (TGD):	$DILUTION := 10$
Factor (1+Kp * SUSPwater):	$FACTOR := 1$

Emission per day:

$$Elocal_{water} := \frac{TONNAGE \cdot Fmainsource \cdot f_{emission}}{Temission} \qquad Elocal_{water} = 22.5 \circ kg \cdot d^{-1}$$

Influent concentration:

$$Clocal_{inf} := \frac{Elocal_{water}}{EFFLUENT_{stp}} \qquad Clocal_{inf} = 11.25 \circ mg \cdot l^{-1}$$

Effluent concentration:

$$Clocal_{eff} := Clocal_{inf} \cdot Fstp_{water} \qquad Clocal_{eff} = 1.42 \circ mg \cdot l^{-1}$$

Concentration in surface water:

$$Clocal_{water} := \frac{Clocal_{eff}}{FACTOR \cdot DILUTION} \qquad Clocal_{water} = 141.8 \circ \mu g \cdot l^{-1}$$

Total release for the regional model (without elimination in STPs):

$$RELEASE := TONNAGE \cdot f_{emission} \qquad RELEASE = 11.25 \circ tonne \cdot a^{-1}$$

Annual average local concentration in water:

$$Clocal_{water\_ann} := Clocal_{water} \cdot \frac{Temission}{365 \cdot d \cdot a^{-1}} \qquad Clocal_{water\_ann} = 116.5 \circ \mu g \cdot l^{-1}$$

Appendix 2-4

PEC local_water

Scenario IC/UC 14/48

Industrial Use – 5,000 t/a

Estimation of Clocal$_{water}$ of chemicals used as a solvent in paint during industrial processing (IC = 14) **status: TGD,A+B table, IC - 14**

$\mu g := 10^{-9} \cdot kg$

$d := 86400 \cdot s$

$a := 365 \cdot d$

chemical : 2-EEA CAS-Nr.: 111-15-9

Total annual tonnage of chemical:	$TONNAGE := 375 \cdot tonne \cdot a^{-1}$
Release factor (A 3.15):	$f_{emission} := 0.1$
Fraction of main source (B 3.13):	$Fmainsource := 0.15$
Waste water flow of wwtp:	$EFFLUENT_{stp} := 2000 \cdot m^3 \cdot d^{-1}$
Duration of emission (B 3.13):	$Temission := 300 \cdot d \cdot a^{-1}$
Fraction of emission directed to water: (SimpleTreat; k:1 h^{-1}; logPow:0.24 ; logH:-0.81)	$Fstp_{water} := 12.6 \cdot \%$
Dilution factor (TGD):	$DILUTION := 10$
Factor (1+Kp * SUSPwater):	$FACTOR := 1$

***Emission per day*:**

$$Elocal_{water} := \frac{TONNAGE \cdot Fmainsource \cdot f_{emission}}{Temission} \qquad Elocal_{water} = 18.75 \circ kg \cdot d^{-1}$$

Influent concentration:

$$Clocal_{inf} := \frac{Elocal_{water}}{EFFLUENT_{stp}} \qquad Clocal_{inf} = 9.38 \circ mg \cdot l^{-1}$$

Effluent concentration:

$$Clocal_{eff} := Clocal_{inf} \cdot Fstp_{water} \qquad Clocal_{eff} = 1.18 \circ mg \cdot l^{-1}$$

Concentration in surface water:

$$Clocal_{water} := \frac{Clocal_{eff}}{FACTOR \cdot DILUTION} \qquad Clocal_{water} = 118.1 \circ \mu g \cdot l^{-1}$$

Total release for the regional model (without elimination in STPs):

$$RELEASE := TONNAGE \cdot f_{emission} \qquad RELEASE = 37.5 \circ tonne \cdot a^{-1}$$

Annual average local concentration in water:

$$Clocal_{water\_ann} := Clocal_{water} \cdot \frac{Temission}{365 \cdot d \cdot a^{-1}} \qquad Clocal_{water\_ann} = 97.1 \circ \mu g \cdot l^{-1}$$

Appendix 2-5

PEC local_water

Scenario IC/UC 2/48

1,000 t/a

Estimation of Clocal$_{water}$ of chemicals used as a solvent in chemical industry (IC = 2) status: TGD,A+B table, IC - 2

$\mu g := 10^{-9} \cdot kg$

$d := 86400 \cdot s$

$a := 365 \cdot d$

chemical : 2-EEA CAS-Nr.: 111-15-9

Total annual tonnage of chemical: $TONNAGE := 100 \cdot tonne \cdot a^{-1}$

Release factor (A 3.2): $f_{emission} := 0.8$

Fraction of main source (B 3.2): $Fmainsource := 0.5$

Waste water flow of wwtp: $EFFLUENT_{stp} := 2000 \cdot m^3 \cdot d^{-1}$

Duration of emission (B 3.2): $Temission := 20 \cdot d \cdot a^{-1}$

Fraction of emission directed to water:
(SimpleTreat; k:1 h^{-1}; logPow:0.24 ; logH:-0.81) $Fstp_{water} := 12.6 \cdot \%$

Dilution factor (TGD): $DILUTION := 10$

Factor (1+Kp * SUSPwater): $FACTOR := 1$

Emission per day:

$$Elocal_{water} := \frac{TONNAGE \cdot Fmainsource \cdot f_{emission}}{Temission} \qquad Elocal_{water} = 2 \cdot 10^{3} \cdot kg \cdot d^{-1}$$

Influent concentration:

$$Clocal_{inf} := \frac{Elocal_{water}}{EFFLUENT_{stp}} \qquad Clocal_{inf} = 1 \cdot 10^{3} \cdot mg \cdot l^{-1}$$

Effluent concentration:

$$Clocal_{eff} := Clocal_{inf} \cdot Fstp_{water} \qquad Clocal_{eff} = 126 \cdot mg \cdot l^{-1}$$

Concentration in surface water:

$$Clocal_{water} := \frac{Clocal_{eff}}{FACTOR \cdot DILUTION} \qquad Clocal_{water} = 1.3 \cdot 10^{4} \cdot \mu g \cdot l^{-1}$$

Total release for the regional model (without elimination in STPs):

$$RELEASE := TONNAGE \cdot f_{emission} \qquad RELEASE = 80 \cdot tonne \cdot a^{-1}$$

Annual average local concentration in water:

$$Clocal_{water\_ann} := Clocal_{water} \cdot \frac{Temission}{365 \cdot d \cdot a^{-1}} \qquad Clocal_{water\_ann} = 690.4 \cdot \mu g \cdot l^{-1}$$

Appendix 2-6

PEC local_water

Scenario IC/UC 2/48

5,000 t/a

Estimation of Clocal$_{water}$ of chemicals used as a solvent in chemical industry (IC = 2) status: TGD,A+B table, IC - 2

$\mu g := 10^{-9} \cdot kg$

$d := 86400 \cdot s$

$a := 365 \cdot d$

chemical : 2-EEA CAS-Nr.: 111-15-9

Total annual tonnage of chemical:	$TONNAGE := 500 \cdot tonne \cdot a^{-1}$
Release factor (A 3.2):	$f_{emission} := 0.8$
Fraction of main source (B 3.2):	$Fmainsource := 0.4$
Waste water flow of wwtp:	$EFFLUENT_{stp} := 2000 \cdot m^{3} \cdot d^{-1}$
Duration of emission (B 3.2):	$Temission := 50 \cdot d \cdot a^{-1}$
Fraction of emission directed to water: (SimpleTreat; k:1 h^{-1}; logPow:0.24 ; logH:-0.81)	$Fstp_{water} := 12.6 \cdot \%$
Dilution factor (TGD):	$DILUTION := 10$
Factor (1+Kp * SUSPwater):	$FACTOR := 1$

Emission per day:

$$Elocal_{water} := \frac{TONNAGE \cdot Fmainsource \cdot f_{emission}}{Temission} \qquad Elocal_{water} = 3.2 \cdot 10^{3} \; kg \cdot d^{-1}$$

Influent concentration:

$$Clocal_{inf} := \frac{Elocal_{water}}{EFFLUENT_{stp}} \qquad Clocal_{inf} = 1.6 \cdot 10^{3} \; mg \cdot l^{-1}$$

Effluent concentration:

$$Clocal_{eff} := Clocal_{inf} \cdot Fstp_{water} \qquad Clocal_{eff} = 201.6 \; mg \cdot l^{-1}$$

Concentration in surface water:

$$Clocal_{water} := \frac{Clocal_{eff}}{FACTOR \cdot DILUTION} \qquad Clocal_{water} = 2 \cdot 10^{4} \; \mu g \cdot l^{-1}$$

Total release for the regional model (without elimination in STPs):

$$RELEASE := TONNAGE \cdot f_{emission} \qquad RELEASE = 400 \; tonne \cdot a^{-1}$$

Annual average local concentration in water:

$$Clocal_{water\_ann} := Clocal_{water} \cdot \frac{Temission}{365 \cdot d \cdot a^{-1}} \qquad Clocal_{water\_ann} = 2.8 \cdot 10^{3} \; \mu g \cdot l^{-1}$$

Appendix 2-7

PEC local_water

Scenario IC/UC 3/33

Industrial Use – 1,000 t/a

Estimation of $Clocal_{water}$ of chemicals used as an intermediate (IC = 3)

status: TGD,A+B table, IC - 3

$\mu g := 10^{-9} \cdot kg$

$d := 86400 \cdot s$

$a := 365 \cdot d$

chemical : 2-EEA CAS-Nr.: 111-15-9

Total annual tonnage of chemical: $TONNAGE := 150 \cdot tonne \cdot a^{-1}$

Release factor (A 3.3): $f_{emission} := 0.02$

Fraction of main source (B 3.2): $Fmainsource := 0.5$

Waste water flow of wwtp: $EFFLUENT_{stp} := 10000 \cdot m^{3} \cdot d^{-1}$

Duration of emission (B 3.2): $Temission := 30 \cdot d \cdot a^{-1}$

Fraction of emission directed to water:
(SimpleTreat; k:1 h^{-1}; logPow:0.24 ; logH:-0.81) $Fstp_{water} := 12.6 \cdot \%$

Dilution factor (TGD): $DILUTION := 40$

Factor (1+Kp * SUSPwater): $FACTOR := 1$

Emission per day:

$$Elocal_{water} := \frac{TONNAGE \cdot Fmainsource \cdot f_{emission}}{Temission} \qquad Elocal_{water} = 50 \circ kg \cdot d^{-1}$$

Influent concentration:

$$Clocal_{inf} := \frac{Elocal_{water}}{EFFLUENT_{stp}} \qquad Clocal_{inf} = 5 \circ mg \cdot l^{-1}$$

Effluent concentration:

$$Clocal_{eff} := Clocal_{inf} \cdot Fstp_{water} \qquad Clocal_{eff} = 0.63 \circ mg \cdot l^{-1}$$

Concentration in surface water:

$$Clocal_{water} := \frac{Clocal_{eff}}{FACTOR \cdot DILUTION} \qquad Clocal_{water} = 15.7 \circ \mu g \cdot l^{-1}$$

Total release for the regional model (without elimination in STPs):

$$RELEASE := TONNAGE \cdot f_{emission} \qquad RELEASE = 3 \circ tonne \cdot a^{-1}$$

Annual average local concentration in water:

$$Clocal_{water\_ann} := Clocal_{water} \cdot \frac{Temission}{365 \cdot d \cdot a^{-1}} \qquad Clocal_{water\_ann} = 1.3 \circ \mu g \cdot l^{-1}$$

Appendix 2-8

PEC local_water

Scenario IC/UC 3/33

Industrial Use – 5,000 t/a

Estimation of Clocal$_{water}$ of chemicals used as an intermediate (IC = 3)

status: TGD,A+B table, IC - 3

$\mu g := 10^{-9} \cdot kg$

$d := 86400 \cdot s$

$a := 365 \cdot d$

chemical : 2-EEA CAS-Nr.: 111-15-9

Total annual tonnage of chemical:	$TONNAGE := 750 \cdot tonne \cdot a^{-1}$
Release factor (A 3.3):	$f_{emission} := 0.02$
Fraction of main source (B 3.2):	$Fmainsource := 0.4$
Waste water flow of wwtp:	$EFFLUENT_{stp} := 10000 \cdot m^3 \cdot d^{-1}$
Duration of emission (B 3.2):	$Temission := 75 \cdot d \cdot a^{-1}$
Fraction of emission directed to water: (SimpleTreat; k:1 h^{-1}; logPow:0.24 ; logH:-0.81)	$Fstp_{water} := 12.6 \cdot \%$
Dilution factor (TGD):	$DILUTION := 40$
Factor (1+Kp * SUSPwater):	$FACTOR := 1$

Emission per day:

$$Elocal_{water} := \frac{TONNAGE \cdot Fmainsource \cdot f_{emission}}{Temission} \qquad Elocal_{water} = 80 \circ kg \cdot d^{-1}$$

Influent concentration:

$$Clocal_{inf} := \frac{Elocal_{water}}{EFFLUENT_{stp}} \qquad Clocal_{inf} = 8 \circ mg \cdot l^{-1}$$

Effluent concentration:

$$Clocal_{eff} := Clocal_{inf} \cdot Fstp_{water} \qquad Clocal_{eff} = 1.01 \circ mg \cdot l^{-1}$$

Concentration in surface water:

$$Clocal_{water} := \frac{Clocal_{eff}}{FACTOR \cdot DILUTION} \qquad Clocal_{water} = 25.2 \circ \mu g \cdot l^{-1}$$

Total release for the regional model (without elimination in STPs):

$$RELEASE := TONNAGE \cdot f_{emission} \qquad RELEASE = 15 \circ tonne \cdot a^{-1}$$

Annual average local concentration in water:

$$Clocal_{water\_ann} := Clocal_{water} \cdot \frac{Temission}{365 \cdot d \cdot a^{-1}} \qquad Clocal_{water\_ann} = 5.2 \circ \mu g \cdot l^{-1}$$

Appendix 3-1

PEC local_air

Scenario IC/UC 14/48

Formulation – 1,000 t/a

Atmosphere (OPS-model)

Calculation of Clocal $_{air}$ and PEC local $_{air}$

substance: 2-EEA CAS-Nr.: 111-15-9

stage of life cycle: IC 14, UC 48, Formulation

$d := 86400 \cdot s$

$a := 365 \cdot d$

$mg := 1 \cdot 10^{-6} \cdot kg$

tonnage for specific scenario: $\mathrm{TONNAGE} := 750 \cdot tonne \cdot a^{-1}$

release factor (A 3.2): $f_{emission} := 0.01$

fraction of main source (B 3.2): $\mathrm{Fmainsource} := 0.8$

days of use per year (B 3.2): $\mathrm{Temission} := 300 \cdot d \cdot a^{-1}$

release during life cycle to air: $\mathrm{RELEASE} := \mathrm{TONNAGE} \cdot f_{emission}$

$\mathrm{RELEASE} = 7.5 \circ tonne \cdot a^{-1}$

local emission during episode to air: $\mathrm{Elocal}_{air} := \frac{\mathrm{Fmainsource} \cdot \mathrm{RELEASE}}{\mathrm{Temission}}$

$\mathrm{Elocal}_{air} = 20 \circ kg \cdot d^{-1}$

concentration in air at source strength of 1kg/d: $\mathrm{Cstd}_{air} := 2.78 \cdot 10^{-4} \cdot mg \cdot m^{-3} \cdot kg^{-1} \cdot d$

fraction of the emission to air from STP (App.II): $\mathrm{Fstp}_{air} := 0.1 \cdot \%$

local emission rate to water during emission episode: $\mathrm{Elocal}_{water} := 40.0 \cdot kg \cdot d^{-1}$

local emission to air from STP during emission episode: $\mathrm{Estp}_{air} := \mathrm{Fstp}_{air} \cdot \mathrm{Elocal}_{water}$

$\mathrm{Estp}_{air} = 0.04 \circ kg \cdot d^{-1}$

local concentation in air during emission episode: $\mathrm{Clocal}_{air} := \mathrm{wenn}\left(\mathrm{Elocal}_{air} > \mathrm{Estp}_{air}, \mathrm{Elocal}_{air} \cdot \mathrm{Cstd}_{air}, \mathrm{Estp}_{air} \cdot \mathrm{Cstd}_{air}\right)$

$\mathrm{Clocal}_{air} = 5.56 \bullet 10^{-3} \circ mg \cdot m^{-3}$

annual average concentration in air, 100m from point source: $\mathrm{Clocal}_{air\_ann} := \mathrm{Clocal}_{air} \cdot \frac{\mathrm{Temission}}{365 \cdot d \cdot a^{-1}}$

$\mathrm{Clocal}_{air\_ann} = 4.57 \bullet 10^{-3} \circ mg \cdot m^{-3}$

regional concentration in air: $\mathrm{PECregional}_{air} := 3.34 \cdot 10^{-7} \cdot mg \cdot m^{-3}$

annual average predicted environmental concentration in air: $\mathrm{PEClocal}_{air\_ann} := \mathrm{Clocal}_{air\_ann} + \mathrm{PECregional}_{air}$

$\mathrm{PEClocal}_{air\_ann} = 4.57 \bullet 10^{-3} \circ mg \cdot m^{-3}$

Calculation of the deposition rate

standard deposition flux of aerosol-bound compounds at a source strength of 1kg/d

$$\mathrm{DEPstd}_{\mathrm{aer}} := 1\cdot 10^{-2}\cdot \mathrm{mg}\cdot \mathrm{m}^{-2}\cdot \mathrm{d}^{-1}\cdot \mathrm{kg}^{-1}\cdot \mathrm{d}$$

fraction of the chemical bound to aerosol (see: Distribution and Fate)

$$\mathrm{Fass}_{\mathrm{aer}} := 3.7\cdot 10^{-7}$$

deposition flux of gaseous compounds as a function of Henry`s Law coefficient,at a source strength of 1kg/d

logH<-2	$5*10^{-4}$ mg*m^{-2}*d^{-1}
-2<logH<2	$4*10^{-4}$ mg*m^{-2}*d^{-1}
logH>2	$3*10^{-4}$ mg*m^{-2}*d^{-1}

$$\mathrm{DEPstd}_{\mathrm{gas}} := 4\cdot 10^{-4}\cdot \mathrm{mg}\cdot \mathrm{m}^{-2}\cdot \mathrm{d}^{-1}\cdot \mathrm{kg}^{-1}\cdot \mathrm{d}$$

total deposition flux during emission episode

$$\mathrm{DEPtotal} := \left(\mathrm{Elocal}_{\mathrm{air}} + \mathrm{Estp}_{\mathrm{air}}\right)\cdot\left[\mathrm{Fass}_{\mathrm{aer}}\cdot \mathrm{DEPstd}_{\mathrm{aer}} + \left(1 - \mathrm{Fass}_{\mathrm{aer}}\right)\cdot \mathrm{DEPstd}_{\mathrm{gas}}\right]$$

$$\mathrm{DEPtotal} = 8.016\cdot 10^{-3}\ \circ \mathrm{mg}\cdot \mathrm{m}^{-2}\cdot \mathrm{d}^{-1}$$

annual average total depostion flux

$$\mathrm{DEPtotal}_{\mathrm{ann}} := \mathrm{DEPtotal}\cdot \frac{\mathrm{Temission}}{365\cdot \mathrm{d}\cdot \mathrm{a}^{-1}}$$

$$\mathrm{DEPtotal}_{\mathrm{ann}} = 6.589\cdot 10^{-3}\ \circ \mathrm{mg}\cdot \mathrm{m}^{-2}\cdot \mathrm{d}^{-1}$$

Appendix 3-2

PEC local_air

Scenario IC/UC 14/48

Industrial Use – 1,000 t/a

Atmosphere (OPS-model)

Calculation of Clocal $_{air}$ and PEC local $_{air}$

substance: 2-EEA CAS-Nr.: 111-15-9

stage of life cycle: IC 14, UC 48, Industrial Use

$d := 86400 \cdot s$

$a := 365 \cdot d$

$mg := 1 \cdot 10^{-6} \cdot kg$

tonnage for specific scenario: $TONNAGE := 75 \cdot tonne \cdot a^{-1}$

release factor (A 3.2): $f_{emission} := 0.9$

fraction of main source (B 3.2): $Fmainsource := 0.15$

days of use per year (B 3.2): $Temission := 300 \cdot d \cdot a^{-1}$

release during life cycle to air: $RELEASE := TONNAGE \cdot f_{emission}$

$RELEASE = 67.5 \circ tonne \cdot a^{-1}$

local emission during episode to air: $Elocal_{air} := \dfrac{Fmainsource \cdot RELEASE}{Temission}$

$Elocal_{air} = 33.75 \circ kg \cdot d^{-1}$

concentration in air at source strength of 1kg/d: $Cstd_{air} := 2.78 \cdot 10^{-4} \cdot mg \cdot m^{-3} \cdot kg^{-1} \cdot d$

fraction of the emission to air from STP (App.II): $Fstp_{air} := 0.1 \cdot \%$

local emission rate to water during emission episode: $Elocal_{water} := 3.75 \cdot kg \cdot d^{-1}$

local emission to air from STP during emission episode: $Estp_{air} := Fstp_{air} \cdot Elocal_{water}$

$Estp_{air} = 3.75 \bullet 10^{-3} \circ kg \cdot d^{-1}$

local concentation in air during emission episode: $Clocal_{air} := wenn\left(Elocal_{air} > Estp_{air}, Elocal_{air} \cdot Cstd_{air}, Estp_{air} \cdot Cstd_{air}\right)$

$Clocal_{air} = 9.383 \bullet 10^{-3} \circ mg \cdot m^{-3}$

annual average concentration in air, 100m from point source: $Clocal_{air\_ann} := Clocal_{air} \cdot \dfrac{Temission}{365 \cdot d \cdot a^{-1}}$

$Clocal_{air\_ann} = 7.712 \bullet 10^{-3} \circ mg \cdot m^{-3}$

regional concentration in air: $PECregional_{air} := 3.34 \cdot 10^{-7} \cdot mg \cdot m^{-3}$

annual average predicted environmental concentration in air: $PEClocal_{air\_ann} := Clocal_{air\_ann} + PECregional_{air}$

$PEClocal_{air\_ann} = 7.712 \bullet 10^{-3} \circ mg \cdot m^{-3}$

Calculation of the deposition rate

standard deposition flux of aerosol-bound compounds at a source strength of 1kg/d

$DEPstd_{aer} := 1\cdot 10^{-2}\cdot mg\cdot m^{-2}\cdot d^{-1}\cdot kg^{-1}\cdot d$

fraction of the chemical bound to aerosol (see: Distribution and Fate)

$Fass_{aer} := 3.7\cdot 10^{-7}$

deposition flux of gaseous compounds as a function of Henry`s Law coefficient,at a source strength of 1kg/d

logH<-2	$5*10^{-4}$ $mg*m^{-2}*d^{-1}$
-2<logH<2	$4*10^{-4}$ $mg*m^{-2}*d^{-1}$
logH>2	$3*10^{-4}$ $mg*m^{-2}*d^{-1}$

$DEPstd_{gas} := 4\cdot 10^{-4}\cdot mg\cdot m^{-2}\cdot d^{-1}\cdot kg^{-1}\cdot d$

total deposition flux during emission episode

$$DEPtotal := \left(Elocal_{air} + Estp_{air}\right)\cdot\left[Fass_{aer}\cdot DEPstd_{aer} + \left(1 - Fass_{aer}\right)\cdot DEPstd_{gas}\right]$$

$$DEPtotal = 0.014\,mg\cdot m^{-2}\cdot d^{-1}$$

annual average total depostion flux

$$DEPtotal_{ann} := DEPtotal\cdot\frac{Temission}{365\cdot d\cdot a^{-1}}$$

$$DEPtotal_{ann} = 0.011\,mg\cdot m^{-2}\cdot d^{-1}$$

Appendix 3-3

PEC local_air

Scenario IC/UC 2/48

1,000 t/a

Atmosphere (OPS-model)

Calculation of Clocal $_{air}$ and PEC local $_{air}$

substance: 2-EEA CAS-Nr.: 111-15-9

stage of life cycle: IC 2, UC 48

$$d := 86400 \cdot s$$

$$a := 365 \cdot d$$

$$mg := 1 \cdot 10^{-6} \cdot kg$$

tonnage for specific scenario:

$$TONNAGE := 100 \cdot tonne \cdot a^{-1}$$

release factor (A 3.2):

$$f_{emission} := 0.1$$

fraction of main source (B 3.2):

$$Fmainsource := 0.5$$

days of use per year (B 3.2):

$$Temission := 20 \cdot d \cdot a^{-1}$$

release during life cycle to air:

$$RELEASE := TONNAGE \cdot f_{emission}$$

$$RELEASE = 10 \circ tonne \cdot a^{-1}$$

local emission during episode to air:

$$Elocal_{air} := \frac{Fmainsource \cdot RELEASE}{Temission}$$

$$Elocal_{air} = 250 \circ kg \cdot d^{-1}$$

concentration in air at source
strength of 1kg/d

$$Cstd_{air} := 2.78 \cdot 10^{-4} \cdot mg \cdot m^{-3} \cdot kg^{-1} \cdot d$$

fraction of the emission to air from STP
(App.II)

$$Fstp_{air} := 0.1 \cdot \%$$

local emission rate to water during
emission episode

$$Elocal_{water} := 2000 \cdot kg \cdot d^{-1}$$

local emission to air from STP during
emission episode

$$Estp_{air} := Fstp_{air} \cdot Elocal_{water}$$

$$Estp_{air} = 2 \circ kg \cdot d^{-1}$$

local concentation in air
during emission episode:

$$Clocal_{air} := wenn\left(Elocal_{air} > Estp_{air}, Elocal_{air} \cdot Cstd_{air}, Estp_{air} \cdot Cstd_{air}\right)$$

$$Clocal_{air} = 0.069 \circ mg \cdot m^{-3}$$

annual average concentration in air,
100m from point source

$$Clocal_{air\_ann} := Clocal_{air} \cdot \frac{Temission}{365 \cdot d \cdot a^{-1}}$$

$$Clocal_{air\_ann} = 3.808 \bullet 10^{-3} \circ mg \cdot m^{-3}$$

regional concentration in air

$$PECregional_{air} := 3.34 \cdot 10^{-7} \cdot mg \cdot m^{-3}$$

annual average predicted environmental
concentration in air

$$PEClocal_{air\_ann} := Clocal_{air\_ann} + PECregional_{air}$$

$$PEClocal_{air\_ann} = 3.809 \bullet 10^{-3} \circ mg \cdot m^{-3}$$

Calculation of the deposition rate

standard deposition flux of aerosol-bound compounds at a source strength of 1kg/d

$$DEPstd_{aer} := 1\cdot10^{-2}\cdot mg\cdot m^{-2}\cdot d^{-1}\cdot kg^{-1}\cdot d$$

fraction of the chemical bound to aerosol
(see: Distribution and Fate)

$$Fass_{aer} := 3.7\cdot10^{-7}$$

deposition flux of gaseous compounds as a function of Henry`s Law coefficient,at a source strength of 1kg/d

logH<-2	5*10 $^{-4}$ mg*m^{-2}*d^{-1}
-2<logH<2	4*10^{-4} mg*m^{-2}*d^{-1}
logH>2	3*10^{-4} mg*m^{-2}*d^{-1}

$$DEPstd_{gas} := 4\cdot10^{-4}\cdot mg\cdot m^{-2}\cdot d^{-1}\cdot kg^{-1}\cdot d$$

total deposition flux during emission episode

$$DEPtotal := \left(Elocal_{air} + Estp_{air}\right)\cdot\left[Fass_{aer}\cdot DEPstd_{aer} + \left(1 - Fass_{aer}\right)\cdot DEPstd_{gas}\right]$$

$$DEPtotal = 0.101\circ mg\cdot m^{-2}\cdot d^{-1}$$

annual average total depostion flux

$$DEPtotal_{ann} := DEPtotal\cdot\frac{Temission}{365\cdot d\cdot a^{-1}}$$

$$DEPtotal_{ann} = 5.523\bullet10^{-3}\ \circ mg\cdot m^{-2}\cdot d^{-1}$$

Appendix 3-4

PEC local_air

Scenario IC/UC 3/33

1,000 t/a

Atmosphere (OPS-model)

Calculation of Clocal $_{air}$ and PEC local $_{air}$

substance: 2-EEA CAS-Nr.: 111-15-9

stage of life cycle: IC 3, UC 33

$d := 86400 \cdot s$

$a := 365 \cdot d$

$mg := 1 \cdot 10^{-6} \cdot kg$

tonnage for specific scenario:

$TONNAGE := 150 \cdot tonne \cdot a^{-1}$

release factor (A 3.3):

$f_{emission} := 0.01$

fraction of main source (B 3.2):

$Fmainsource := 0.5$

days of use per year (B 3.2):

$Temission := 30 \cdot d \cdot a^{-1}$

release during life cycle to air:

$RELEASE := TONNAGE \cdot f_{emission}$

$RELEASE = 1.5 \cdot tonne \cdot a^{-1}$

local emission during episode to air:

$$Elocal_{air} := \frac{Fmainsource \cdot RELEASE}{Temission}$$

$Elocal_{air} = 25 \cdot kg \cdot d^{-1}$

concentration in air at source strength of 1kg/d

$Cstd_{air} := 2.78 \cdot 10^{-4} \cdot mg \cdot m^{-3} \cdot kg^{-1} \cdot d$

fraction of the emission to air from STP (App.II)

$Fstp_{air} := 0.1 \cdot \%$

local emission rate to water during emission episode

$Elocal_{water} := 50.0 \cdot kg \cdot d^{-1}$

local emission to air from STP during emission episode

$Estp_{air} := Fstp_{air} \cdot Elocal_{water}$

$Estp_{air} = 0.05 \cdot kg \cdot d^{-1}$

local concentation in air during emission episode:

$Clocal_{air} := wenn\left(Elocal_{air} > Estp_{air}, Elocal_{air} \cdot Cstd_{air}, Estp_{air} \cdot Cstd_{air}\right)$

$Clocal_{air} = 6.95 \cdot 10^{-3} \cdot mg \cdot m^{-3}$

annual average concentration in air, 100m from point source

$$Clocal_{air\_ann} := Clocal_{air} \cdot \frac{Temission}{365 \cdot d \cdot a^{-1}}$$

$Clocal_{air\_ann} = 5.712 \cdot 10^{-4} \cdot mg \cdot m^{-3}$

regional concentration in air

$PECregional_{air} := 3.34 \cdot 10^{-7} \cdot mg \cdot m^{-3}$

annual average predicted environmental concentration in air

$PEClocal_{air\_ann} := Clocal_{air\_ann} + PECregional_{air}$

$PEClocal_{air\_ann} = 5.716 \cdot 10^{-4} \cdot mg \cdot m^{-3}$

Calculation of the deposition rate

standard deposition flux of aerosol-bound compounds at a source strength of 1kg/d

$$DEPstd_{aer} := 1 \cdot 10^{-2} \cdot mg \cdot m^{-2} \cdot d^{-1} \cdot kg^{-1} \cdot d$$

fraction of the chemical bound to aerosol (see: Distribution and Fate)

$$Fass_{aer} := 3.7 \cdot 10^{-7}$$

deposition flux of gaseous compounds as a function of Henry`s Law coefficient,at a source strength of 1kg/d

logH<-2	$5*10^{-4}$ $mg*m^{-2}*d^{-1}$
-2<logH<2	$4*10^{-4}$ $mg*m^{-2}*d^{-1}$
logH>2	$3*10^{-4}$ $mg*m^{-2}*d^{-1}$

$$DEPstd_{gas} := 4 \cdot 10^{-4} \cdot mg \cdot m^{-2} \cdot d^{-1} \cdot kg^{-1} \cdot d$$

total deposition flux during emission episode

$$DEPtotal := \left(Elocal_{air} + Estp_{air}\right) \cdot \left[Fass_{aer} \cdot DEPstd_{aer} + \left(1 - Fass_{aer}\right) \cdot DEPstd_{gas}\right]$$

$$DEPtotal = 0.01 \circ mg \cdot m^{-2} \cdot d^{-1}$$

annual average total depostion flux

$$DEPtotal_{ann} := DEPtotal \cdot \frac{Temission}{365 \cdot d \cdot a^{-1}}$$

$$DEPtotal_{ann} = 8.236 \bullet 10^{-4} \circ mg \cdot m^{-2} \cdot d^{-1}$$

Appendix 3-5

PEC local_air

Scenario IC/UC 14/48

Formulation – 5,000 t/a

Atmosphere (OPS-model)

Calculation of Clocal $_{air}$ and PEC local $_{air}$

substance: 2-EEA CAS-Nr.: 111-15-9

stage of life cycle: IC 14, UC 48, Formulation

$d := 86400 \cdot s$

$a := 365 \cdot d$

$mg := 1 \cdot 10^{-6} \cdot kg$

tonnage for specific scenario:

$TONNAGE := 3750 \cdot tonne \cdot a^{-1}$

release factor (A 3.2):

$f_{emission} := 0.01$

fraction of main source (B 3.2):

$Fmainsource := 0.6$

days of use per year (B 3.2):

$Temission := 300 \cdot d \cdot a^{-1}$

release during life cycle to air:

$RELEASE := TONNAGE \cdot f_{emission}$

$RELEASE = 37.5 \circ tonne \cdot a^{-1}$

local emission during episode to air:

$$Elocal_{air} := \frac{Fmainsource \cdot RELEASE}{Temission}$$

$Elocal_{air} = 75 \circ kg \cdot d^{-1}$

concentration in air at source strength of 1kg/d

$Cstd_{air} := 2.78 \cdot 10^{-4} \cdot mg \cdot m^{-3} \cdot kg^{-1} \cdot d$

fraction of the emission to air from STP (App.II)

$Fstp_{air} := 0.1 \cdot \%$

local emission rate to water during emission episode

$Elocal_{water} := 22.5\, kg \cdot d^{-1}$

local emission to air from STP during emission episode

$Estp_{air} := Fstp_{air} \cdot Elocal_{water}$

$Estp_{air} = 0.023 \circ kg \cdot d^{-1}$

local concentation in air during emission episode:

$$Clocal_{air} := wenn\left(Elocal_{air} > Estp_{air}, Elocal_{air} \cdot Cstd_{air}, Estp_{air} \cdot Cstd_{air}\right)$$

$Clocal_{air} = 0.021 \circ mg \cdot m^{-3}$

annual average concentration in air, 100m from point source

$$Clocal_{air\_ann} := Clocal_{air} \cdot \frac{Temission}{365 \cdot d \cdot a^{-1}}$$

$Clocal_{air\_ann} = 0.017 \circ mg \cdot m^{-3}$

regional concentration in air

$PECregional_{air} := 1.67 \cdot 10^{-6} \cdot mg \cdot m^{-3}$

annual average predicted environmental concentration in air

$PEClocal_{air\_ann} := Clocal_{air\_ann} + PECregional_{air}$

$PEClocal_{air\_ann} = 0.017 \circ mg \cdot m^{-3}$

Calculation of the deposition rate

standard deposition flux of aerosol-bound compounds at a source strength of 1kg/d

$$DEPstd_{aer} := 1\cdot10^{-2}\cdot mg\cdot m^{-2}\cdot d^{-1}\cdot kg^{-1}\cdot d$$

fraction of the chemical bound to aerosol
(see: Distribution and Fate)

$$Fass_{aer} := 3.7\cdot10^{-7}$$

deposition flux of gaseous compounds as a function of Henry`s Law coefficient,at a source strength of 1kg/d

logH<-2	$5*10^{-4}$ $mg*m^{-2}*d^{-1}$
-2<logH<2	$4*10^{-4}$ $mg*m^{-2}*d^{-1}$
logH>2	$3*10^{-4}$ $mg*m^{-2}*d^{-1}$

$$DEPstd_{gas} := 4\cdot10^{-4}\cdot mg\cdot m^{-2}\cdot d^{-1}\cdot kg^{-1}\cdot d$$

total deposition flux during emission episode

$$DEPtotal := \left(Elocal_{air} + Estp_{air}\right)\cdot\left[Fass_{aer}\cdot DEPstd_{aer} + \left(1 - Fass_{aer}\right)\cdot DEPstd_{gas}\right]$$

$$DEPtotal = 0.03\,mg\cdot m^{-2}\cdot d^{-1}$$

annual average total depostion flux

$$DEPtotal_{ann} := DEPtotal\cdot\frac{Temission}{365\cdot d\cdot a^{-1}}$$

$$DEPtotal_{ann} = 0.025\,mg\cdot m^{-2}\cdot d^{-1}$$

Appendix 3-6

PEC local_air

Scenario IC/UC 14/48

Industrial Use – 5,000 t/a

Atmosphere (OPS-model)

Calculation of Clocal $_{air}$ and PEC local $_{air}$

substance: 2-EEA CAS-Nr.: 111-15-9

$d := 86400 \cdot s$

$a := 365 \cdot d$

$mg := 1 \cdot 10^{-6} \cdot kg$

stage of life cycle: IC 14, UC 48, Industrial Use

tonnage for specific scenario: $TONNAGE := 375 \cdot tonne \cdot a^{-1}$

release factor (A 3.2): $f_{emission} := 0.9$

fraction of main source (B 3.2): $Fmainsource := 0.15$

days of use per year (B 3.2): $Temission := 300 \cdot d \cdot a^{-1}$

release during life cycle to air: $RELEASE := TONNAGE \cdot f_{emission}$

$RELEASE = 337.5 \circ tonne \cdot a^{-1}$

local emission during episode to air:

$$Elocal_{air} := \frac{Fmainsource \cdot RELEASE}{Temission}$$

$Elocal_{air} = 168.75 \circ kg \cdot d^{-1}$

concentration in air at source strength of 1kg/d: $Cstd_{air} := 2.78 \cdot 10^{-4} \cdot mg \cdot m^{-3} \cdot kg^{-1} \cdot d$

fraction of the emission to air from STP (App.II): $Fstp_{air} := 0.1 \cdot \%$

local emission rate to water during emission episode: $Elocal_{water} := 18.75 \cdot kg \cdot d^{-1}$

local emission to air from STP during emission episode: $Estp_{air} := Fstp_{air} \cdot Elocal_{water}$

$Estp_{air} = 0.019 \circ kg \cdot d^{-1}$

local concentation in air during emission episode:

$$Clocal_{air} := wenn\left(Elocal_{air} > Estp_{air}, Elocal_{air} \cdot Cstd_{air}, Estp_{air} \cdot Cstd_{air}\right)$$

$Clocal_{air} = 0.047 \circ mg \cdot m^{-3}$

annual average concentration in air, 100m from point source:

$$Clocal_{air\_ann} := Clocal_{air} \cdot \frac{Temission}{365 \cdot d \cdot a^{-1}}$$

$Clocal_{air\_ann} = 0.039 \circ mg \cdot m^{-3}$

regional concentration in air: $PECregional_{air} := 1.67 \cdot 10^{-6} \cdot mg \cdot m^{-3}$

annual average predicted environmental concentration in air:

$$PEClocal_{air\_ann} := Clocal_{air\_ann} + PECregional_{air}$$

$PEClocal_{air\_ann} = 0.039 \circ mg \cdot m^{-3}$

Calculation of the deposition rate

standard deposition flux of aerosol-bound compounds at a source strength of 1kg/d

$$DEPstd_{aer} := 1\cdot 10^{-2}\cdot mg\cdot m^{-2}\cdot d^{-1}\cdot kg^{-1}\cdot d$$

fraction of the chemical bound to aerosol (see: Distribution and Fate)

$$Fass_{aer} := 3.7\cdot 10^{-7}$$

deposition flux of gaseous compounds as a function of Henry`s Law coefficient,at a source strength of 1kg/d

logH<-2	$5*10^{-4}$ $mg*m^{-2}*d^{-1}$
-2<logH<2	$4*10^{-4}$ $mg*m^{-2}*d^{-1}$
logH>2	$3*10^{-4}$ $mg*m^{-2}*d^{-1}$

$$DEPstd_{gas} := 4\cdot 10^{-4}\cdot mg\cdot m^{-2}\cdot d^{-1}\cdot kg^{-1}\cdot d$$

total deposition flux during emission episode

$$DEPtotal := \left(Elocal_{air} + Estp_{air}\right)\cdot\left[Fass_{aer}\cdot DEPstd_{aer} + \left(1 - Fass_{aer}\right)\cdot DEPstd_{gas}\right]$$

$$DEPtotal = 0.068\,mg\cdot m^{-2}\cdot d^{-1}$$

annual average total depostion flux

$$DEPtotal_{ann} := DEPtotal\cdot\frac{Temission}{365\cdot d\cdot a^{-1}}$$

$$DEPtotal_{ann} = 0.055\,mg\cdot m^{-2}\cdot d^{-1}$$

Appendix 3-7

PEC local_air

Scenario IC/UC 2/48

5,000 t/a

Atmosphere (OPS-model)

Calculation of Clocal $_{air}$ and PEC local $_{air}$

substance: 2-EEA CAS-Nr.: 111-15-9

$d := 86400 \cdot s$

$a := 365 \cdot d$

$mg := 1 \cdot 10^{-6} \cdot kg$

stage of life cycle: IC 2, UC 48

tonnage for specific scenario: $TONNAGE := 500 \cdot tonne \cdot a^{-1}$

release factor (A 3.2): $f_{emission} := 0.1$

fraction of main source (B 3.2): $Fmainsource := 0.4$

days of use per year (B 3.2): $Temission := 50 \cdot d \cdot a^{-1}$

release during life cycle to air: $RELEASE := TONNAGE \cdot f_{emission}$

$RELEASE = 50 \circ tonne \cdot a^{-1}$

local emission during episode to air: $Elocal_{air} := \frac{Fmainsource \cdot RELEASE}{Temission}$

$Elocal_{air} = 400 \circ kg \cdot d^{-1}$

concentration in air at source strength of 1kg/d: $Cstd_{air} := 2.78 \cdot 10^{-4} \cdot mg \cdot m^{-3} \cdot kg^{-1} \cdot d$

fraction of the emission to air from STP (App.II): $Fstp_{air} := 0.1 \cdot \%$

local emission rate to water during emission episode: $Elocal_{water} := 3200 \cdot kg \cdot d^{-1}$

local emission to air from STP during emission episode: $Estp_{air} := Fstp_{air} \cdot Elocal_{water}$

$Estp_{air} = 3.2 \circ kg \cdot d^{-1}$

local concentation in air during emission episode: $Clocal_{air} := wenn\left(Elocal_{air} > Estp_{air}, Elocal_{air} \cdot Cstd_{air}, Estp_{air} \cdot Cstd_{air}\right)$

$Clocal_{air} = 0.111 \circ mg \cdot m^{-3}$

annual average concentration in air, 100m from point source: $Clocal_{air\_ann} := Clocal_{air} \cdot \frac{Temission}{365 \cdot d \cdot a^{-1}}$

$Clocal_{air\_ann} = 0.015 \circ mg \cdot m^{-3}$

regional concentration in air: $PECregional_{air} := 1.67 \cdot 10^{-6} \cdot mg \cdot m^{-3}$

annual average predicted environmental concentration in air: $PEClocal_{air\_ann} := Clocal_{air\_ann} + PECregional_{air}$

$PEClocal_{air\_ann} = 0.015 \circ mg \cdot m^{-3}$

Calculation of the deposition rate

standard deposition flux of aerosol-bound compounds at a source strength of 1kg/d

$$DEPstd_{aer} := 1 \cdot 10^{-2} \cdot mg \cdot m^{-2} \cdot d^{-1} \cdot kg^{-1} \cdot d$$

fraction of the chemical bound to aerosol (see: Distribution and Fate)

$$Fass_{aer} := 3.7 \cdot 10^{-7}$$

deposition flux of gaseous compounds as a function of Henry`s Law coefficient,at a source strength of 1kg/d

logH<-2	$5*10^{-4}$ $mg*m^{-2}*d^{-1}$
-2<logH<2	$4*10^{-4}$ $mg*m^{-2}*d^{-1}$
logH>2	$3*10^{-4}$ $mg*m^{-2}*d^{-1}$

$$DEPstd_{gas} := 4 \cdot 10^{-4} \cdot mg \cdot m^{-2} \cdot d^{-1} \cdot kg^{-1} \cdot d$$

total deposition flux during emission episode

$$DEPtotal := \left(Elocal_{air} + Estp_{air}\right) \cdot \left[Fass_{aer} \cdot DEPstd_{aer} + \left(1 - Fass_{aer}\right) \cdot DEPstd_{gas}\right]$$

$$DEPtotal = 0.161 \circ mg \cdot m^{-2} \cdot d^{-1}$$

annual average total depostion flux

$$DEPtotal_{ann} := DEPtotal \cdot \frac{Temission}{365 \cdot d \cdot a^{-1}}$$

$$DEPtotal_{ann} = 0.022 \circ mg \cdot m^{-2} \cdot d^{-1}$$

Appendix 3-8

PEC local_air

Scenario IC/UC 3/33

5,000 t/a

Atmosphere (OPS-model)

Calculation of Clocal $_{air}$ and PEC local $_{air}$

substance: 2-EEA CAS-Nr.: 111-15-9

$d := 86400 \cdot s$

$a := 365 \cdot d$

$mg := 1 \cdot 10^{-6} \cdot kg$

stage of life cycle: IC 3, UC 33

tonnage for specific scenario:

$TONNAGE := 750 \cdot tonne \cdot a^{-1}$

release factor (A 3.3):

$f_{emission} := 0.01$

fraction of main source (B 3.2):

$Fmainsource := 0.4$

days of use per year (B 3.2):

$Temission := 75 \cdot d \cdot a^{-1}$

release during life cycle to air:

$RELEASE := TONNAGE \cdot f_{emission}$

$RELEASE = 7.5 \circ tonne \cdot a^{-1}$

local emission during episode to air:

$$Elocal_{air} := \frac{Fmainsource \cdot RELEASE}{Temission}$$

$Elocal_{air} = 40 \circ kg \cdot d^{-1}$

concentration in air at source strength of 1kg/d

$Cstd_{air} := 2.78 \cdot 10^{-4} \cdot mg \cdot m^{-3} \cdot kg^{-1} \cdot d$

fraction of the emission to air from STP (App.II)

$Fstp_{air} := 0.1 \cdot \%$

local emission rate to water during emission episode

$Elocal_{water} := 80.0 \cdot kg \cdot d^{-1}$

local emission to air from STP during emission episode

$Estp_{air} := Fstp_{air} \cdot Elocal_{water}$

$Estp_{air} = 0.08 \circ kg \cdot d^{-1}$

local concentation in air during emission episode:

$$Clocal_{air} := wenn\left(Elocal_{air} > Estp_{air}, Elocal_{air} \cdot Cstd_{air}, Estp_{air} \cdot Cstd_{air}\right)$$

$Clocal_{air} = 0.011 \circ mg \cdot m^{-3}$

annual average concentration in air, 100m from point source

$$Clocal_{air\_ann} := Clocal_{air} \cdot \frac{Temission}{365 \cdot d \cdot a^{-1}}$$

$Clocal_{air\_ann} = 2.285 \bullet 10^{-3} \circ mg \cdot m^{-3}$

regional concentration in air

$PECregional_{air} := 1.67 \cdot 10^{-6} \cdot mg \cdot m^{-3}$

annual average predicted environmental concentration in air

$PEClocal_{air\_ann} := Clocal_{air\_ann} + PECregional_{air}$

$PEClocal_{air\_ann} = 2.287 \bullet 10^{-3} \circ mg \cdot m^{-3}$

Calculation of the deposition rate

standard deposition flux of aerosol-bound compounds at a source strength of 1kg/d

$$DEPstd_{aer} := 1 \cdot 10^{-2} \cdot mg \cdot m^{-2} \cdot d^{-1} \cdot kg^{-1} \cdot d$$

fraction of the chemical bound to aerosol (see: Distribution and Fate)

$$Fass_{aer} := 3.7 \cdot 10^{-7}$$

deposition flux of gaseous compounds as a function of Henry`s Law coefficient,at a source strength of 1kg/d

logH<-2	$5*10^{-4}$ $mg*m^{-2}*d^{-1}$
-2<logH<2	$4*10^{-4}$ $mg*m^{-2}*d^{-1}$
logH>2	$3*10^{-4}$ $mg*m^{-2}*d^{-1}$

$$DEPstd_{gas} := 4 \cdot 10^{-4} \cdot mg \cdot m^{-2} \cdot d^{-1} \cdot kg^{-1} \cdot d$$

total deposition flux during emission episode

$$DEPtotal := \left(Elocal_{air} + Estp_{air}\right) \cdot \left[Fass_{aer} \cdot DEPstd_{aer} + \left(1 - Fass_{aer}\right) \cdot DEPstd_{gas}\right]$$

$$DEPtotal = 0.016 \, mg \cdot m^{-2} \cdot d^{-1}$$

annual average total depostion flux

$$DEPtotal_{ann} := DEPtotal \cdot \frac{Temission}{365 \cdot d \cdot a^{-1}}$$

$$DEPtotal_{ann} = 3.294 \cdot 10^{-3} \, mg \cdot m^{-2} \cdot d^{-1}$$

Appendix 3-9

PEC local_soil

Scenario IC/UC 14/48

Industrial Use – 1,000 t/a

Exposure of Soil

chemical: 2 – EEA

Defaults:

mixing depth of soil:

$$DEPTHsoil_i := \begin{array}{|c|}\hline 0.2\cdot m \\ \hline 0.2\cdot m \\ \hline 0.1\cdot m \\ \hline \end{array}$$

bulk density of soil: $RHO_{soil} := 1700\cdot kg\cdot m^{-3}$

average time for exposure:

$$T_i := \begin{array}{|c|}\hline 30\cdot d \\ \hline 180\cdot d \\ \hline 180\cdot d \\ \hline \end{array}$$

partial mass transfer coefficient at air-side of the air-soil interface: $kasl_{air} := 120\cdot m\cdot d^{-1}$

partial mass transfer coefficient at soilair-side of the air-soil interface: $kasl_{soilair} := 0.48\cdot m\cdot d^{-1}$

partial mass transfer coefficient at soilwater-side of the air-soil interface: $kasl_{soilwater} := 4.8\cdot 10^{-5}\cdot m\cdot d^{-1}$

fraction of rain water that infiltrates into soil: $Finf_{soil} := 0.25$

rate of wet precipitation: $RAINrate := 1.92\cdot 10^{-3}\cdot m\cdot d^{-1}$

dry sludge application rate:

$$APPLsludge_i := \begin{array}{|c|}\hline 0.5\cdot kg\cdot m^{-2}\cdot a^{-1} \\ \hline 0.5\cdot kg\cdot m^{-2}\cdot a^{-1} \\ \hline 0.1\cdot kg\cdot m^{-2}\cdot a^{-1} \\ \hline \end{array}$$

Input:

annual average total deposition flux: $DEPtotal_{ann} := 0.011\cdot mg\cdot m^{-2}\cdot d^{-1}$

soil-water partitioning coefficient: $K_{soil\_water} := 0.619$

concentration in dry sewage sludge: $C_{sludge} := 0.0\cdot mg\cdot kg^{-1}$

air-water partitioning coefficient: $K_{air\_water} := 6.39\cdot 10^{-5}$

rate constant for for removal from top soil: $kbio_{soil} := 0.023\cdot d^{-1}$

PECregional: $PECregional_{natural\_soil} := 2.11\cdot 10^{-6}\cdot mg\cdot kg^{-1}$

Calculation:

aerial deposition flux per kg of soil:

$$D_{air_i} := \frac{DEPtotal_{ann}}{DEPTHsoil_i \cdot RHO_{soil}}$$

rate constant for valatilisation from soil:

$$k_{volat_i} := \left[\left(\frac{1}{kasl_{air} \cdot K_{air\_water}} + \frac{1}{kasl_{soilair} \cdot K_{air\_water} + kasl_{soilwater}} \right) \cdot K_{soil\_water} \cdot DEPTHsoil_i \right]^{-1}$$

rate constant for leaching from soil layer:

$$k_{leach_i} := \frac{Finf_{soil} \cdot RAINrate}{K_{soil\_water} \cdot DEPTHsoil_i}$$

removal from top soil:

$$k_i := k_{volat_i} + k_{leach_i} + kbio_{soil}$$

concentration in soil

concentration in soil due to 10 years of continuous deposition:

$$Cdep_{soil\_10_i} := \frac{D_{air_i}}{k_i} \cdot \left(1 - \exp(-365 \cdot d \cdot 10 \cdot k_i)\right)$$

concentration just after the first year of sludge application:

$$Csludge_{soil\_1_i} := \frac{C_{sludge} \cdot APPLsludge_i \cdot a}{DEPTHsoil_i \cdot RHO_{soil}}$$

initial concentration in soil after 10 applications of sludge:

$$Csludge_{soil\_10_i} := Csludge_{soil\_1_i} \cdot \left(1 + \sum_{n=1}^{9} \exp(-365 \cdot d \cdot n \cdot k_i)\right)$$

sum of the concentrations due to both processes:

$$C_{soil\_10_i} := Cdep_{soil\_10_i} + Csludge_{soil\_10_i}$$

average concentration in soil over T days:

$$Clocal_{soil_i} := \frac{D_{air_i}}{k_i} + \frac{1}{k_i \cdot T_i} \cdot \left(C_{soil\_10_i} - \frac{D_{air_i}}{k_i} \right) \cdot \left(1 - \exp\left(-k_i \cdot T_i \right) \right)$$

$$PEClocal_{soil_i} := Clocal_{soil_i} + PECregional_{natural\_soil}$$

	$Clocal_{soil_i}$ ppt		$PEClocal_{soil_i}$ ppt
$Clocal_{soil}$ =	$1.1762 \cdot 10^{3}$	$PEClocal_{soil}$ =	$1.1783 \cdot 10^{3}$
$Clocal_{agr.soil}$ =	$1.1762 \cdot 10^{3}$	$PEClocal_{agr.soil}$ =	$1.1783 \cdot 10^{3}$
$Clocal_{grassland}$ =	$2.0213 \cdot 10^{3}$	$PEClocal_{grassland}$ =	$2.0234 \cdot 10^{3}$

Indicating persistency of the substance in soil

initial concentration after 10 years:

$C_{soil\_10_i}$ ppt
$1.1762 \cdot 10^{3}$
$1.1762 \cdot 10^{3}$
$2.0213 \cdot 10^{3}$

initial concentration in steady-state situation:

$$C_{soil\_ss_i} := \frac{D_{air_i}}{k_i} + Csludge_{soil\_1_i} \cdot \left(\frac{1}{1 - \exp\left(-365 \cdot d \cdot k_i \right)} \right)$$

$C_{soil\_ss_i}$ ppt
$1.1762 \cdot 10^{3}$
$1.1762 \cdot 10^{3}$
$2.0213 \cdot 10^{3}$

fraction of steady-state in soil achieved:

$$Fst\_st_i := \frac{C_{soil\_10_i}}{C_{soil\_ss_i}}$$

Fst_st_i
1
1
1

calculated k-values

	k_{volat_i} d^{-1}	k_{leach_i} d^{-1}	k_i d^{-1}
soil	$6.2902 \cdot 10^{-4}$	$3.8772 \cdot 10^{-3}$	0.0275
agriculture soil	$6.2902 \cdot 10^{-4}$	$3.8772 \cdot 10^{-3}$	0.0275
grassland	$1.258 \cdot 10^{-3}$	$7.7544 \cdot 10^{-3}$	0.032

concentration in pore water

$$Clocal_{soil\_porew_i} := \frac{Clocal_{soil_i} \cdot RHO_{soil}}{K_{soil\_water}}$$

$\frac{Clocal_{soil\_porew_i}}{ng \cdot l^{-1}}$
$3.2303 \cdot 10^3$
$3.2303 \cdot 10^3$
$5.5511 \cdot 10^3$

$Clocal_{soil\_porew}$ =

$Clocal_{agr.soil\_porew}$ =

$Clocal_{grassland\_porew}$ =

$$PEClocal_{soil\_porew_i} := \frac{PEClocal_{soil_i} \cdot RHO_{soil}}{K_{soil\_water}}$$

$\frac{PEClocal_{soil\_porew_i}}{ng \cdot l^{-1}}$
$3.2361 \cdot 10^3$
$3.2361 \cdot 10^3$
$5.5569 \cdot 10^3$

$PEClocal_{soil\_porew}$ =

$PEClocal_{agr.soil\_porew}$ =

$PEClocal_{grassland\_porew}$ =

concentration in ground water

$PEClocal_{grw} = PEClocal_{agr\_soil\_porew}$

Appendix 3-10

PEC local_soil

Scenario IC/UC 14/48

Industrial Use – 5,000 t/a

Exposure of Soil

chemical: 2 – EEA

Defaults:

mixing depth of soil: $DEPTHsoil_i :=$

$0.2 \cdot m$
$0.2 \cdot m$
$0.1 \cdot m$

bulk density of soil: $RHO_{soil} := 1700 \cdot kg \cdot m^{-3}$

average time for exposure: $T_i :=$

$30 \cdot d$
$180 \cdot d$
$180 \cdot d$

partial mass transfer coefficient at air-side of the air-soil interface: $kasl_{air} := 120 \cdot m \cdot d^{-1}$

partial mass transfer coefficient at soilair-side of the air-soil interface: $kasl_{soilair} := 0.48 \cdot m \cdot d^{-1}$

partial mass transfer coefficient at soilwater-side of the air-soil interface: $kasl_{soilwater} := 4.8 \cdot 10^{-5} \cdot m \cdot d^{-1}$

fraction of rain water that infiltrates into soil: $Finf_{soil} := 0.25$

rate of wet precipitation: $RAINrate := 1.92 \cdot 10^{-3} \cdot m \cdot d^{-1}$

dry sludge application rate: $APPLsludge_i :=$

$0.5 \cdot kg \cdot m^{-2} \cdot a^{-1}$
$0.5 \cdot kg \cdot m^{-2} \cdot a^{-1}$
$0.1 \cdot kg \cdot m^{-2} \cdot a^{-1}$

Input:

annual average total deposition flux: $DEPtotal_{ann} := 0.055 \cdot mg \cdot m^{-2} \cdot d^{-1}$

soil-water partitioning coefficient: $K_{soil\_water} := 0.619$

concentration in dry sewage sludge: $C_{sludge} := 0.0 \cdot mg \cdot kg^{-1}$

air-water partitioning coefficient: $K_{air\_water} := 6.39 \cdot 10^{-5}$

rate constant for for removal from top soil: $kbio_{soil} := 0.023 \cdot d^{-1}$

PECregional: $PECregional_{natural\_soil} := 1.05 \cdot 10^{-5} \cdot mg \cdot kg^{-1}$

Calculation:

aerial deposition flux per kg of soil:

$$D_{air_i} := \frac{DEPtotal_{ann}}{DEPTHsoil_i \cdot RHO_{soil}}$$

rate constant for valatilisation from soil:

$$k_{volat_i} := \left[\left(\frac{1}{kasl_{air} \cdot K_{air\_water}} + \frac{1}{kasl_{soilair} \cdot K_{air\_water} + kasl_{soilwater}}\right) \cdot K_{soil\_water} \cdot DEPTHsoil_i\right]^{-1}$$

rate constant for leaching from soil layer:

$$k_{leach_i} := \frac{Finf_{soil} \cdot RAINrate}{K_{soil\_water} \cdot DEPTHsoil_i}$$

removal from top soil:

$$k_i := k_{volat_i} + k_{leach_i} + kbio_{soil}$$

concentration in soil

concentration in soil due to 10 years of continuous deposition:

$$Cdep_{soil\_10_i} := \frac{D_{air_i}}{k_i} \cdot \left(1 - \exp\left(-365 \cdot d \cdot 10 \cdot k_i\right)\right)$$

concentration just after the first year of sludge application:

$$Csludge_{soil\_1_i} := \frac{C_{sludge} \cdot APPLsludge_i \cdot a}{DEPTHsoil_i \cdot RHO_{soil}}$$

initial concentration in soil after 10 applications of sludge:

$$Csludge_{soil\_10_i} := Csludge_{soil\_1_i} \cdot \left(1 + \sum_{n=1}^{9} \exp\left(-365 \cdot d \cdot n \cdot k_i\right)\right)$$

sum of the concentrations due to both processes:

$$C_{soil\_10_i} := Cdep_{soil\_10_i} + Csludge_{soil\_10_i}$$

average concentration in soil over T days:

$$\mathrm{Clocal}_{\mathrm{soil}_i} := \frac{D_{\mathrm{air}_i}}{k_i} + \frac{1}{k_i \cdot T_i} \cdot \left(C_{\mathrm{soil\_10}_i} - \frac{D_{\mathrm{air}_i}}{k_i} \right) \cdot \left(1 - \exp\left(-k_i \cdot T_i \right) \right)$$

$$\mathrm{PEClocal}_{\mathrm{soil}_i} := \mathrm{Clocal}_{\mathrm{soil}_i} + \mathrm{PECregional}_{\mathrm{natural\_soil}}$$

	$\mathrm{Clocal}_{\mathrm{soil}_i}$ (ppt)		$\mathrm{PEClocal}_{\mathrm{soil}_i}$ (ppt)
$\mathrm{Clocal}_{\mathrm{soil}}$ =	$5.881 \cdot 10^{3}$	$\mathrm{PEClocal}_{\mathrm{soil}}$ =	$5.8915 \cdot 10^{3}$
$\mathrm{Clocal}_{\mathrm{agr.soil}}$ =	$5.881 \cdot 10^{3}$	$\mathrm{PEClocal}_{\mathrm{agr.soil}}$ =	$5.8915 \cdot 10^{3}$
$\mathrm{Clocal}_{\mathrm{grassland}}$ =	$1.0106 \cdot 10^{4}$	$\mathrm{PEClocal}_{\mathrm{grassland}}$ =	$1.0117 \cdot 10^{4}$

Indicating persistency of the substance in soil

initial concentration after 10 years:

$C_{\mathrm{soil\_10}_i}$ (ppt)
$5.881 \cdot 10^{3}$
$5.881 \cdot 10^{3}$
$1.0106 \cdot 10^{4}$

initial concentration in steady-state situation:

$$C_{\mathrm{soil\_ss}_i} := \frac{D_{\mathrm{air}_i}}{k_i} + \mathrm{Csludge}_{\mathrm{soil\_1}_i} \cdot \left(\frac{1}{1 - \exp\left(-365 \cdot d \cdot k_i \right)} \right)$$

$C_{\mathrm{soil\_ss}_i}$ (ppt)
$5.881 \cdot 10^{3}$
$5.881 \cdot 10^{3}$
$1.0106 \cdot 10^{4}$

fraction of steady-state in soil achieved:

$$\mathrm{Fst\_st}_i := \frac{C_{\mathrm{soil\_10}_i}}{C_{\mathrm{soil\_ss}_i}}$$

$\mathrm{Fst\_st}_i$
1
1
1

calculated k-values

	k_{volat_i} (d^{-1})	k_{leach_i} (d^{-1})	k_i (d^{-1})
soil	$6.2902 \cdot 10^{-4}$	$3.8772 \cdot 10^{-3}$	0.0275
agriculture soil	$6.2902 \cdot 10^{-4}$	$3.8772 \cdot 10^{-3}$	0.0275
grassland	$1.258 \cdot 10^{-3}$	$7.7544 \cdot 10^{-3}$	0.032

concentration in pore water

$$Clocal_{soil\_porew_i} := \frac{Clocal_{soil_i} \cdot RHO_{soil}}{K_{soil\_water}}$$

$\dfrac{Clocal_{soil\_porew_i}}{ng \cdot l^{-1}}$

Variable	=	Value
$Clocal_{soil\_porew}$	=	$1.6151 \cdot 10^{4}$
$Clocal_{agr.soil\_porew}$	=	$1.6151 \cdot 10^{4}$
$Clocal_{grassland\_porew}$	=	$2.7756 \cdot 10^{4}$

$$PEClocal_{soil\_porew_i} := \frac{PEClocal_{soil_i} \cdot RHO_{soil}}{K_{soil\_water}}$$

$\dfrac{PEClocal_{soil\_porew_i}}{ng \cdot l^{-1}}$

Variable	=	Value
$PEClocal_{soil\_porew}$	=	$1.618 \cdot 10^{4}$
$PEClocal_{agr.soil\_porew}$	=	$1.618 \cdot 10^{4}$
$PEClocal_{grassland\_porew}$	=	$2.7785 \cdot 10^{4}$

concentration in ground water

$PEClocal_{grw} = PEClocal_{agr\_soil\_porew}$

Appendix 4-1

Indirect exposure via the environment

Scenario IC/UC 14/48

1,000 t/a

Industrial Use

INDIRECT EXPOSURE VIA THE ENVIRONMENT

(TGD On New and Existing Chemicals, chapter 2)

Parameter [Unit]	*Symbol*

Definitions (for the use in this document)

definition of the unit 'kg$_{bw}$' for body weight	$kg_{bw} := 1 \cdot kg$
definition of the unit 'd' for day	$d := 1 \cdot Tag$
	$scenario := 1 .. 2$
	$local := 1$ $regional := 2$

Constants

gas - constant R	$R := 8.314 \cdot J \cdot K^{-1} \cdot Mol^{-1}$

Defaults

volumefraction air in plant tissue [-]	$Fair_{plant} := 0.3$
volumefraction water in plant tissue [-]	$Fwater_{plant} := 0.65$
volumefraction lipids in plant tissue [-]	$Flipid_{plant} := 0.01$
bulk density of plant tissue [$kg_{wet\ plant} * m_{plant}^{-3}$]	$RHO_{plant} := 700 \cdot kg \cdot m^{-3}$
leaf surface area [m^2]	$AREA_{plant} := 5 \cdot m^2$
conductance (0.001 $m*s^{-1}$) [$m*d^{-1}$]	$g_{plant} := 0.001 \cdot m \cdot s^{-1}$
shoot volume [m^3]	$V_{leaf} := 0.002 \cdot m^3$
transpiration stream [m^3*d^{-1}]	$Q_{transp} := 1 \cdot 10^{-3} \cdot m^3 \cdot d^{-1}$
correction exponent for differences between plant lipids and octanol [-]	$b := 0.95$
growth rate constant for dilution by growth [d^{-1}]	$kgrowth_{plant} := 0.035 \cdot d^{-1}$
pseudo-first order rate constant for metabolism in plants [d^{-1}]	$kmetab_{plant} := 0 \cdot d^{-1}$
pseudo-first order rate constant for photolysis in plants [d^{-1}]	$kphoto_{plant} := 0 \cdot d^{-1}$

concentration in meat and milk

daily intake of grass
[$kg_{wetgrass}$*d^{-1}]

$IC_{grass} := 67.6 \cdot kg \cdot d^{-1}$

daily intake of soil
[$kg_{wet\ soil}$*d^{-1}]

$IC_{soil} := 0.46 \cdot kg \cdot d^{-1}$

daily intake of air
[$m_{air}{}^{3}$*d^{-1}]

$IC_{air} := 122 \cdot m^{3} \cdot d^{-1}$

daily intake of drinkingwater
[l*d^{-1}]

$IC_{drw} := 55 \cdot l \cdot d^{-1}$

daily intake for human

daily intake for the several pathways
[kg_{chem}*d^{-1}] or [$m^{3*}d^{-1}$]

$IH_{drw} := 2 \cdot l \cdot d^{-1}$

$IH_{fish} := 0.115 \cdot kg \cdot d^{-1}$

$IH_{stem} := 1.2 \cdot kg \cdot d^{-1}$

$IH_{root} := 0.384 \cdot kg \cdot d^{-1}$

$IH_{meat} := 0.301 \cdot kg \cdot d^{-1}$

$IH_{milk} := 0.561 \cdot kg \cdot d^{-1}$

$IH_{air} := 20 \cdot m^{3} \cdot d^{-1}$

bioavailability through route of intake
[-]

$BIO_{inh} := 0.75$

$BIO_{oral} := 1.0$

average body weight of human
[kg]

$BW := 70 \cdot kg_{bw}$

Input

chemical properties

	$\mathrm{logK_{OW}} := 0.24$
octanol-water partitioning coefficient [-]	$\mathrm{K_{OW}} := 10^{\mathrm{logK_{OW}}}$
Henry - partitioning coefficient [Pa*m^3*mol^{-1}]	$\mathrm{HENRY} := 0.16 \cdot \mathrm{Pa} \cdot \mathrm{m}^3 \cdot \mathrm{Mol}^{-1}$
air-water partitioning coefficient [-]	$\mathrm{K_{air\_water}} := 6.4 \cdot 10^{-5}$
fraction of the chemical associated with aerosol particles [-]	$\mathrm{F_{ass\_aer}} := 3.7 \cdot 10^{-7}$
half-life for biodegration in surface water [d]	$\mathrm{DT_{50\_bio\_water}} := 15 \cdot \mathrm{d}$

environmental concentrations

annual average local PEC in surface water (dissolved) [mg$_{chem}$ * l$_{water}$$^{-1}$] , (from open use)	$\mathrm{PEClocal_{water\_ann}} := 0.0194 \cdot \mathrm{mg} \cdot \mathrm{l}^{-1}$
annual average local PEC in air (total) [mg$_{chem}$ * m$_{air}$$^{-3}$] (from open use)	$\mathrm{PEClocal_{air\_ann}} := 7.7 \cdot 10^{-3} \cdot \mathrm{mg} \cdot \mathrm{m}^{-3}$
local PEC in grassland (total), averaged over 180 days [mg$_{chem}$ * kg$_{soil}$$^{-1}$]	$\mathrm{PEClocal_{grassland}} := 2.02 \cdot 10^{-3} \cdot \mathrm{mg} \cdot \mathrm{kg}^{-}$
local PEC in porewater of agriculture soil [mg$_{chem}$ * l$_{porewater}$$^{-1}$]	$\mathrm{PEClocal_{agr\_soil\_porew}} := 3.24 \cdot 10^{-3} \cdot \mathrm{mg} \cdot \mathrm{l}^{-1}$
local PEC in porewater of grassland [mg$_{chem}$ * l$_{porewater}$$^{-1}$]	$\mathrm{PEClocal_{grassland\_porew}} := 5.56 \cdot 10^{-3} \cdot \mathrm{mg} \cdot \mathrm{l}^{-1}$
local PEC in groundwater under agriculture soil [mg$_{chem}$ * l$_{water}$$^{-1}$]	$\mathrm{PEClocal_{grw}} := 3.24 \cdot 10^{-3} \cdot \mathrm{mg} \cdot \mathrm{l}^{-1}$
regional PEC in surface water (dissolved) [mg$_{chem}$ * l$_{water}$$^{-1}$]	$\mathrm{PECregional_{water}} := 3.41 \cdot 10^{-5} \cdot \mathrm{mg} \cdot \mathrm{l}^{-1}$
regional PEC in air (total) [mg$_{chem}$ * m$_{air}$$^{-3}$]	$\mathrm{PECregional_{air}} := 3.34 \cdot 10^{-7} \cdot \mathrm{mg} \cdot \mathrm{m}^{-3}$
regional PEC in agriculture soil (total) [mg$_{chem}$*kg$_{soil}$$^{-1}$	$\mathrm{PECregional_{agr\_soil}} := 9.50 \cdot 10^{-7} \cdot \mathrm{mg} \cdot \mathrm{kg}^{-1}$
regional PEC in porewater of agriculture soils [mg$_{chem}$*l$_{water}$$^{-1}$	$\mathrm{PECregional_{agr\_soil\_porew}} := 2.61 \cdot 10^{-6} \cdot \mathrm{mg} \cdot \mathrm{l}^{-}$

Definition of the concentrations used for indirect exposure

$Cwater_{local} := PEClocal_{water\_ann}$

$Cair_{local} := PEClocal_{air\_ann}$

$Cgrassland_{local} := PEClocal_{grassland}$

$Cagr\_porew_{local} := PEClocal_{agr\_soil\_porew}$

$Cgrass\_porew_{local} := PEClocal_{grassland\_porew}$

$Cgrw_{local} := PEClocal_{grw}$

$Cwater_{regional} := PECregional_{water}$

$Cair_{regional} := PECregional_{air}$

$Cgrassland_{regional} := PECregional_{agr\_soil}$

$Cagr\_porew_{regional} := PECregional_{agr\_soil\_porew}$

$Cgrass\_porew_{regional} := PECregional_{agr\_soil\_porew}$

$Cgrw_{regional} := PECregional_{agr\_soil\_porew}$

bioconcentration in fish

bioconcentration factor for fish
[$m_{water}{}^{3}*kg_{chem}{}^{-1}$]

$$BCF_{fish} := 10^{0.85\cdot logK_{OW}-0.7}\cdot l\cdot kg^{-1}$$

modified equation for logKow > 6

$$BCF_{fish} := wenn\left[logK_{OW} > 6, \left(-0.278\cdot logK_{OW}{}^{2} + 3.38\cdot logK_{OW} - 5.94\right)\cdot l\cdot kg^{-1}, BCF_{fish}\right]$$

$$Cfish_{scenario} := BCF_{fish}\cdot Cwater_{scenario}$$

bioconcentration in plants

$$K_{plant\_water} := Fwater_{plant} + Flipid_{plant}\cdot K_{OW}{}^{b}$$

$$Croot_{agr\_plant}{}_{scenario} := \frac{K_{plant\_water}\cdot C_{agr\_porew}{}_{scenario}}{RHO_{plant}}$$

$$TSCF := 0.784\cdot e^{\frac{-\left(logK_{OW}-1.78\right)^{2}}{2.44}}$$

remark: for $logK_{ow}$ out of the range from -0.5 to 4.5
the TSCF is limited by the values for $logK_{ow}$ = -0.5 resp. 4.5

$$TSCF := wenn\left(logK_{OW} < -0.5, 0.903, TSCF\right)$$

$$TSCF := wenn\left(logK_{OW} > 4.5, 0.832, TSCF\right)$$

$$K_{leaf\_air} := Fair_{plant} + \frac{K_{plant\_water}}{K_{air\_water}}$$

$$kelim_{plant} := kmetab_{plant} + kphoto_{plant}$$

$$\alpha := \frac{AREA_{plant}\cdot g_{plant}}{K_{leaf\_air}\cdot V_{leaf}} + kelim_{plant} + kgrowth_{plant}$$

$$\beta_{agr\_plant_{scenario}} := C_{agr\_porew_{scenario}} \cdot TSCF \cdot \frac{Q_{transp}}{V_{leaf}} + \left(1 - F_{ass\_aer}\right) \cdot C_{air_{scenario}} \cdot g_{plant} \cdot \frac{AREA_{plant}}{V_{leaf}}$$

$$C_{leaf\_crops_{scenario}} := \frac{\beta_{agr\_plant_{scenario}}}{\alpha \cdot RHO_{plant}}$$

$$\beta_{grass\_plant_{scenario}} := C_{grass\_porew_{scenario}} \cdot TSCF \cdot \frac{Q_{transp}}{V_{leaf}} + \left(1 - F_{ass\_aer}\right) \cdot C_{air_{scenario}} \cdot g_{plant} \cdot \frac{AREA_{plant}}{V_{leaf}}$$

$$C_{leaf\_grass_{scenario}} := \frac{\beta_{grass\_plant_{scenario}}}{\alpha \cdot RHO_{plant}}$$

<u>purification of drinking water</u>

system may defined dependent from the aerobic biodegradation

$$system := wenn\left(DT_{50\_bio\_water} < 10 \cdot d, 0, 1\right)$$

select a column on dependence from log K_{OW}

$$FIndex := wenn\left(logK_{OW} < 4, 0, wenn\left(logK_{OW} > 5, 2, 1\right)\right)$$

$$Fpur_{logKow} := \begin{pmatrix} 1 & \frac{1}{4} & \frac{1}{16} \\ 1 & \frac{1}{2} & \frac{1}{4} \end{pmatrix}$$

$$Fpur := \frac{Fpur_{logKow_{system, FIndex}}}{wenn\left(HENRY > 100 \cdot Pa \cdot m^3 \cdot Mol^{-1}, 2, 1\right)}$$

$$C_{drw_{scenario}} := wenn\left[C_{grw_{scenario}} > \left(C_{water_{scenario}} \cdot Fpur\right), C_{grw_{scenario}}, C_{water_{scenario}} \cdot Fpur\right]$$

<u>Biotransfer to meat and milk</u>

$$BTF_{meat} := 10^{-7.6 + logK_{OW}} \cdot kg^{-1} \cdot d$$

remark: for logK_{OW} out of the range from 1.5 to 6.5
the BTF $_{meat}$ is limited by the values for logK_{OW} = 1.5 resp. 6.5

$$BTF_{meat} := wenn\left(logK_{OW} < 1.5, 7.943 \cdot 10^{-7} \cdot kg^{-1} \cdot d, BTF_{meat}\right)$$

$$BTF_{meat} := wenn\left(logK_{OW} > 6.5, 0.07943 \cdot kg^{-1} \cdot d, BTF_{meat}\right)$$

$$C_{meat_{scenario}} := BTF_{meat} \cdot \left(C_{leaf\_grass_{scenario}} \cdot IC_{grass} + C_{grassland_{scenario}} \cdot IC_{soil} \cdots + C_{air_{scenario}} \cdot IC_{air} + C_{drw_{scenario}} \cdot IC_{drw}\right)$$

$$BTF_{milk} := 10^{-8.1+logK_{OW}} \cdot kg^{-1} \cdot d$$

remark: for logK$_{OW}$ out of the range from 3 to 6.5
the BTF $_{milk}$ is limited by the values for logK$_{OW}$ = 1.5 resp. 6.5

$$BTF_{milk} := wenn\left(logK_{OW} < 3, 7.943 \cdot 10^{-6} \cdot kg^{-1} \cdot d, BTF_{milk}\right)$$

$$BTF_{milk} := wenn\left(logK_{OW} > 6.5, 0.02512 \cdot kg^{-1} \cdot d, BTF_{milk}\right)$$

$$C_{milk_{scenario}} := BTF_{milk} \cdot \left(C_{leaf\_grass_{scenario}} \cdot IC_{grass} + C_{grassland_{scenario}} \cdot IC_{soil} \dots + C_{air_{scenario}} \cdot IC_{air} + C_{drw_{scenario}} \cdot IC_{drw}\right)$$

total daily intake for human

daily dose through intake of several pathways

[$kg_{chem}*kg_{bw}^{-1}*d^{-1}$]

$$DOSE_{drw_{scenario}} := \frac{C_{drw_{scenario}} \cdot IH_{drw}}{BW}$$

$$DOSE_{air_{scenario}} := \frac{C_{air_{scenario}} \cdot IH_{air} \cdot BIO_{inh}}{BW \cdot BIO_{oral}}$$

$$DOSE_{stem_{scenario}} := \frac{C_{leaf\_crops_{scenario}} \cdot IH_{stem}}{BW}$$

$$DOSE_{root_{scenario}} := \frac{Croot_{agr\_plant_{scenario}} \cdot IH_{root}}{BW}$$

$$DOSE_{meat_{scenario}} := \frac{C_{meat_{scenario}} \cdot IH_{meat}}{BW}$$

$$DOSE_{milk_{scenario}} := \frac{C_{milk_{scenario}} \cdot IH_{milk}}{BW}$$

$$DOSE_{fish_{scenario}} := \frac{C_{fish_{scenario}} \cdot IH_{fish}}{BW}$$

total daily intake for human

total daily intake for human as sum of each pathway

[$kg_{chem}*kg_{bw}^{-1}*d^{-1}$]

$$DOSE_{tot_{scenario}} := DOSE_{drw_{scenario}} + DOSE_{fish_{scenario}} + DOSE_{stem_{scenario}} + DOSE_{root_{scenario}} \cdots + DOSE_{meat_{scenario}} + DOSE_{milk_{scenario}} + DOSE_{air_{scenario}}$$

relative doses of specific different pathway (%)

$$RDOSE_{drw_{scenario}} := \frac{DOSE_{drw_{scenario}} \cdot 100 \cdot \%}{DOSE_{tot_{scenario}}}$$

$$RDOSE_{air_{scenario}} := \frac{DOSE_{air_{scenario}} \cdot 100 \cdot \%}{DOSE_{tot_{scenario}}}$$

$$RDOSE_{stem_{scenario}} := \frac{DOSE_{stem_{scenario}} \cdot 100 \cdot \%}{DOSE_{tot_{scenario}}}$$

$$RDOSE_{root_{scenario}} := \frac{DOSE_{root_{scenario}} \cdot 100 \cdot \%}{DOSE_{tot_{scenario}}}$$

$$RDOSE_{meat_{scenario}} := \frac{DOSE_{meat_{scenario}} \cdot 100 \cdot \%}{DOSE_{tot_{scenario}}}$$

$$RDOSE_{milk_{scenario}} := \frac{DOSE_{milk_{scenario}} \cdot 100 \cdot \%}{DOSE_{tot_{scenario}}}$$

$$RDOSE_{fish_{scenario}} := \frac{DOSE_{fish_{scenario}} \cdot 100 \cdot \%}{DOSE_{tot_{scenario}}}$$

Results of calculation

$DOSE_{tot_{local}} = 4.194341 \times 10^{-3} \frac{mg}{kg_{bw} \cdot d}$

$DOSE_{tot_{regional}} = 1.163078 \times 10^{-6} \frac{mg}{kg_{bw} \cdot d}$

$RDOSE_{drw_{local}} = 13.215084\%$

$RDOSE_{drw_{regional}} = 83.76785\%$

$RDOSE_{air_{local}} = 39.338718\%$

$RDOSE_{air_{regional}} = 6.153621\%$

$RDOSE_{stem_{local}} = 46.784377\%$

$RDOSE_{stem_{regional}} = 7.355461\%$

$RDOSE_{root_{local}} = 0.40372\%$

$RDOSE_{root_{regional}} = 1.172817\%$

$RDOSE_{meat_{local}} = 7.937004 \times 10^{-4}\%$

$RDOSE_{meat_{regional}} = 6.619192 \times 10^{-4}\%$

$RDOSE_{milk_{local}} = 0.014793\%$

$RDOSE_{milk_{regional}} = 0.012337\%$

$RDOSE_{fish_{local}} = 0.242515\%$

$RDOSE_{fish_{regional}} = 1.537253\%$

Appendix 4-2

Indirect exposure via the environment

Scenario IC/UC 14/48

5,000 t/a

Industrial Use

INDIRECT EXPOSURE VIA THE ENVIRONMENT

(TGD On New and Existing Chemicals, chapter 2)

Parameter [Unit]	*Symbol*

Definitions (for the use in this document)

definition of the unit 'kg$_{bw}$' for body weight	$kg_{bw} := 1 \cdot kg$
definition of the unit 'd' for day	$d := 1 \cdot Tag$
	$scenario := 1 .. 2$
	$local := 1$ $regional := 2$

Constants

gas - constant R	$R := 8.314 \cdot J \cdot K^{-1} \cdot Mol^{-1}$

Defaults

volumefraction air in plant tissue [-]	$Fair_{plant} := 0.3$
volumefraction water in plant tissue [-]	$Fwater_{plant} := 0.65$
volumefraction lipids in plant tissue [-]	$Flipid_{plant} := 0.01$
bulk density of plant tissue [$kg_{wet\ plant} * m_{plant}^{-3}$]	$RHO_{plant} := 700 \cdot kg \cdot m^{-3}$
leaf surface area [m^2]	$AREA_{plant} := 5 \cdot m^2$
conductance (0.001 $m*s^{-1}$) [$m*d^{-1}$]	$g_{plant} := 0.001 \cdot m \cdot s^{-1}$
shoot volume [m^3]	$V_{leaf} := 0.002 \cdot m^3$
transpiration stream [m^3*d^{-1}]	$Q_{transp} := 1 \cdot 10^{-3} \cdot m^3 \cdot d^{-1}$
correction exponent for differences between plant lipids and octanol [-]	$b := 0.95$
growth rate constant for dilution by growth [d^{-1}]	$kgrowth_{plant} := 0.035 \cdot d^{-1}$
pseudo-first order rate constant for metabolism in plants [d^{-1}]	$kmetab_{plant} := 0 \cdot d^{-1}$
pseudo-first order rate constant for photolysis in plants [d^{-1}]	$kphoto_{plant} := 0 \cdot d^{-1}$

concentration in meat and milk

daily intake of grass
$[kg_{wetgrass}*d^{-1}]$ $IC_{grass} := 67.6 \cdot kg \cdot d^{-1}$

daily intake of soil
$[kg_{wet\ soil}*d^{-1}]$ $IC_{soil} := 0.46 \cdot kg \cdot d^{-1}$

daily intake of air
$[m_{air}{}^{3}*d^{-1}]$ $IC_{air} := 122 \cdot m^{3} \cdot d^{-1}$

daily intake of drinkingwater $IC_{drw} := 55 \cdot l \cdot d^{-1}$
$[l*d^{-1}]$

daily intake for human

daily intake for the several pathways
$[kg_{chem}*d^{-1}]$ or $[m^{3*}d^{-1}]$

$IH_{drw} := 2 \cdot l \cdot d^{-1}$

$IH_{fish} := 0.115 \cdot kg \cdot d^{-1}$

$IH_{stem} := 1.2 \cdot kg \cdot d^{-1}$

$IH_{root} := 0.384 \cdot kg \cdot d^{-1}$

$IH_{meat} := 0.301 \cdot kg \cdot d^{-1}$

$IH_{milk} := 0.561 \cdot kg \cdot d^{-1}$

$IH_{air} := 20 \cdot m^{3} \cdot d^{-1}$

bioavailability through route of intake
[-]

$BIO_{inh} := 0.75$

$BIO_{oral} := 1.0$

average body weight of human $BW := 70 \cdot kg_{bw}$
[kg]

Name: 2-EEA CAS - No.: 111 – 15 – 9

Input

chemical properties

$\mathrm{logK}_{OW} := 0.24$

octanol-water partitioning coefficient
[-]

$K_{OW} := 10^{\mathrm{logK}_{OW}}$

Henry - partitioning coefficient
[Pa*m^{3}*mol^{-1}]

$\mathrm{HENRY} := 0.16 \cdot \mathrm{Pa} \cdot \mathrm{m}^{3} \cdot \mathrm{Mol}^{-1}$

air-water partitioning coefficient
[-]

$K_{air\_water} := 6.4 \cdot 10^{-5}$

fraction of the chemical associated
with aerosol particles
[-]

$F_{ass\_aer} := 3.7 \cdot 10^{-7}$

half-life for biodegration in surface water
[d]

$DT_{50\_bio\_water} := 15 \cdot d$

environmental concentrations

annual average local PEC in surface water (dissolved)
[mg$_{chem}$ * l$_{water}$$^{-1}$] , (from open use)

$\mathrm{PEClocal}_{water\_ann} := 0.1 \cdot \mathrm{mg} \cdot \mathrm{l}^{-1}$

annual average local PEC in air (total)
[mg$_{chem}$ * m$_{air}$$^{-3}$] (from open use)

$\mathrm{PEClocal}_{air\_ann} := 0.039 \cdot \mathrm{mg} \cdot \mathrm{m}^{-3}$

local PEC in grassland (total), averaged over 180 days
[mg$_{chem}$ * kg$_{soil}$$^{-1}$]

$\mathrm{PEClocal}_{grassland} := 1.01 \cdot 10^{-2} \cdot \mathrm{mg} \cdot \mathrm{kg}^{-}$

local PEC in porewater of agriculture soil
[mg$_{chem}$ * l$_{porewater}$$^{-1}$]

$\mathrm{PEClocal}_{agr\_soil\_porew} := 6.47 \cdot 10^{-3} \cdot \mathrm{mg} \cdot \mathrm{l}^{-1}$

local PEC in porewater of grassland
[mg$_{chem}$ * l$_{porewater}$$^{-1}$]

$\mathrm{PEClocal}_{grassland\_porew} := 2.8 \cdot 10^{-2} \cdot \mathrm{mg} \cdot \mathrm{l}^{-1}$

local PEC in groundwater under agriculture soil
[mg$_{chem}$ * l$_{water}$$^{-1}$]

$\mathrm{PEClocal}_{grw} := 1.6 \cdot 10^{-2} \cdot \mathrm{mg} \cdot \mathrm{l}^{-1}$

regional PEC in surface water (dissolved)
[mg$_{chem}$ * l$_{water}$$^{-1}$]

$\mathrm{PECregional}_{water} := 1.50 \cdot 10^{-4} \cdot \mathrm{mg} \cdot \mathrm{l}^{-1}$

regional PEC in air (total)
[mg$_{chem}$ * m$_{air}$$^{-3}$]

$\mathrm{PECregional}_{air} := 1.67 \cdot 10^{-6} \cdot \mathrm{mg} \cdot \mathrm{m}^{-3}$

regional PEC in agriculture soil (total)
[mg$_{chem}$*kg$_{soil}$$^{-1}$

$\mathrm{PECregional}_{agr\_soil} := 4.74 \cdot 10^{-6} \cdot \mathrm{mg} \cdot \mathrm{kg}^{-1}$

regional PEC in porewater of agriculture soils
[mg$_{chem}$*l$_{water}$$^{-1}$

$\mathrm{PECregional}_{agr\_soil\_porew} := 1.3 \cdot 10^{-5} \cdot \mathrm{mg} \cdot \mathrm{l}^{-1}$

Definition of the concentrations used for indirect exposure

$Cwater_{local} := PEClocal_{water\_ann}$

$Cair_{local} := PEClocal_{air\_ann}$

$Cgrassland_{local} := PEClocal_{grassland}$

$Cagr\_porew_{local} := PEClocal_{agr\_soil\_porew}$

$Cgrass\_porew_{local} := PEClocal_{grassland\_porew}$

$Cgrw_{local} := PEClocal_{grw}$

$Cwater_{regional} := PECregional_{water}$

$Cair_{regional} := PECregional_{air}$

$Cgrassland_{regional} := PECregional_{agr\_soil}$

$Cagr\_porew_{regional} := PECregional_{agr\_soil\_porew}$

$Cgrass\_porew_{regional} := PECregional_{agr\_soil\_porew}$

$Cgrw_{regional} := PECregional_{agr\_soil\_porew}$

bioconcentration in fish

bioconcentration factor for fish
[$m_{water}{}^{3}$*$kg_{chem}{}^{-1}$]

$$BCF_{fish} := 10^{0.85 \cdot logK_{OW} - 0.7} \cdot l \cdot kg^{-1}$$

modified equation for logKow > 6

$$BCF_{fish} := wenn\left[logK_{OW} > 6, \left(-0.278 \cdot logK_{OW}{}^{2} + 3.38 \cdot logK_{OW} - 5.94\right) \cdot l \cdot kg^{-1}, BCF_{fish}\right]$$

$$Cfish_{scenario} := BCF_{fish} \cdot Cwater_{scenario}$$

bioconcentration in plants

$$K_{plant\_water} := Fwater_{plant} + Flipid_{plant} \cdot K_{OW}{}^{b}$$

$$Croot_{agr\_plant}{}_{scenario} := \frac{K_{plant\_water} \cdot C_{agr\_porew}{}_{scenario}}{RHO_{plant}}$$

$$TSCF := 0.784 \cdot e^{\frac{-\left(logK_{OW} - 1.78\right)^{2}}{2.44}}$$

remark: for $logK_{ow}$ out of the range from -0.5 to 4.5
the TSCF is limited by the values for $logK_{ow}$ = -0.5 resp. 4.5

$$TSCF := wenn\left(logK_{OW} < -0.5, 0.903, TSCF\right)$$

$$TSCF := wenn\left(logK_{OW} > 4.5, 0.832, TSCF\right)$$

$$K_{leaf\_air} := Fair_{plant} + \frac{K_{plant\_water}}{K_{air\_water}}$$

$$kelim_{plant} := kmetab_{plant} + kphoto_{plant}$$

$$\alpha := \frac{AREA_{plant} \cdot g_{plant}}{K_{leaf\_air} \cdot V_{leaf}} + kelim_{plant} + kgrowth_{plant}$$

$$\beta_{agr\_plant_{scenario}} := C_{agr\_porew_{scenario}} \cdot TSCF \cdot \frac{Q_{transp}}{V_{leaf}} + \left(1 - F_{ass\_aer}\right) \cdot C_{air_{scenario}} \cdot g_{plant} \cdot \frac{AREA_{plant}}{V_{leaf}}$$

$$C_{leaf\_crops_{scenario}} := \frac{\beta_{agr\_plant_{scenario}}}{\alpha \cdot RHO_{plant}}$$

$$\beta_{grass\_plant_{scenario}} := C_{grass\_porew_{scenario}} \cdot TSCF \cdot \frac{Q_{transp}}{V_{leaf}} + \left(1 - F_{ass\_aer}\right) \cdot C_{air_{scenario}} \cdot g_{plant} \cdot \frac{AREA_{plant}}{V_{leaf}}$$

$$C_{leaf\_grass_{scenario}} := \frac{\beta_{grass\_plant_{scenario}}}{\alpha \cdot RHO_{plant}}$$

purification of drinking water

system may defined dependent from the aerobic biodegradation

$$system := wenn\left(DT_{50\_bio\_water} < 10 \cdot d, 0, 1\right)$$

select a column on dependence from log K_{ow}

$$FIndex := wenn\left(logK_{OW} < 4, 0, wenn\left(logK_{OW} > 5, 2, 1\right)\right)$$

$$Fpur_{logKow} := \begin{pmatrix} 1 & \frac{1}{4} & \frac{1}{16} \\ 1 & \frac{1}{2} & \frac{1}{4} \end{pmatrix}$$

$$Fpur := \frac{Fpur_{logKow_{system, FIndex}}}{wenn\left(HENRY > 100 \cdot Pa \cdot m^{3} \cdot Mol^{-1}, 2, 1\right)}$$

$$C_{drw_{scenario}} := wenn\left[C_{grw_{scenario}} > \left(C_{water_{scenario}} \cdot Fpur\right), C_{grw_{scenario}}, C_{water_{scenario}} \cdot Fpur\right]$$

Biotransfer to meat and milk

$$BTF_{meat} := 10^{-7.6 + logK_{OW}} \cdot kg^{-1} \cdot d$$

remark: for $logK_{ow}$ out of the range from 1.5 to 6.5
the BTF $_{meat}$ is limited by the values for $logK_{ow} = 1.5$ resp. 6.5

$$BTF_{meat} := wenn\left(logK_{OW} < 1.5, 7.943 \cdot 10^{-7} \cdot kg^{-1} \cdot d, BTF_{meat}\right)$$

$$BTF_{meat} := wenn\left(logK_{OW} > 6.5, 0.07943 \cdot kg^{-1} \cdot d, BTF_{meat}\right)$$

$$C_{meat_{scenario}} := BTF_{meat} \cdot \left(C_{leaf\_grass_{scenario}} \cdot IC_{grass} + C_{grassland_{scenario}} \cdot IC_{soil} \ldots + C_{air_{scenario}} \cdot IC_{air} + C_{drw_{scenario}} \cdot IC_{drw}\right)$$

$$BTF_{milk} := 10^{-8.1+logK_{OW}} \cdot kg^{-1} \cdot d$$

remark: for $logK_{OW}$ out of the range from 3 to 6.5

the BTF $_{milk}$ is limited by the values for $logK_{OW}$ = 1.5 resp. 6.5

$$BTF_{milk} := wenn\left(logK_{OW} < 3, 7.943 \cdot 10^{-6} \cdot kg^{-1} \cdot d, BTF_{milk}\right)$$

$$BTF_{milk} := wenn\left(logK_{OW} > 6.5, 0.02512 \cdot kg^{-1} \cdot d, BTF_{milk}\right)$$

$$C_{milk_{scenario}} := BTF_{milk} \cdot \left(\begin{array}{l} C_{leaf\_grass_{scenario}} \cdot IC_{grass} + C_{grassland_{scenario}} \cdot IC_{soil} \ldots \\ + C_{air_{scenario}} \cdot IC_{air} + C_{drw_{scenario}} \cdot IC_{drw} \end{array}\right)$$

total daily intake for human

daily dose through intake of several pathways

$[kg_{chem}*kg_{bw}^{-1}*d^{-1}]$

$$DOSE_{drw_{scenario}} := \frac{C_{drw_{scenario}} \cdot IH_{drw}}{BW} \qquad DOSE_{air_{scenario}} := \frac{C_{air_{scenario}} \cdot IH_{air} \cdot BIO_{inh}}{BW \cdot BIO_{oral}}$$

$$DOSE_{stem_{scenario}} := \frac{C_{leaf\_crops_{scenario}} \cdot IH_{stem}}{BW} \qquad DOSE_{root_{scenario}} := \frac{Croot_{agr\_plant_{scenario}} \cdot IH_{root}}{BW}$$

$$DOSE_{meat_{scenario}} := \frac{C_{meat_{scenario}} \cdot IH_{meat}}{BW} \qquad DOSE_{milk_{scenario}} := \frac{C_{milk_{scenario}} \cdot IH_{milk}}{BW}$$

$$DOSE_{fish_{scenario}} := \frac{C_{fish_{scenario}} \cdot IH_{fish}}{BW}$$

total daily intake for human

total daily intake for human as sum of each pathway

$[kg_{chem}*kg_{bw}^{-1}*d^{-1}]$

$$DOSE_{tot_{scenario}} := DOSE_{drw_{scenario}} + DOSE_{fish_{scenario}} + DOSE_{stem_{scenario}} + DOSE_{root_{scenario}} \cdots + DOSE_{meat_{scenario}} + DOSE_{milk_{scenario}} + DOSE_{air_{scenario}}$$

relative doses of specific different pathway (%)

$$RDOSE_{drw_{scenario}} := \frac{DOSE_{drw_{scenario}} \cdot 100 \cdot \%}{DOSE_{tot_{scenario}}} \qquad RDOSE_{air_{scenario}} := \frac{DOSE_{air_{scenario}} \cdot 100 \cdot \%}{DOSE_{tot_{scenario}}}$$

$$RDOSE_{stem_{scenario}} := \frac{DOSE_{stem_{scenario}} \cdot 100 \cdot \%}{DOSE_{tot_{scenario}}} \qquad RDOSE_{root_{scenario}} := \frac{DOSE_{root_{scenario}} \cdot 100 \cdot \%}{DOSE_{tot_{scenario}}}$$

$$RDOSE_{meat_{scenario}} := \frac{DOSE_{meat_{scenario}} \cdot 100 \cdot \%}{DOSE_{tot_{scenario}}} \qquad RDOSE_{milk_{scenario}} := \frac{DOSE_{milk_{scenario}} \cdot 100 \cdot \%}{DOSE_{tot_{scenario}}}$$

$$RDOSE_{fish_{scenario}} := \frac{DOSE_{fish_{scenario}} \cdot 100 \cdot \%}{DOSE_{tot_{scenario}}}$$

Results of calculation

$DOSE_{tot_{local}} = 0.021241 \frac{mg}{kg_{bw} \cdot d}$

$RDOSE_{drw_{local}} = 13.451066\%$

$RDOSE_{air_{local}} = 39.344367\%$

$RDOSE_{stem_{local}} = 46.782909\%$

$RDOSE_{root_{local}} = 0.159194\%$

$RDOSE_{meat_{local}} = 7.953507 \times 10^{-4}\%$

$RDOSE_{milk_{local}} = 0.014824\%$

$RDOSE_{fish_{local}} = 0.246845\%$

$DOSE_{tot_{regional}} = 5.218583 \times 10^{-6} \frac{mg}{kg_{bw} \cdot d}$

$RDOSE_{drw_{regional}} = 82.124099\%$

$RDOSE_{air_{regional}} = 6.857362\%$

$RDOSE_{stem_{regional}} = 8.19648\%$

$RDOSE_{root_{regional}} = 1.301936\%$

$RDOSE_{meat_{regional}} = 6.638218 \times 10^{-4}\%$

$RDOSE_{milk_{regional}} = 0.012372\%$

$RDOSE_{fish_{regional}} = 1.507087\%$

Appendix 4-3

Indirect exposure via the environment

Scenario IC/UC 2/48

1,000 t/a

definition of the unit 'd' for day	$d := 1 \cdot Tag$ $scenario := 1 .. 2$ $local := 1$ $regional := 2$

Constants

gas - constant R	$R := 8.314 \cdot J \cdot K^{-1} \cdot Mol^{-1}$

Defaults

volumefraction air in plant tissue [-]	$Fair_{plant} := 0.3$
volumefraction water in plant tissue [-]	$Fwater_{plant} := 0.65$
volumefraction lipids in plant tissue [-]	$Flipid_{plant} := 0.01$
bulk density of plant tissue $[kg_{wet\ plant} *m_{plant}^{-3}]$	$RHO_{plant} := 700 \cdot kg \cdot m^{-3}$
leaf surface area $[m^2]$	$AREA_{plant} := 5 \cdot m^2$
conductance (0.001 $m*s^{-1}$) $[m*d^{-1}]$	$g_{plant} := 0.001 \cdot m \cdot s^{-1}$
shoot volume $[m^3]$	$V_{leaf} := 0.002 \cdot m^3$
transpiration stream $[m^3*d^{-1}]$	$Q_{transp} := 1 \cdot 10^{-3} \cdot m^3 \cdot d^{-1}$
correction exponent for differences between plant lipids and octanol [-]	$b := 0.95$
growth rate constant for dilution by growth $[d^{-1}]$	$kgrowth_{plant} := 0.035 \cdot d^{-1}$
pseudo-first order rate constant for metabolism in plants $[d^{-1}]$	$kmetab_{plant} := 0 \cdot d^{-1}$
pseudo-first order rate constant for photolysis in plants $[d^{-1}]$	$kphoto_{plant} := 0 \cdot d^{-1}$

<u>concentration in meat and milk</u>

daily intake of grass $[kg_{wetgrass}*d^{-1}]$	$IC_{grass} := 67.6 \cdot kg \cdot d^{-1}$
daily intake of soil $[kg *d^{-1}]$	$IC_{soil} := 0.46 \cdot kg \cdot d^{-1}$

concentration in meat and milk

daily intake of grass
[$\text{kg}_{\text{wetgrass}}$*$\text{d}^{-1}$]
$$IC_{grass} := 67.6 \cdot kg \cdot d^{-1}$$

daily intake of soil
[$\text{kg}_{\text{wet soil}}$*$\text{d}^{-1}$]
$$IC_{soil} := 0.46 \cdot kg \cdot d^{-1}$$

daily intake of air
[$\text{m}_{\text{air}}{}^{3}$*$\text{d}^{-1}$]
$$IC_{air} := 122 \cdot m^{3} \cdot d^{-1}$$

daily intake of drinkingwater
[l*d^{-1}]
$$IC_{drw} := 55 \cdot l \cdot d^{-1}$$

daily intake for human

daily intake for the several pathways
[kg_{chem}*d^{-1}] or [m^{3}*d^{-1}]

$$IH_{drw} := 2 \cdot l \cdot d^{-1}$$

$$IH_{fish} := 0.115 \cdot kg \cdot d^{-1}$$

$$IH_{stem} := 1.2 \cdot kg \cdot d^{-1}$$

$$IH_{root} := 0.384 \cdot kg \cdot d^{-1}$$

$$IH_{meat} := 0.301 \cdot kg \cdot d^{-1}$$

$$IH_{milk} := 0.561 \cdot kg \cdot d^{-1}$$

$$IH_{air} := 20 \cdot m^{3} \cdot d^{-1}$$

bioavailability through route of intake
[-]
$$BIO_{inh} := 0.75$$
$$BIO_{oral} := 1.0$$

average body weight of human
[kg]
$$BW := 70 \cdot kg_{bw}$$

Name: 2-EEA CAS - No.: 111 – 15 – 9

Input

chemical properties

$\log K_{OW} := 0.24$

octanol-water partitioning coefficient
[-]
$K_{OW} := 10^{\log K_{OW}}$

Henry - partitioning coefficient
[Pa*m^3*mol^{-1}]
$HENRY := 0.16 \cdot Pa \cdot m^3 \cdot Mol^{-1}$

air-water partitioning coefficient
[-]
$K_{air\_water} := 6.4 \cdot 10^{-5}$

fraction of the chemical associated
with aerosol particles
[-]
$F_{ass\_aer} := 3.7 \cdot 10^{-7}$

half-life for biodegration in surface water
[d]
$DT_{50\_bio\_water} := 15 \cdot d$

environmental concentrations

annual average local PEC in surface water (dissolved)
[mg$_{chem}$ * l$_{water}^{-1}$] , (from open use)
$PEClocal_{water\_ann} := 0.694 \cdot mg \cdot l^{-1}$

annual average local PEC in air (total)
[mg$_{chem}$ * m$_{air}^{-3}$] (from open use)
$PEClocal_{air\_ann} := 3.8 \cdot 10^{-3} \cdot mg \cdot m^{-3}$

local PEC in grassland (total), averaged over 180 days
[mg$_{chem}$ * kg$_{soil}^{-1}$]
$PEClocal_{grassland} := 1.01 \cdot 10^{-3} \cdot mg \cdot kg^{-}$

local PEC in porewater of agriculture soil
[mg$_{chem}$ * l$_{porewater}^{-1}$]
$PEClocal_{agr\_soil\_porew} := 1.62 \cdot 10^{-3} \cdot mg \cdot l^{-1}$

local PEC in porewater of grassland
[mg$_{chem}$ * l$_{porewater}^{-1}$]
$PEClocal_{grassland\_porew} := 2.78 \cdot 10^{-3} \cdot mg \cdot l^{-1}$

local PEC in groundwater under agriculture soil
[mg$_{chem}$ * l$_{water}^{-1}$]
$PEClocal_{grw} := 1.62 \cdot 10^{-3} \cdot mg \cdot l^{-1}$

regional PEC in surface water (dissolved)
[mg$_{chem}$ * l$_{water}^{-1}$]
$PECregional_{water} := 3.41 \cdot 10^{-5} \cdot mg \cdot l^{-1}$

regional PEC in air (total)
[mg$_{chem}$ * m$_{air}^{-3}$]
$PECregional_{air} := 3.34 \cdot 10^{-7} \cdot mg \cdot m^{-3}$

regional PEC in agriculture soil (total)
[mg$_{chem}$*kg$_{soil}^{-1}$
$PECregional_{agr\_soil} := 9.50 \cdot 10^{-7} \cdot mg \cdot kg^{-1}$

regional PEC in porewater of agriculture soils
[mg$_{chem}$*l$_{water}^{-1}$
$PECregional_{agr\_soil\_porew} := 2.61 \cdot 10^{-6} \cdot mg \cdot l^{-}$

Definition of the concentrations used for indirect exposure

$C_{water_{local}} := PEClocal_{water\_ann}$

$C_{air_{local}} := PEClocal_{air\_ann}$

$C_{grassland_{local}} := PEClocal_{grassland}$

$C_{agr\_porew_{local}} := PEClocal_{agr\_soil\_porew}$

$C_{grass\_porew_{local}} := PEClocal_{grassland\_porew}$

$C_{grw_{local}} := PEClocal_{grw}$

$C_{water_{regional}} := PECregional_{water}$

$C_{air_{regional}} := PECregional_{air}$

$C_{grassland_{regional}} := PECregional_{agr\_soil}$

$C_{agr\_porew_{regional}} := PECregional_{agr\_soil\_porew}$

$C_{grass\_porew_{regional}} := PECregional_{agr\_soil\_porew}$

$C_{grw_{regional}} := PECregional_{agr\_soil\_porew}$

bioconcentration in fish

bioconcentration factor for fish
$[m_{water}{}^{3} * kg_{chem}{}^{-1}]$

$$BCF_{fish} := 10^{0.85\cdot \log K_{OW}-0.7}\cdot 1\cdot kg^{-1}$$

modified equation for logKow > 6

$$BCF_{fish} := wenn\left[\log K_{OW} > 6, \left(-0.278\cdot \log K_{OW}{}^{2} + 3.38\cdot \log K_{OW} - 5.94\right)\cdot 1\cdot kg^{-1}, BCF_{fish}\right]$$

$$C_{fish_{scenario}} := BCF_{fish}\cdot C_{water_{scenario}}$$

bioconcentration in plants

$$K_{plant\_water} := Fwater_{plant} + Flipid_{plant}\cdot K_{OW}{}^{b}$$

$$Croot_{agr\_plant_{scenario}} := \frac{K_{plant\_water}\cdot C_{agr\_porew_{scenario}}}{RHO_{plant}}$$

$$TSCF := 0.784\cdot e^{\frac{-\left(\log K_{OW}-1.78\right)^{2}}{2.44}}$$

remark: for $\log K_{OW}$ out of the range from -0.5 to 4.5
the TSCF is limited by the values for $\log K_{OW} = -0.5$ resp. 4.5

$$TSCF := wenn\left(\log K_{OW} < -0.5, 0.903, TSCF\right)$$

$$TSCF := wenn\left(\log K_{OW} > 4.5, 0.832, TSCF\right)$$

$$K_{leaf\_air} := Fair_{plant} + \frac{K_{plant\_water}}{K_{air\_water}}$$

$$kelim_{plant} := kmetab_{plant} + kphoto_{plant}$$

$$\alpha := \frac{AREA_{plant}\cdot g_{plant}}{K_{leaf\_air}\cdot V_{leaf}} + kelim_{plant} + kgrowth_{plant}$$

$$\beta_{agr\_plant_{scenario}} := C_{agr\_porew_{scenario}} \cdot TSCF \cdot \frac{Q_{transp}}{V_{leaf}} + \left(1 - F_{ass\_aer}\right) \cdot C_{air_{scenario}} \cdot g_{plant} \cdot \frac{AREA_{plant}}{V_{leaf}}$$

$$C_{leaf\_crops_{scenario}} := \frac{\beta_{agr\_plant_{scenario}}}{\alpha \cdot RHO_{plant}}$$

$$\beta_{grass\_plant_{scenario}} := C_{grass\_porew_{scenario}} \cdot TSCF \cdot \frac{Q_{transp}}{V_{leaf}} + \left(1 - F_{ass\_aer}\right) \cdot C_{air_{scenario}} \cdot g_{plant} \cdot \frac{AREA_{plant}}{V_{leaf}}$$

$$C_{leaf\_grass_{scenario}} := \frac{\beta_{grass\_plant_{scenario}}}{\alpha \cdot RHO_{plant}}$$

purification of drinking water

system may defined dependent from the aerobic biodegradation

$$system := wenn\left(DT_{50\_bio\_water} < 10 \cdot d, 0, 1\right)$$

select a column on dependence from log K_{ow}

$$FIndex := wenn\left(logK_{OW} < 4, 0, wenn\left(logK_{OW} > 5, 2, 1\right)\right)$$

$$Fpur_{logKow} := \begin{pmatrix} 1 & \frac{1}{4} & \frac{1}{16} \\ 1 & \frac{1}{2} & \frac{1}{4} \end{pmatrix}$$

$$Fpur := \frac{Fpur_{logKow_{system, FIndex}}}{wenn\left(HENRY > 100 \cdot Pa \cdot m^3 \cdot Mol^{-1}, 2, 1\right)}$$

$$C_{drw_{scenario}} := wenn\left[C_{grw_{scenario}} > \left(C_{water_{scenario}} \cdot Fpur\right), C_{grw_{scenario}}, C_{water_{scenario}} \cdot Fpur\right]$$

Biotransfer to meat and milk

$$BTF_{meat} := 10^{-7.6 + logK_{OW}} \cdot kg^{-1} \cdot d$$

remark: for logK_{OW} out of the range from 1.5 to 6.5
the BTF $_{meat}$ is limited by the values for logK_{OW} = 1.5 resp. 6.5

$$BTF_{meat} := wenn\left(logK_{OW} < 1.5, 7.943 \cdot 10^{-7} \cdot kg^{-1} \cdot d, BTF_{meat}\right)$$

$$BTF_{meat} := wenn\left(logK_{OW} > 6.5, 0.07943 \cdot kg^{-1} \cdot d, BTF_{meat}\right)$$

$$C_{meat_{scenario}} := BTF_{meat} \cdot \left(C_{leaf\_grass_{scenario}} \cdot IC_{grass} + C_{grassland_{scenario}} \cdot IC_{soil} \ldots + C_{air_{scenario}} \cdot IC_{air} + C_{drw_{scenario}} \cdot IC_{drw}\right)$$

$$BTF_{milk} := 10^{-8.1+\log K_{OW}} \cdot kg^{-1} \cdot d$$

remark: for $\log K_{OW}$ out of the range from 3 to 6.5
the BTF_{milk} is limited by the values for $\log K_{OW}$ = 1.5 resp. 6.5

$$BTF_{milk} := \text{wenn}\left(\log K_{OW} < 3, 7.943 \cdot 10^{-6} \cdot kg^{-1} \cdot d, BTF_{milk}\right)$$

$$BTF_{milk} := \text{wenn}\left(\log K_{OW} > 6.5, 0.02512 \cdot kg^{-1} \cdot d, BTF_{milk}\right)$$

$$C_{milk_{scenario}} := BTF_{milk} \cdot \left(\begin{array}{l} C_{leaf\_grass_{scenario}} \cdot IC_{grass} + C_{grassland_{scenario}} \cdot IC_{soil} \ldots \\ + C_{air_{scenario}} \cdot IC_{air} + C_{drw_{scenario}} \cdot IC_{drw} \end{array}\right)$$

total daily intake for human

daily dose through intake of several pathways

[$kg_{chem}*kg_{bw}^{-1}*d^{-1}$]

$$DOSE_{drw_{scenario}} := \frac{C_{drw_{scenario}} \cdot IH_{drw}}{BW} \qquad DOSE_{air_{scenario}} := \frac{C_{air_{scenario}} \cdot IH_{air} \cdot BIO_{inh}}{BW \cdot BIO_{oral}}$$

$$DOSE_{stem_{scenario}} := \frac{C_{leaf\_crops_{scenario}} \cdot IH_{stem}}{BW} \qquad DOSE_{root_{scenario}} := \frac{Croot_{agr\_plant_{scenario}} \cdot IH_{root}}{BW}$$

$$DOSE_{meat_{scenario}} := \frac{C_{meat_{scenario}} \cdot IH_{meat}}{BW} \qquad DOSE_{milk_{scenario}} := \frac{C_{milk_{scenario}} \cdot IH_{milk}}{BW}$$

$$DOSE_{fish_{scenario}} := \frac{C_{fish_{scenario}} \cdot IH_{fish}}{BW}$$

total daily intake for human

total daily intake for human as sum of each pathway

[$kg_{chem}*kg_{bw}^{-1}*d^{-1}$]

$$DOSE_{tot_{scenario}} := DOSE_{drw_{scenario}} + DOSE_{fish_{scenario}} + DOSE_{stem_{scenario}} + DOSE_{root_{scenario}} \cdots + DOSE_{meat_{scenario}} + DOSE_{milk_{scenario}} + DOSE_{air_{scenario}}$$

relative doses of specific different pathway (%)

$$RDOSE_{drw_{scenario}} := \frac{DOSE_{drw_{scenario}} \cdot 100 \cdot \%}{DOSE_{tot_{scenario}}} \qquad RDOSE_{air_{scenario}} := \frac{DOSE_{air_{scenario}} \cdot 100 \cdot \%}{DOSE_{tot_{scenario}}}$$

$$RDOSE_{stem_{scenario}} := \frac{DOSE_{stem_{scenario}} \cdot 100 \cdot \%}{DOSE_{tot_{scenario}}} \qquad RDOSE_{root_{scenario}} := \frac{DOSE_{root_{scenario}} \cdot 100 \cdot \%}{DOSE_{tot_{scenario}}}$$

$$RDOSE_{meat_{scenario}} := \frac{DOSE_{meat_{scenario}} \cdot 100 \cdot \%}{DOSE_{tot_{scenario}}} \qquad RDOSE_{milk_{scenario}} := \frac{DOSE_{milk_{scenario}} \cdot 100 \cdot \%}{DOSE_{tot_{scenario}}}$$

$$RDOSE_{fish_{scenario}} := \frac{DOSE_{fish_{scenario}} \cdot 100 \cdot \%}{DOSE_{tot_{scenario}}}$$

Results of calculation

$DOSE_{tot_{local}} = 0.021986 \frac{mg}{kg_{bw} \cdot d}$

$RDOSE_{drw_{local}} = 90.185367\%$

$RDOSE_{air_{local}} = 3.703578\%$

$RDOSE_{stem_{local}} = 4.404573\%$

$RDOSE_{root_{local}} = 0.038509\%$

$RDOSE_{meat_{local}} = 6.594965 \times 10^{-4}\%$

$RDOSE_{milk_{local}} = 0.012292\%$

$RDOSE_{fish_{local}} = 1.655023\%$

$DOSE_{tot_{regional}} = 1.163078 \times 10^{-6} \frac{mg}{kg_{bw} \cdot d}$

$RDOSE_{drw_{regional}} = 83.76785\%$

$RDOSE_{air_{regional}} = 6.153621\%$

$RDOSE_{stem_{regional}} = 7.355461\%$

$RDOSE_{root_{regional}} = 1.172817\%$

$RDOSE_{meat_{regional}} = 6.619192 \times 10^{-4}\%$

$RDOSE_{milk_{regional}} = 0.012337\%$

$RDOSE_{fish_{regional}} = 1.537253\%$

Appendix 4-4

Indirect exposure via the environment

Scenario IC/UC 2/48

5000 t/a

INDIRECT EXPOSURE VIA THE ENVIRONMENT

(TGD On New and Existing Chemicals, chapter 2)

Definitions (for the use in this document)

Parameter [Unit]	*Symbol*
definition of the unit 'kg$_{bw}$' for body weight	$kg_{bw} := 1 \cdot kg$
definition of the unit 'd' for day	$d := 1 \cdot Tag$
	$scenario := 1 .. 2$
	$local := 1$ $regional := 2$

Constants

Parameter [Unit]	*Symbol*
gas - constant R	$R := 8.314 \cdot J \cdot K^{-1} \cdot Mol^{-1}$

Defaults

Parameter [Unit]	*Symbol*
volumefraction air in plant tissue [-]	$Fair_{plant} := 0.3$
volumefraction water in plant tissue [-]	$Fwater_{plant} := 0.65$
volumefraction lipids in plant tissue [-]	$Flipid_{plant} := 0.01$
bulk density of plant tissue [kg$_{wet\ plant}$ *m$_{plant}$$^{-3}$]	$RHO_{plant} := 700 \cdot kg \cdot m^{-3}$
leaf surface area [m^2]	$AREA_{plant} := 5 \cdot m^2$
conductance (0.001 m*s^{-1}) [m*d^{-1}]	$g_{plant} := 0.001 \cdot m \cdot s^{-1}$
shoot volume [m^3]	$V_{leaf} := 0.002 \cdot m^3$
transpiration stream [m^3*d^{-1}]	$Q_{transp} := 1 \cdot 10^{-3} \cdot m^3 \cdot d^{-1}$
correction exponent for differences between plant lipids and octanol [-]	$b := 0.95$
growth rate constant for dilution by growth [d^{-1}]	$kgrowth_{plant} := 0.035 \cdot d^{-1}$
pseudo-first order rate constant for metabolism in plants [d^{-1}]	$kmetab_{plant} := 0 \cdot d^{-1}$
pseudo-first order rate constant for photolysis in plants [d^{-1}]	$kphoto_{plant} := 0 \cdot d^{-1}$

concentration in meat and milk

daily intake of grass [$kg_{wetgrass}$*d^{-1}]	$IC_{grass} := 67.6 \cdot kg \cdot d^{-1}$
daily intake of soil [$kg_{wet\ soil}$*d^{-1}]	$IC_{soil} := 0.46 \cdot kg \cdot d^{-1}$
daily intake of air [$m_{air}{}^{3}$*d^{-1}]	$IC_{air} := 122 \cdot m^{3} \cdot d^{-1}$
daily intake of drinkingwater [l*d^{-1}]	$IC_{drw} := 55 \cdot l \cdot d^{-1}$

daily intake for human

daily intake for the several pathways [kg_{chem}*d^{-1}] or [m^{3}*d^{-1}]	$IH_{drw} := 2 \cdot l \cdot d^{-1}$
	$IH_{fish} := 0.115 \cdot kg \cdot d^{-1}$
	$IH_{stem} := 1.2 \cdot kg \cdot d^{-1}$
	$IH_{root} := 0.384 \cdot kg \cdot d^{-1}$
	$IH_{meat} := 0.301 \cdot kg \cdot d^{-1}$
	$IH_{milk} := 0.561 \cdot kg \cdot d^{-1}$
	$IH_{air} := 20 \cdot m^{3} \cdot d^{-1}$

bioavailability through route of intake [-]	$BIO_{inh} := 0.75$
	$BIO_{oral} := 1.0$
average body weight of human [kg]	$BW := 70 \cdot kg_{bw}$

Input

chemical properties

$\log K_{OW} := 0.24$

octanol-water partitioning coefficient
[-]

$K_{OW} := 10^{\log K_{OW}}$

Henry - partitioning coefficient
$[Pa*m^{3}*mol^{-1}]$

$HENRY := 0.16\cdot Pa\cdot m^{3}\cdot Mol^{-1}$

air-water partitioning coefficient
[-]

$K_{air\_water} := 6.4\cdot 10^{-5}$

fraction of the chemical associated
with aerosol particles
[-]

$F_{ass\_aer} := 3.7\cdot 10^{-7}$

half-life for biodegration in surface water
[d]

$DT_{50\_bio\_water} := 15\cdot d$

environmental concentrations

annual average local PEC in surface water (dissolved)
$[mg_{chem} * l_{water}^{-1}]$, (from open use)

$PEClocal_{water\_ann} := 2.8\cdot mg\cdot l^{-1}$

annual average local PEC in air (total)
$[mg_{chem} * m_{air}^{-3}]$ (from open use)

$PEClocal_{air\_ann} := 0.015\cdot mg\cdot m^{-3}$

local PEC in grassland (total), averaged over 180 days
$[mg_{chem} * kg_{soil}^{-1}]$

$PEClocal_{grassland} := 4.05\cdot 10^{-3}\cdot mg\cdot kg^{-}$

local PEC in porewater of agriculture soil
$[mg_{chem} * l_{porewater}^{-1}]$

$PEClocal_{agr\_soil\_porew} := 4.49\cdot 10^{-3}\cdot mg\cdot l^{-1}$

local PEC in porewater of grassland
$[mg_{chem} * l_{porewater}^{-1}]$

$PEClocal_{grassland\_porew} := 1.11\cdot 10^{-2}\cdot mg\cdot l^{-1}$

local PEC in groundwater under agriculture soil
$[mg_{chem} * l_{water}^{-1}]$

$PEClocal_{grw} := 4.49\cdot 10^{-3}\cdot mg\cdot l^{-1}$

regional PEC in surface water (dissolved)
$[mg_{chem} * l_{water}^{-1}]$

$PECregional_{water} := 1.50\cdot 10^{-4}\cdot mg\cdot l^{-1}$

regional PEC in air (total)
$[mg_{chem} * m_{air}^{-3}]$

$PECregional_{air} := 1.67\cdot 10^{-6}\cdot mg\cdot m^{-3}$

regional PEC in agriculture soil (total)
$[mg_{chem}*kg_{soil}^{-1}$

$PECregional_{agr\_soil} := 4.74\cdot 10^{-6}\cdot mg\cdot kg^{-1}$

regional PEC in porewater of agriculture soils
$[mg_{chem}*l_{water}^{-1}$

$PECregional_{agr\_soil\_porew} := 1.30\cdot 10^{-5}\cdot mg\cdot l^{-}$

Definition of the concentrations used for indirect exposure

$$\mathrm{Cwater}_{\mathrm{local}} := \mathrm{PEClocal}_{\mathrm{water\_ann}} \qquad \mathrm{Cwater}_{\mathrm{regional}} := \mathrm{PECregional}_{\mathrm{water}}$$

$$\mathrm{Cair}_{\mathrm{local}} := \mathrm{PEClocal}_{\mathrm{air\_ann}} \qquad \mathrm{Cair}_{\mathrm{regional}} := \mathrm{PECregional}_{\mathrm{air}}$$

$$\mathrm{Cgrassland}_{\mathrm{local}} := \mathrm{PEClocal}_{\mathrm{grassland}} \qquad \mathrm{Cgrassland}_{\mathrm{regional}} := \mathrm{PECregional}_{\mathrm{agr\_soil}}$$

$$\mathrm{Cagr\_porew}_{\mathrm{local}} := \mathrm{PEClocal}_{\mathrm{agr\_soil\_porew}} \qquad \mathrm{Cagr\_porew}_{\mathrm{regional}} := \mathrm{PECregional}_{\mathrm{agr\_soil\_porew}}$$

$$\mathrm{Cgrass\_porew}_{\mathrm{local}} := \mathrm{PEClocal}_{\mathrm{grassland\_porew}} \qquad \mathrm{Cgrass\_porew}_{\mathrm{regional}} := \mathrm{PECregional}_{\mathrm{agr\_soil\_porew}}$$

$$\mathrm{Cgrw}_{\mathrm{local}} := \mathrm{PEClocal}_{\mathrm{grw}} \qquad \mathrm{Cgrw}_{\mathrm{regional}} := \mathrm{PECregional}_{\mathrm{agr\_soil\_porew}}$$

<u>bioconcentration in fish</u>

bioconcentration factor for fish
[$m_{water}{}^{3}$*$kg_{chem}{}^{-1}$]

$$\mathrm{BCF}_{\mathrm{fish}} := 10^{0.85\cdot \log K_{OW}-0.7}\cdot 1\cdot \mathrm{kg}^{-1}$$

modified equation for logKow > 6

$$\mathrm{BCF}_{\mathrm{fish}} := \mathrm{wenn}\left[\log K_{OW} > 6, \left(-0.278\cdot \log K_{OW}{}^{2} + 3.38\cdot \log K_{OW} - 5.94\right)\cdot 1\cdot \mathrm{kg}^{-1}, \mathrm{BCF}_{\mathrm{fish}}\right]$$

$$\mathrm{Cfish}_{\mathrm{scenario}} := \mathrm{BCF}_{\mathrm{fish}}\cdot \mathrm{Cwater}_{\mathrm{scenario}}$$

<u>bioconcentration in plants</u>

$$K_{\mathrm{plant\_water}} := \mathrm{Fwater}_{\mathrm{plant}} + \mathrm{Flipid}_{\mathrm{plant}}\cdot K_{OW}{}^{b}$$

$$\mathrm{Croot}_{\mathrm{agr\_plant}_{\mathrm{scenario}}} := \frac{K_{\mathrm{plant\_water}}\cdot C_{\mathrm{agr\_porew}_{\mathrm{scenario}}}}{\mathrm{RHO}_{\mathrm{plant}}}$$

$$\mathrm{TSCF} := 0.784\cdot e^{\frac{-\left(\log K_{OW}-1.78\right)^{2}}{2.44}}$$

remark: for $\log K_{ow}$ out of the range from -0.5 to 4.5
the TSCF is limited by the values for $\log K_{ow}$ = -0.5 resp. 4.5

$$\mathrm{TSCF} := \mathrm{wenn}\left(\log K_{OW} < -0.5, 0.903, \mathrm{TSCF}\right)$$

$$\mathrm{TSCF} := \mathrm{wenn}\left(\log K_{OW} > 4.5, 0.832, \mathrm{TSCF}\right)$$

$$K_{\mathrm{leaf\_air}} := \mathrm{Fair}_{\mathrm{plant}} + \frac{K_{\mathrm{plant\_water}}}{K_{\mathrm{air\_water}}}$$

$$\mathrm{kelim}_{\mathrm{plant}} := \mathrm{kmetab}_{\mathrm{plant}} + \mathrm{kphoto}_{\mathrm{plant}}$$

$$\alpha := \frac{\mathrm{AREA}_{\mathrm{plant}}\cdot g_{\mathrm{plant}}}{K_{\mathrm{leaf\_air}}\cdot V_{\mathrm{leaf}}} + \mathrm{kelim}_{\mathrm{plant}} + \mathrm{kgrowth}_{\mathrm{plant}}$$

$$\beta_{agr\_plant_{scenario}} := C_{agr\_porew_{scenario}} \cdot TSCF \cdot \frac{Q_{transp}}{V_{leaf}} + \left(1 - F_{ass\_aer}\right) \cdot C_{air_{scenario}} \cdot g_{plant} \cdot \frac{AREA_{plant}}{V_{leaf}}$$

$$C_{leaf\_crops_{scenario}} := \frac{\beta_{agr\_plant_{scenario}}}{\alpha \cdot RHO_{plant}}$$

$$\beta_{grass\_plant_{scenario}} := C_{grass\_porew_{scenario}} \cdot TSCF \cdot \frac{Q_{transp}}{V_{leaf}} + \left(1 - F_{ass\_aer}\right) \cdot C_{air_{scenario}} \cdot g_{plant} \cdot \frac{AREA_{plant}}{V_{leaf}}$$

$$C_{leaf\_grass_{scenario}} := \frac{\beta_{grass\_plant_{scenario}}}{\alpha \cdot RHO_{plant}}$$

<u>purification of drinking water</u>

system may defined dependent from the aerobic biodegradation

$$system := wenn\left(DT_{50\_bio\_water} < 10 \cdot d, 0, 1\right)$$

select a column on dependence from log K_{ow}

$$FIndex := wenn\left(logK_{OW} < 4, 0, wenn\left(logK_{OW} > 5, 2, 1\right)\right)$$

$$Fpur_{logKow} := \begin{pmatrix} 1 & \frac{1}{4} & \frac{1}{16} \\ 1 & \frac{1}{2} & \frac{1}{4} \end{pmatrix}$$

$$Fpur := \frac{Fpur_{logKow_{system, FIndex}}}{wenn\left(HENRY > 100 \cdot Pa \cdot m^3 \cdot Mol^{-1}, 2, 1\right)}$$

$$C_{drw_{scenario}} := wenn\left[C_{grw_{scenario}} > \left(C_{water_{scenario}} \cdot Fpur\right), C_{grw_{scenario}}, C_{water_{scenario}} \cdot Fpur\right]$$

<u>Biotransfer to meat and milk</u>

$$BTF_{meat} := 10^{-7.6 + logK_{OW}} \cdot kg^{-1} \cdot d$$

remark: for logK_{OW} out of the range from 1.5 to 6.5
the BTF $_{meat}$ is limited by the values for logK_{OW} = 1.5 resp. 6.5

$$BTF_{meat} := wenn\left(logK_{OW} < 1.5, 7.943 \cdot 10^{-7} \cdot kg^{-1} \cdot d, BTF_{meat}\right)$$

$$BTF_{meat} := wenn\left(logK_{OW} > 6.5, 0.07943 \cdot kg^{-1} \cdot d, BTF_{meat}\right)$$

$$C_{meat_{scenario}} := BTF_{meat} \cdot \begin{pmatrix} C_{leaf\_grass_{scenario}} \cdot IC_{grass} + C_{grassland_{scenario}} \cdot IC_{soil} \cdots \\ + C_{air_{scenario}} \cdot IC_{air} + C_{drw_{scenario}} \cdot IC_{drw} \end{pmatrix}$$

$$BTF_{milk} := 10^{-8.1+logK_{OW}} \cdot kg^{-1} \cdot d$$

remark: for $logK_{OW}$ out of the range from 3 to 6.5
the BTF $_{milk}$ is limited by the values for $logK_{OW}$ = 1.5 resp. 6.5

$$BTF_{milk} := wenn\left(logK_{OW} < 3, 7.943 \cdot 10^{-6} \cdot kg^{-1} \cdot d, BTF_{milk}\right)$$

$$BTF_{milk} := wenn\left(logK_{OW} > 6.5, 0.02512 \cdot kg^{-1} \cdot d, BTF_{milk}\right)$$

$$C_{milk_{scenario}} := BTF_{milk} \cdot \left(\begin{array}{l} C_{leaf\_grass_{scenario}} \cdot IC_{grass} + C_{grassland_{scenario}} \cdot IC_{soil} \ldots \\ + C_{air_{scenario}} \cdot IC_{air} + C_{drw_{scenario}} \cdot IC_{drw} \end{array}\right)$$

total daily intake for human

daily dose through intake of several pathways
[$kg_{chem}*kg_{bw}^{-1}*d^{-1}$]

$$DOSE_{drw_{scenario}} := \frac{C_{drw_{scenario}} \cdot IH_{drw}}{BW} \qquad DOSE_{air_{scenario}} := \frac{C_{air_{scenario}} \cdot IH_{air} \cdot BIO_{inh}}{BW \cdot BIO_{oral}}$$

$$DOSE_{stem_{scenario}} := \frac{C_{leaf\_crops_{scenario}} \cdot IH_{stem}}{BW} \qquad DOSE_{root_{scenario}} := \frac{Croot_{agr\_plant_{scenario}} \cdot IH_{root}}{BW}$$

$$DOSE_{meat_{scenario}} := \frac{C_{meat_{scenario}} \cdot IH_{meat}}{BW} \qquad DOSE_{milk_{scenario}} := \frac{C_{milk_{scenario}} \cdot IH_{milk}}{BW}$$

$$DOSE_{fish_{scenario}} := \frac{C_{fish_{scenario}} \cdot IH_{fish}}{BW}$$

total daily intake for human

total daily intake for human as sum of each pathway
[$kg_{chem}*kg_{bw}^{-1}*d^{-1}$]

$$DOSE_{tot_{scenario}} := DOSE_{drw_{scenario}} + DOSE_{fish_{scenario}} + DOSE_{stem_{scenario}} + DOSE_{root_{scenario}} \cdots + DOSE_{meat_{scenario}} + DOSE_{milk_{scenario}} + DOSE_{air_{scenario}}$$

relative doses of specific different pathway (%)

$$RDOSE_{drw_{scenario}} := \frac{DOSE_{drw_{scenario}} \cdot 100 \cdot \%}{DOSE_{tot_{scenario}}} \qquad RDOSE_{air_{scenario}} := \frac{DOSE_{air_{scenario}} \cdot 100 \cdot \%}{DOSE_{tot_{scenario}}}$$

$$RDOSE_{stem_{scenario}} := \frac{DOSE_{stem_{scenario}} \cdot 100 \cdot \%}{DOSE_{tot_{scenario}}} \qquad RDOSE_{root_{scenario}} := \frac{DOSE_{root_{scenario}} \cdot 100 \cdot \%}{DOSE_{tot_{scenario}}}$$

$$RDOSE_{meat_{scenario}} := \frac{DOSE_{meat_{scenario}} \cdot 100 \cdot \%}{DOSE_{tot_{scenario}}} \qquad RDOSE_{milk_{scenario}} := \frac{DOSE_{milk_{scenario}} \cdot 100 \cdot \%}{DOSE_{tot_{scenario}}}$$

$$RDOSE_{fish_{scenario}} := \frac{DOSE_{fish_{scenario}} \cdot 100 \cdot \%}{DOSE_{tot_{scenario}}}$$

Results of calculation

$DOSE_{tot_{local}} = 0.08854\frac{mg}{kg_{bw}\cdot d}$

$DOSE_{tot_{regional}} = 5.218583\times 10^{-6}\frac{mg}{kg_{bw}\cdot d}$

$RDOSE_{drw_{local}} = 90.35499\%$

$RDOSE_{drw_{regional}} = 82.124099\%$

$RDOSE_{air_{local}} = 3.630334\%$

$RDOSE_{air_{regional}} = 6.857362\%$

$RDOSE_{stem_{local}} = 4.31709\%$

$RDOSE_{stem_{regional}} = 8.19648\%$

$RDOSE_{root_{local}} = 0.026504\%$

$RDOSE_{root_{regional}} = 1.301936\%$

$RDOSE_{meat_{local}} = 6.592961\times 10^{-4}\%$

$RDOSE_{meat_{regional}} = 6.638218\times 10^{-4}\%$

$RDOSE_{milk_{local}} = 0.012288\%$

$RDOSE_{milk_{regional}} = 0.012372\%$

$RDOSE_{fish_{local}} = 1.658135\%$

$RDOSE_{fish_{regional}} = 1.507087\%$

The report provides the comprehensive risk assessment of the substance 2-ethoxyethyl acetate. 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 human health risk assessment has not been performed because production, import and use of the substance in the EU ceased entirely by 2002. The environmental risk assessment was however performed at a much earlier stage, and in order not to loose the results of this assessment, the current risk assessment report covering the environmental part is published.

The evaluation considers the emissions and the resulting exposure to the environment 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 risk assessment concludes that there are no risks for the environment identified based on the former production and use pattern.