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Priority Assessment of Toxic Substances in the frame of LCA

**Development and application of the multi-media
fate, exposure and effect model USES-LCA**

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Abstract

Up till now, in the calculation of toxicity potentials, fate of an emitted substance was only taken into account by using unrealistic system settings in multi media fate models. Moreover, in most cases a considerable amount of questionable default values are used as inputs in the computation of toxicity potentials. This report outlines the global nested multi media fate model USES-LCA, based on the Uniform System for the Evaluation of Substances 2.0 (USES 2.0), which is used to calculate new toxicity potentials for LCA purposes. Although artificial changes in the system settings are not needed in this model, a number of LCA-specific changes are still necessary in the use of risk assessment models, such as USES 2.0. The most important LCA-specific model changes are (1) the minimisation of the local and regional scale, (2) the change of worst-case input parameters in more realistic values, (3) the switch off of most economic processes that are part of the USES 2.0 model, (4) the use of standard emissions at the continental scale, (5) the aggregation of risk characterisation ratios (RCRs) at the continental and global scale, and (6) the introduction of a reference substance and reference compartments. In addition to the LCA-specific model changes, some general model improvements are introduced, such as the inclusion of transport of a chemical from the troposphere to the stratosphere. Moreover, the model is modified for the modelling of dissociating substances and heavy metals.

The adapted model, called USES-LCA, calculates toxicity potentials for the impact categories human toxicity, aquatic ecotoxicity, sediment ecotoxicity and terrestrial ecotoxicity after initial emission to the compartments air, fresh water, sea water, industrial soil and agricultural soil, respectively. Toxicity potentials are calculated for 181 substances, using empirical substance-specific input data as much as possible. Differences of several orders of magnitude can be found between the new toxicity potentials and toxicity potentials calculated previously. Although both method and input data are improved, still a number of further improvements should be addressed. First, model improvements, such as the inclusion of a groundwater, are needed. Furthermore, a more sophisticated aggregation procedure of RCRs for aquatic and terrestrial ecotoxicity may be used. A discussion is also needed about which toxic impact categories should be distinguished, and whether worst-case safety factors in the derivation of human and ecotoxicological no-effect values need to be replaced by typical estimates. This discussion may lead to further improvements. Finally, it is necessary to compute toxicity potentials for additional substances, and to perform an uncertainty analysis to operationalise data uncertainty in the computation of toxicity potentials.

1. Introduction

Life Cycle Assessment (LCA) is a tool for the assessment of the potential environmental impact of a product system (Heijungs et al., 1992). Not only potential impacts due to the usage of a product, but also production, transportation, maintenance, and waste disposal are considered (viz. its entire life cycle). According to ISO standardisation guidelines, an LCA study can be divided into four steps: goal and scope definition, inventory analysis, impact assessment, and interpretation (ISO, 1997a,b; 1998a,b). In the goal and scope definition, the aim and the subject of an LCA study are determined and a *functional unit* is defined. An example of a functional unit is 'watching 100 hours of television' with, for instance, the aim to compare the environmental impacts of different type of televisions. In the inventory analysis, all extractions of resources and emissions of substances attributable to the studied functional unit are listed. From this list, overall life cycle emissions of specified substances can be identified. In the impact assessment, it is first determined which impact categories have to be considered and which extractions and emissions contribute to which impact categories. Impact categories are environmental problem types like human toxicity or ozone depletion. Next, the magnitude of the potential impact of individual substances within each impact category is determined. This is done by multiplying, for each individual substance specifically, emission data with characterisation factors per impact category. Characterisation factors are substance-specific, quantitative representations of potential impacts and are usually calculated with specific computer models. Thus, within one impact category, characterisation factors are used as weighting factors to determine the relative contribution of a substance to an impact category, and not to determine environmental risks. A characterisation factor is also called 'a potential', such as Human Toxicity Potential (HTP), and Ozone Depletion Potential (ODP). The last (optional) step in the impact assessment is the calculation of an environmental index by aggregation the impact categories with each other. This can be done by attributing weighting factors to the several impact categories. The final step in an LCA study is the interpretation of the results from the previous three steps, to draw conclusions, and to formulate recommendations.

This report concentrates on the calculation of toxicity potentials for LCA purposes. In current product life cycle assessments (LCAs) it is possible to include a full fate and exposure analysis in the assessment of potential human health and ecotoxicological impacts of pollutants. Guinée et al. (1996a) used the multi media fate and exposure model *Uniform System for the Evaluation of Substances 1.0* (USES 1.0), developed by RIVM et al. (1994), for the computation of toxicity potentials. Hertwich et al. (1998) used the CalTOX multimedia fate model, developed by McKone (1993), for the same purpose. Although multi media fate modelling is a potentially powerful tool to compute toxicity potentials, some drawbacks can be identified in the models used up to now. First, these models are originally developed for regional risk assessment purposes allowing import and export of pollutants across their system boundaries. As a consequence of the open character of the system in USES 1.0 and CalTOX, the fate of an emitted substance could not be taken fully into account. Therefore, to prevent substance flows across the system boundaries the open system must be transformed into a closed system by setting wind speed and water flow to an extremely low level in the calculations (Guinée et al., 1996a; Hertwich et al., 1998). This makes these models

less realistic. Furthermore, not all relevant compartments are included in these models. For instance, the sea is omitted. Finally, a considerable amount of questionable default values (e.g. as to degradation rates) are used as inputs in the computation of toxicity potentials by Guinée et al. (1996a). Thus, improvements in the model structure and using substance-specific input data instead of unrealistic defaults may lead to more reliable toxicity potentials.

The artificial change to a closed system and the lacking of relevant compartments in the currently used multi media fate models can be overcome by modelling a larger part of the world. Recently, RIVM et al. (1998) developed the second version of the *Uniform System for the Evaluation of Substances* (USES 2.0) which includes the nested multi media fate model Simplebox 2.0 (Brandes et al., 1996). The model optionally includes a regional scale, a continental scale and a global scale. The major advantage of using USES 2.0 for computing toxicity potentials is that it is not necessary to artificially change system parameters, such as wind speed and water flow, and that the sea compartment is included. However, some changes, related to the use of fate models for LCA purposes, are still needed in USES 2.0.

This report outlines the system settings and adaptations in USES 2.0 needed for the computation of LCA toxicity potentials. Furthermore, it describes the selection of substance-specific input data. Using the adapted model, called USES-LCA, and substance-specific input data, toxicity potentials for 181 substances are calculated and for 12 substances a comparison is made with the toxicity potentials calculated by Guinée et al. (1996a). Finally, this paper discusses the validity of the toxicity potentials calculated with USES-LCA.

2. Multi-media modelling for LCA purposes

2.1 USES 2.0

'USES 2.0 has been developed for quantitative assessment of the risks posed by new and existing chemical substances as well as agricultural and non-agricultural pesticides to man and the environment' (RIVM et al., 1998). USES 2.0 is divided in six modules: (1) an input module for substance-specific data; (2) an emission module; (3) a distribution module; (4) an exposure module; (5) an effects module; and (6) a risk characterisation module.

Basic substance-specific input data, such as solubility, K_{ow} , degradation potential, etc., is required to run USES 2.0. These input data can be entered in the input module. In the emission module, emission factors for various life-cycle stages are taken from a database on the basis of the properties, uses and functions of a substance. Local fate models and the nested¹ multi-media fate model Simplebox 2.0 are part of the distribution module in USES 2.0. In multi-media fate models environmental compartments (air, water, sediment, soil) are modelled as homogeneous and well-mixed boxes, and inter-media transport and transformation are represented by first-order processes. Although these models can produce time-dependent concentrations,

¹ Nested means that chemicals can be transported from one scale to a higher scale and vice versa

most commonly used is steady-state calculation. This is also applied in USES 2.0 (RIVM et al., 1998). Simplebox 2.0 has five spatial scales, which are a regional, a continental and a global scale consisting of three parts, reflecting arctic, moderate and tropic geographic zones of the Northern hemisphere (Figure 1; Brandes et al., 1996). The regional and continental scales each consist of six compartments: air, fresh water, seawater, natural soil, agricultural soil, and industrial soil. All three climate zones of the global scale consist each of three compartments: air, (sea)water, and soil. Because the global scale is modelled as a closed system without transport across the system boundaries, emitted substances cannot 'leave' the system as was the case in USES 1.0. Furthermore, in USES 2.0 temperature dependence of chemical properties as vapour pressure, solubility, Henry's Law constant and biodegradation rates can be taken into account. Moreover, the soil depth, which is set equal to the chemical penetration depth in the model, of natural, agricultural and industrially/urban used soil can be related to the properties of the chemical under consideration at the regional and the continental scale. In addition, both a fresh water and a sea water compartment are separately implemented at the regional and continental scale; (Brandes et al., 1996; RIVM et al., 1998). Other more detailed differences between USES 1.0 and USES 2.0 in both model structure and default values can be found in RIVM et al. (1998).

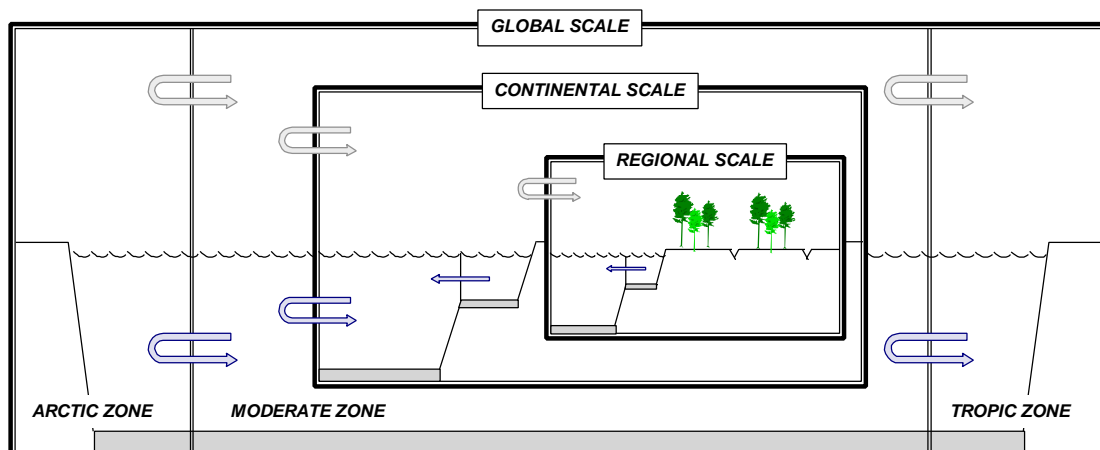


Figure 1: Schematic representation of SimpleBox 2.0 (Brandes *et al.*, 1996).

Human exposure through the environment and secondary poisoning of predating birds and mammals is estimated on the basis of predicted environmental concentrations (PECs) on the regional and/or the local scale. Workplace exposure and consumer exposure can also be estimated in the exposure assessment module. In the effects assessment module, a Predicted No-Effect Concentration (PNEC) is calculated for aquatic ecosystems, terrestrial ecosystems, sediment ecosystems, fish-eating predators, worm-eating predators, and micro-organisms in sewage treatment plants. A PNEC is preferably derived from ecotoxicological data and is considered to be that concentration below which an unacceptable effect is unlikely to occur. If no toxicity data for soil and/or sediment organisms are available, a PNEC for soil and sediment are calculated from the aquatic PNEC, using the equilibrium-partitioning method. In human toxicological effects assessment, a 'No-Observed-Adverse-Effect' Level (NOAEL) or 'Lowest-Observed-Adverse-Effect' Level (LOAEL) for inhalation and oral intake are derived from available data. If either an oral or inhalatory N(L)OAEL for a substance is not available, route-to-route extrapolation on the basis of absorption

rates or acute toxicity for inhalation and oral uptake may be performed. Finally, the outcomes of the exposure assessment and the effects assessment modules are integrated into a Risk Characterisation Ratio (RCR) for each of the seven above-mentioned protection targets on the local and/or the regional scale. In an RCR, the exposure level of a substance due to an emission is compared to the substance-specific PNEC or N(L)OAEL. These RCRs are indicators for the likelihood of adverse effects occurring.

2.2 Adaptations in USES 2.0

Because changes in the model structure of USES 2.0 are not possible in the current model environment, the complete model is programmed in the spreadsheet program Microsoft Excel© 7.0 (Microsoft, 1995). General changes in the model structure are described in section 2.2.1 and LCA-specific changes in section 2.2.2.

2.2.1 General adaptations

Fate analysis

In USES 2.0 temperature dependency of OH-radical reaction rates can not be taken into account. In USES-LCA, however, this option has been added and temperature dependent OH-radical reaction rates of 14 substances, based on information in Atkinson (1986) and Brubaker & Hites (1997), have been taken into account. Furthermore, a chemical-specific penetration depth in the soil is taken into account in the USES-LCA calculations. In USES 2.0 it is possible to use a chemical-specific penetration depth on the regional and continental scale. In USES-LCA this option is extended to the three global scales. Moreover, transport of a chemical from the troposphere to the stratosphere is included in USES-LCA. A tropospheric residence time of 60 years for transport to the stratosphere is assumed (D. Mackay, pers. comm.). This means that every year 1/60th of the volume of the air in the troposphere advects to the stratosphere. It also appeared that some default system parameters are incorrect in USES 2.0 (→ Table 1; Jager & Hamers, 1997; H. den Hollander, pers. comm.).

Table 1: Changes in system parameters in USES 2.0

Parameter	Unit	USES 2.0	USES-LCA
Arctic system area ^a	km ²	2.55·10 ⁷	4.25·10 ⁷
Moderate system area ^b	km ²	3.89·10 ⁷	7.78·10 ⁷
Tropical system area ^c	km ²	8.93·10 ⁷	1.28·10 ⁸
Volume fraction of fat in plant roots	m ³ .m ⁻³	0.01	0.005
Volume fraction of water in plant roots	m ³ .m ⁻³	0.65	0.93
Bulk density of plant root tissue	kg _{wwt} .m ⁻³	700	1000
Bulk density of plant leaf tissue	kg _{wwt} .m ⁻³	700	800

^a the area of the arctic scale is defined as the area between 60° and 90° NL, excluding Norway, Sweden and Finland; ^b the area of the moderate scale is defined as the area between 30° and 60° NL, excluding the area of the continental scale; ^c the tropical scale is defined as the area between 0° and 30° NL

Another adaptation in the fate part of USES 2.0 is that pH-dependency of some substance-specific characteristics is taken into account in the model calculations. This is important for (1) the solubility and organic carbon-water partition coefficient (K_{oc}) of dissociating substances, such as chlorophenols, and (2) hydrolysis rates in water, soil and sediments (see also Section 2.3). A typical pH value per environmental compartment must be defined (\rightarrow Table 2).

Table 2: Assumed pH for respectively water, soil, sediment, and rain water

Compartment	pH
fresh water [C]	7
sea water [C, M, A, T]	8
fresh water sediment [C]	7
sea water sediment [C, M, A, T]	8
natural soil [C]	6
agricultural soil [C]	7
industrial soil [C]	6
soil [M, A, T]	7
rainwater [C, M, A, T]	6

C = Continent; M = Moderate scale; A = Arctic scale; T = Tropical scale.

Solubility and K_{oc} of dissociating substances is estimated at the pH of every compartment separately, following the calculation procedure suggested by Shiu et al. (1994):

$$X_{N(x,m)} = \frac{1}{1 + 10^{pH(m) - pKa(x)}} \quad (1)$$

$$SOL_{T(x,m)} = \frac{SOL_{N(x)}}{X_{N(x,m)}} \quad (2)$$

$$Koc_{T(x,m)} = \frac{1.26 \times Kow_{N(x)}^{0.81}}{1000} \times X_{N(x,m)} \quad (3)$$

where,

- $X_{N(x,m)}$ = non-ionic fraction of substance x in compartment m (-)
- $pH(m)$ = pH in compartment m (-)
- $pKa(x)$ = dissociation constant of substance x (-)
- $SOL_{T(x,m)}$ = solubility of the ionic and neutral species of substance x in compartment m ($mg.l^{-1}$)
- $SOL_{N(x)}$ = solubility of the neutral species of substance x ($mg.l^{-1}$)
- $Koc_{T(x,m)}$ = organic carbon-water partition coefficient of the ionic and neutral species of substance x in compartment m ($m^3.kg^{-1}$)
- $Kow_{N(x)}$ = octanol-water partition coefficient of the neutral species of substance x (dimensionless)

The correction of K_{oc} -values for acid dissociation is, however, only appropriate, if the dissociated fraction does not exceed approximately 80%. If the dissociated fraction exceeds the 80%, the adsorption is dominated by characteristics of the dissociated molecule and calculation of pH-dependent K_{oc} -values may lead to a severe underestimation (1-2 orders of magnitude) of adsorption compared to experimental

data (Bockting et al., 1993). Therefore, equation 16 is only used for estimating the $K_{ocT(x,m)}$ if no experimental data are available and if the the non-ionic fraction does not exceed 80% at an environmental pH of 6 and 7.²

Human exposure assessment

USES 2.0 does not cover all potential relevant exposure and uptake routes in the human exposure assessment. For instance, chemical uptake via direct ingestion of soil particles is disregarded, although this route may be an important human exposure route for metals and persistent organic substances present in the soil (Mennes et al., 1998). This may lead to an underestimation of human uptake of these substances. Therefore, soil ingestion is included in the human exposure assessment (→ Section 3.1).

For dissociating substances the estimation of chemical uptake by plants, needed in the human exposure assessment, must be changed in the model calculations, because the model equations are only suitable for non-dissociating organic substances (RIVM et al., 1998). Briggs et al. (1987) give some guidance in estimating the uptake by roots and translocation to shoots of dissociating substances. Their results indicate that entry of these substances into plant tissue is primarily caused by diffusion of the undissociated form, which permeates membranes much more rapidly than their anions. Once inside the cell, dissociation occurs and the anions are unable to diffuse out, leading to accumulation inside the cells when the pH of the surrounding environment is less than that of the protoplasm. The magnitude of the accumulation of dissociating substances into plant tissue can be predicted using a form of the so-called ion-trap equation (see Briggs et al., 1987). There are, however, two problems with the use of the ion-trap equation. First, the permeability ratio of a substance must be known which is not the case for most substances. Furthermore, the ion trap equation does not estimate root concentrations very well for an environmental pH of 7, which is assumed to be the case in agricultural soils. Here, a practical solution is adopted. The results of Briggs et al. (1987) indicate that at an environmental pH of 7, the Root Concentration Factor (RCF) of the investigated acids lay close together (between 0.5 and 0.9 l.kg(wwt)^{-1})³. The same is the case for the Transpiration Stream Concentration Factor (TSCF) (between 0.02-0.05 l.l^{-1}). As a first approximation, a typical RCF of 0.7 l.kg(wwt)^{-1} and a typical TSCF of 0.04 l.l^{-1} is used in the calculations for dissociating substances. However, for the chlorophenols, included in this assessment, the dissociated fraction is not very large at an environmental pH of 7 (typically < 0.2). Therefore, it is chosen to use the USES 2.0 default estimation formulas for uptake in plants for these substances.

² Equation 16 can be used at an environmental pH of 6, if the pKa-value of the substance is larger than 5.4; at an environmental pH of 7, the pKa value must be larger than 6.4

³ 4-(2,4-dichlorophenoxy) phenoxyacetic acid is the only substance which has a larger root concentration factor than 0.9 l.kg(wwt)^{-1} at an environmental pH of 7 (RCF=4.8). This may be explained by the fact that the measured Kow (12.6) at pH=7 is much larger than the expected Kow (0.08) based on the calculation procedure of Shiu et al. (1994)

2.2.2 LCA-specific adaptations

Worst-case estimates

Some system parameters are set to worst-case values in USES 2.0. Worst-case values may be appropriate for initial risk assessment purposes, their use in LCA is, however, debatable. Because LCA is not directly concerned with unacceptable environmental risks, there is no reason for the use of extreme values. Therefore, extreme values are replaced by 'reasonable' estimates. In USES 2.0 a worst-case approach is followed for the computation of chemical concentrations in drinking water. The highest concentration of the chemical in surface water after purification and groundwater without purification is taken as the drinking water concentration used in the indirect exposure assessment. In this assessment chemical concentrations in drinking water on the continental scale are calculated, using both surface water concentrations after purification and groundwater concentrations in a ratio of 4:6 (Thissen, 1999).⁴ On the global scales it is assumed that drinking water is solely produced with ground water as no fresh surface water is modelled on the global scales. Another worst-case approach is found in the estimation of purification factors for drinking water. In USES 2.0 purification factors for drinking water are conservatively estimated, based on the properties of the substance under consideration. According to Jager et al. (1997), it may be more realistic to use an overall purification factor of dissolved organic substances, because the substance-dependent derivation of purification factors is based on a limited dataset of 8 organic compounds, and the physico-chemical properties have only a limited predictive ability. Jager et al. (1997) derived a median purification factor of 0.15 for organic substances, which means that it is expected that 85% of the dissolved concentration of an organic substance is removed from the surface water during drinking water purification processes. This factor is used in the assessment for all organic substances. No information was found for removal percentages of dissolved metals. As a first approximation, the median purification factor of organic substances is also used for dissolved metals. Thirdly, the worst-case human exposure scenario in USES 2.0 is altered in a 'more reasonable' exposure estimates (→ Section 3.1). Finally, if the equilibrium partitioning method is used to derive the soil and sediment MPCs for organic chemicals and the octanol-water partitioning coefficient is larger than $1 \cdot 10^5$, USES 2.0 increases the predicted environmental concentration in the soil by a factor of 10 in the calculation of the RCR_{soil} to account for chemical uptake via ingestion of soil and sediment by organisms (RIVM et al., 1998). However, an increase with a factor 2 seems to be more realistic (Belfroid et al., 1996; T. Jager, pers. comm.). Increase with a factor 2 is also applied for metals, if the the no-effect parameter for metals is derived with the equilibrium partitioning method and if the K_p -values for soil and sediment are larger than 300 l.kg^{-1} and 700 l.kg^{-1} , respectively.⁵

⁴ The ratio surface water: ground water of 4:6 is derived from the 1995 water supply information of all the European Union member states, except Finland, Greece and Ireland. No water supply information were found for these three countries

⁵ Calculation of the soil K_p -value of a substance with a Kow of $1 \cdot 10^5$ results in $\pm 300 \text{ l.kg}^{-1}$, while the sediment K_p -value becomes $\pm 700 \text{ l.kg}^{-1}$ in USES-LCA

Environmental system

In this study the local and regional scale are not taken into account in the model calculations.⁶ In current life cycle inventories emissions are summed up per pollutant type regardless of the spatial context of these emissions which results in an inventory outcome lacking any retrievable relation with a particular region. As a consequence, the local and regional scale in USES 2.0 are not appropriate to use in the computation of toxicity potentials. The continental scale is defined here as the Western part of Europe.⁷ Furthermore, in contrast to the model settings for USES 1.0 in Guinée et al. (1996a), (1) wind speed and (2) water flow are not minimised in USES-LCA, because the fate model is already a closed system. As pointed out before, these changes were implemented in USES 1.0 to prevent pollutant flows across the model system boundaries.

Economic system

In LCA there is a strict distinction between economic processes which should all be taken into account in the inventory analysis and the impact assessment in which the potential impact of these emissions is estimated. Waste water treatment and pesticide application in the agricultural sector, which are both part of USES 2.0, are considered as economic processes and should therefore be dealt with in the inventory analysis (Guinée et al., 1996a). As a consequence, these processes are switched off in the computation of toxicity potentials. For the purification of drinking water an exception is made. In practice, this process is not taken into account in the inventory analysis, while the impact of drinking water purification on indirect human exposure to pollutants may be substantial (Guinée et al., 1996a). Therefore, drinking water purification is taken into account in the computation of toxicity potentials.

Another change in the economic part of the model is that the release of the chemical must be specified in terms fit the LCA methodology (Guinée et al., 1996a). The built-in emission estimation procedures of USES 2.0 are not used, but standard emissions ($1 \cdot 10^6 \text{ kg} \cdot \text{day}^{-1}$) to the different environmental compartments are implemented at the continental scale. Separate calculations are performed for standard releases to air, sea water, fresh water, industrial soil and agricultural soil. By using standard emissions at the continental scale in the computation of toxicity potentials, it is implicitly assumed that the accumulated emissions related to the complete life cycle of a product system, i.e. the outcome of a life cycle inventory, (1) take all place in Western Europe and (2) are uniformly distributed over the initial emission compartment.

Human effects assessment

No extrapolation of NOAELs or LOAELs for mammals to oral and inhalatory Human Limit Values (HLVs) is performed in the human effects assessment of USES 2.0. Furthermore, in USES 2.0 an effects assessment of genotoxic and (possibly) carcinogenic chemicals can not be performed. Using HLVs for all substances is, however, a prerequisite for an equal comparison between substances. Therefore, it is chosen to use chronic HLVs as published by the Health Council of the Netherlands,

⁶ This is done by leaving out the local scale and using a very small surface area ($1 \cdot 10^{-50} \text{ km}^2$) for the regional scale

⁷ Austria, Belgium, Luxembourg, Denmark, Finland, France, Germany, Greece, Ireland, Italy, the Netherlands, Norway, Portugal, Spain, Sweden, Switzerland and United Kingdom are considered to be part of Western Europe (land: $3.53 \cdot 10^6 \text{ km}^2$; surface water: $5.4 \cdot 10^4 \text{ km}^2$; sea: $3.58 \cdot 10^6 \text{ km}^2$)

WHO, RIVM, USEPA and others (→ Section 3.2, effects assessment). Every type of impact that firstly occurs, is used in the derivation of HLVs. For substances which are genotoxic or (possibly) carcinogenic by a genotoxic mechanism of action the human intake value corresponding with an extra life-time risk of 1.10^{-6} is used. This dose is sometimes referred to as the virtually safe dose (VSD; Food Safety Council, 1980; Chen & Gaylor, 1987; Crump & Howe, 1985) or as the risk-specific dose (RSD; Krewski et al., 1990).

Risk Characterisation Ratios

RCRs are calculated by dividing the estimated exposure level after substance release with a no-effect parameter of that particular substance. Although USES 2.0 gives the possibility to assess the potential impact for various impact categories, this research focuses on human toxicity, aquatic ecotoxicity, terrestrial ecotoxicity and sediment ecotoxicity. Micro-organisms in waste water plants are not considered to be part of the environment and are therefore not an impact category in LCA. Calculation of toxicity potentials for fish-eating predators and worm-eating predators are out of the scope of the assessment, although toxicity potentials for these impact categories may be very useful for LCA purposes (→ Section 5).

The RCRs for humans are calculated by

$$RCR_{human, x, s, e} = \sum_{r=1}^{r=n} \frac{PDI_{r, x, s, e}}{HLV_{r, x}} \quad (4)$$

- $RCR_{human, x, s, e}$ = Risk Characterisation Ratio of substance x for humans at geographical scale s after emission to compartment e (-)
 $PDI_{r, x, s, e}$ = Predicted Daily Intake via exposure route r of substance x for humans at geographical scale s after emission to compartment e ($kg \cdot kg \text{ bwt}^{-1} \cdot \text{day}^{-1}$)
 $HLV_{r, x}$ = Human Limit Value for exposure route r of substance x ($kg \cdot kg \text{ bwt}^{-1} \cdot \text{day}^{-1}$)

An exception is made for the inorganic substances nitrogen dioxide (NO₂), sulphur dioxide (SO₂), ammonia (NH₃), hydrogen sulphide (H₂S), hydrogen chloride (HCl) and primary fine particulate matter (PM10). Because USES 2.0 can not be used to calculate concentrations in other compartments than air for these substances, only inhalatory exposure is taken into account in the calculation of human RCRs.

For the aquatic, terrestrial and sediment ecosystems the RCR is calculated by

$$RCR_{x, c, e} = \frac{PEC_{x, c, e}}{PNEC_{x, c}} \quad (5)$$

- $RCR_{x, c, e}$ = Risk Characterisation Ratio of substance x for aquatic, terrestrial or sediment compartment c after emission to compartment e (-)
 $PEC_{x, c, e}$ = Predicted Environmental Concentration of substance x for aquatic, terrestrial or sediment compartment c after emission to compartment e ($kg \cdot m^{-3}$)
 $PNEC_{x, c}$ = Predicted No-Effect Concentration of substance x for aquatic, terrestrial or sediment compartment c ($kg \cdot m^{-3}$)

As stated before, USES 2.0 gives the possibility to compute RCRs for human toxicity,

aquatic ecotoxicity, terrestrial ecotoxicity and sediment ecotoxicity on a local and regional scale. However, these scales are not taken into account in the computation of toxicity potentials. As a logic consequence of earlier choices, RCRs must be computed on the continental scale, and the three global scales for every impact category. As a result, four RCRs for human toxicity, five RCRs for aquatic ecotoxicity, six RCRs for terrestrial ecotoxicity, and five RCRs for sediment ecotoxicity are computed per initial emission compartment. But one is still left with the problem that several RCRs are computed for the same impact category. Here, it is decided to define the following six impact categories: (1) human toxicity, (2) terrestrial ecotoxicity, (3) fresh water ecotoxicity, (4) sea water ecotoxicity, (5) fresh water sediment ecotoxicity, and (6) sea sediment ecotoxicity related to the salt water compartment. Computation of one toxicity potential per initial emission compartment for the six impact categories, respectively, can only take place by aggregation of RCRs for the different environmental scales. The proposed aggregation procedures per impact category are described below.

For sea water ecotoxicity it is proposed to aggregate the RCRs on the basis of their volumes. For sea sediment ecotoxicity and terrestrial ecotoxicity it is proposed to aggregate the RCRs on the basis of their total mass. The larger a compartment, the linearly more important the predicted RCR for that compartment is assumed. For human beings it is chosen to aggregate the human RCRs for the continental, the moderate, tropic and arctic scale on the basis of population figures. The larger the exposed population, the larger the importance of the human RCR related to that particular scale. The aggregated RCRs are called "weighted RCRs" and the general formula to calculate them is

$$\text{Weighted RCR}_{i,x,e} = \sum_{c/s=1}^{c/s=n} \text{RCR}_{i,x,e,c/s} \times W_{i,c/s} \quad (6)$$

Weighted $\text{RCR}_{i, x, e}$ = Weighted Risk Characterisation Ratio of impact category i for substance x after emission to compartment e (-, m^3 or $\text{kg}(\text{wwt})$)
 $\text{RCR}_{i, x, e, c/s}$ = Risk Characterisation Ratio of impact category i for substance x at compartment c or geographical scale s after emission to compartment e (-)
 $W_{i, c/s}$ = Impact-specific weighting factor of compartment c or scale s (-, m^3 or $\text{kg}(\text{wwt})$)

Table 4 lists the total volumes of the four sea water compartments, the total weights of the six soil and four sea sediment compartments, and population figures for the four geographical scales in USES-LCA.

Reference substance

Guinée et al. (1996a) give an extensive overview of a range of options to overcome the difference between the emission flux necessary to implement in a multi media fate model and the artificial emission pulse as outcome of the life cycle inventory. They proposed to use the reference substance 1,4-dichlorobenzene (1,4-DCB) which follows the established use of carbon dioxide (CO_2), ethylene (C_2H_4), and chlorofluorocarbon (CFC11) for evaluating global warming, photochemical ozone formation and stratospheric ozone depletion, respectively. The reference substance approach is also used in this analysis. Table 5 lists the reference substance and reference compartment per impact category. Toxicity potentials are calculated by dividing the aggregated

RCRs of a substance after emission to a certain compartment with the aggregated RCRs of the reference substance after emission to the specific reference compartment (→ Section 2.3).

Table 4: Weighting factors for aggregation of the RCRs on different geographical scales per impact category

Impact category	Humans ^a	Sea water ecosystems ^b	Terrestrial ecosystems ^{b, c}	Sea sediment ecosystems ^b
Weighting factor	number	m ³	kg (wwt)	kg (wwt)
Continental				
- humans	3.67·10 ⁸			
- sea water		7.16·10 ¹⁴		
- natural soil			1.83·10 ¹⁴	
- agricultural soil			3.29·10 ¹⁴	
- industrial soil			3.04·10 ¹³	
- sea water sediment				1.4·10 ¹⁴
Moderate				
humans	2.12·10 ⁹			
water		3.89·10 ¹⁶		
soil			3.31·10 ¹⁵	
sediment				1.52·10 ¹⁵
Tropical				
humans	2.29·10 ⁹			
water		8.93·10 ¹⁶		
soil			3.25·10 ¹⁵	
sediment				3.48·10 ¹⁵
Arctic				
humans	9.91·10 ⁷			
water		2.55·10 ¹⁶		
soil			1.75·10 ¹⁵	
sediment				9.95·10 ¹⁴

^a Anonymous, 1997; ^b RIVM et al. (1998); ^c these are the weighting factors for terrestrial ecosystems using the default soil depth settings in USES-LCA. The weighting factor of a soil compartment will increase, when the chemical dependent penetration depth is larger than the default soil depth.

Table 5: Reference substance and reference compartment for the three impact categories, respectively

Impact category	Reference substance	Reference emission compartment
Humans	1,4-dichlorobenzene (1,4-DCB)	continental air
Fresh water ecosystems	1,4-dichlorobenzene (1,4-DCB)	continental sea water
Seawater ecosystems	1,4-dichlorobenzene (1,4-DCB)	continental fresh water
Fresh water sediment ecosystems	1,4-dichlorobenzene (1,4-DCB)	continental sea water
Sea sediment ecosystems	1,4-dichlorobenzene (1,4-DCB)	continental fresh water
Terrestrial ecosystems	1,4-dichlorobenzene (1,4-DCB)	continental industrial soil

2.3 Toxicity potentials

As stated above, toxicity potentials are calculated for fresh water ecosystems, sea water ecosystems, terrestrial ecosystems, fresh water sediment ecosystems, sea sediment ecosystems and humans. For every substance a fresh water Aquatic EcoToxicity Potential ($AETP_{fresh}$), a salt water Aquatic EcoToxicity Potential ($AETP_{salt}$), a Terrestrial Ecotoxicity Potential (TETP), a fresh water Sediment EcoToxicity Potential ($SETP_{fresh}$), a salt water Sediment EcoToxicity Potential ($SETP_{salt}$) and a Human Toxicity Potential (HTP) is calculated for the initial continental emission compartments air, fresh water, sea water, industrial soil and agricultural soil, resulting in 30 toxicity potentials per substance.

The $AETP_{fresh}$ is calculated with the equation

$$AETP_{fresh, x, i} = \frac{RCR_{freshw, x, i}}{RCR_{freshw, 1, 4DCB, fw}} \quad (7)$$

- $AETP_{fresh, x, i}$ = the fresh water aquatic ecotoxicity potential for substance x released to compartment i (1,4-DCB equivalents);
 $RCR_{freshw, x, i}$ = the fresh water risk characterisation ratio of substance x after release to compartment i (-);
 $RCR_{freshw, 1, 4DCB, fr}$ = the fresh water risk characterisation ratio of reference substance 1,4-DCB after release to the continental fresh water compartment (-).

The $AETP_{salt}$ is calculated with the equation

$$AETP_{salt, x, i} = \frac{\text{Weighted } RCR_{saltw, x, i}}{\text{Weighted } RCR_{saltw, 1, 4DCB, sea}} \quad (8)$$

- $AETP_{salt, x, i}$ = the sea water aquatic ecotoxicity potential for substance x released to compartment i (1,4-DCB equivalents);
 $\text{Weighted } RCR_{saltw, x, i}$ = the weighted sea water aquatic risk characterisation ratio of substance x after release to compartment i (-);
 $\text{Weighted } RCR_{saltw, 1, 4DCB, sea}$ = the weighted sea water aquatic risk characterisation ratio of reference substance 1,4-DCB after release to the continental sea water compartment (-).

The $SETP_{fresh}$ is calculated with the equation

$$SETP_{fresh, x, i} = \frac{RCR_{f sed, x, i}}{RCR_{f sed, 1, 4DCB, fw}} \quad (9)$$

- $SETP_{fresh, x, i}$ = the fresh water sediment ecotoxicity potential for substance x released to compartment i (1,4-DCB equivalents);
 $RCR_{f sed, x, i}$ = the fresh water sediment risk characterisation ratio of substance x after release to compartment i (-);
 $RCR_{f sed, 1, 4DCB, fw}$ = the fresh water sediment risk characterisation ratio of reference substance 1,4-DCB after release to the continental fresh water compartment (-).

The $SETP_{salt}$ is calculated with the equation

$$SETP_{salt, x, i} = \frac{\text{Weighted } RCR_{ssed, x, i}}{\text{Weighted } RCR_{ssed, 1, 4DCB, sea}} \quad (10)$$

$SETP_{x,i}$ = the sea water sediment ecotoxicity potential for substance x released to compartment i (1,4-DCB equivalents);
 Weighted $RCR_{ssed,x,i}$ = the weighted sea water sediment risk characterisation ratio of substance x after release to compartment i (-);
 Weighted $RCR_{ssed,1,4DCB,sea}$ = the weighted sea water sediment risk characterisation ratio of reference substance 1,4-DCB after release to the continental sea water compartment (-).

The TETP is calculated with the equation

$$TETP_{x,i} = \frac{\text{Weighted RCR}_{\text{terr}, x, i}}{\text{Weighted RCR}_{\text{terr}, 1,4\text{DCB}, \text{is}}} \quad (11)$$

- $TETP_{x,i}$ = the terrestrial ecotoxicity potential for substance x released to compartment i (1,4-DCB equivalents);
- Weighted $\text{RCR}_{\text{terr}, x, i}$ = the weighted terrestrial risk characterisation ratio of substance x after release to compartment i (-);
- Weighted $\text{RCR}_{\text{terr}, 1,4\text{DCB}, \text{is}}$ = the weighted terrestrial risk characterisation ratio of reference substance 1,4-DCB after release to the continental industrial soil compartment (-).

The human toxicity potential (HTP) is calculated with the equation

$$HTP_{x,i} = \frac{\text{Weighted RCR}_{\text{human}, x, i}}{\text{Weighted RCR}_{\text{human}, 1,4\text{DCB}, \text{air}}} \quad (12)$$

- $HTP_{x,i}$ = the human toxicity potential for substance x released to compartment i (1,4-DCB equivalents);
- Weighted $\text{RCR}_{\text{human}, x, i}$ = the weighted human risk characterisation ratio of substance x after release to compartment i (-);
- Weighted $\text{RCR}_{\text{human}, 1,4\text{DCB}, \text{air}}$ = the weighted human risk characterisation ratio of reference substance 1,4-DCB after release to the continental air compartment (-).

2.4 Application of toxicity potentials in LCAs

The use of toxicity potentials in current LCAs is relatively straightforward. Scores for the impact categories aquatic ecotoxicity, terrestrial ecotoxicity, sediment ecotoxicity and human toxicity can be calculated with the following formulas:

$$I_{fwa} = \sum_{i=1}^{i=m} \sum_{x=1}^{x=n} AETP_{\text{fresh}, x, i} \times E_{x, i} \quad (13)$$

$$I_{swa} = \sum_{i=1}^{i=m} \sum_{x=1}^{x=n} AETP_{\text{salt}, x, i} \times E_{x, i} \quad (14)$$

$$I_{fws} = \sum \sum SETP_{\text{fresh}, x, i} \times E_{x, i} \quad (15)$$

$$I_{sws} = \sum \sum SETP_{\text{salt}, x, i} \times E_{x, i} \quad (16)$$

$$I_t = \sum_{i=1}^{i=m} \sum_{x=1}^{x=n} TETP_{x, i} \times E_{x, i} \quad (17)$$

$$I_h = \sum_{i=1}^{i=m} \sum_{x=1}^{x=n} HTP_{x,i} \times E_{x,i} \quad (18)$$

where I_{fwa} , I_{swa} , I_{fws} , I_{sws} , I_t , and I_h are the impact scores for fresh water aquatic ecotoxicity, salt water aquatic ecotoxicity, fresh water sediment ecotoxicity, salt water sediment ecotoxicity, terrestrial ecotoxicity, and human toxicity (kg)⁸, respectively, and $E_{x,i}$ is the emission of substance x to compartment i (kg).

3 Input data

3.1 Substance-independent input data

Default values in USES 2.0 for environmental parameters, such as wind speed and soil properties, are used in the calculation of toxicity potentials, except for the changes listed in Section 2.2. These default values can be found in Appendix A.

A problem arises concerning the choice of appropriate human characteristics in the human exposure assessment. Human characteristics, such as food intake values, reflect worst-case assumptions in the human exposure assessment of USES 2.0. A worst-case exposure scenario is implemented by taking the highest country-averaged lifetime-averaged intake rate of each food category in the European Union (RIVM et al., 1998). Furthermore, lifetime-averaged intake rates of drinking water and air are set to high levels. As argued before, worst-case scenarios are in principle less suitable for LCA purposes. Therefore, it is chosen to use average intake rates in the calculation of human toxicity potentials (→ Table 6). One must, however, keep in mind that human characteristics are inherently variable. This means that other choices of human characteristics, related to the choice which part of the human population should be ultimately protected, may also be defensible.

Table 6: Human characteristics in USES-LCA

Parameter	Unit	USES 2.0	USES-LCA	Source
Daily intake of drinking water	l.d ⁻¹	2	1.4	1, 2
Daily intake of fish ^a	kg _{wwt} .d ⁻¹	0.115	0.03	1, 3
Daily intake of leaf crops (incl. fruit and cereals) ^b	kg _{wwt} .d ⁻¹	1.2	0.77	1, 3
Daily intake of root crops ^b	kg _{wwt} .d ⁻¹	0.384	0.18	1, 3
Daily intake of meat	kg _{wwt} .d ⁻¹	0.301	0.26	1, 3
Daily intake of dairy products	kg _{wwt} .d ⁻¹	0.561	0.28	1, 3
Daily inhalation rate	m ³ .d ⁻¹	20	13.3	1, 2
Body weight	kg	70	70	1
Daily soil ingestion ^b	mg _{wwt} .d ⁻¹	-	50	2

^a it is assumed that 90% of the total fish intake (kg_{wwt}) on the continental scale are salt water species and 10% fresh water species (→ Section 2.2.2; personal assessment); ^b an edible fraction of 0.8 for fruit, vegetables and root crops is assumed, following ECETOC (1994); ^c it is assumed that on the continental scale all ingested soil comes from industrial/urban soils; ¹ RIVM et al. (1998); ² USEPA (1997); ³ ECETOC (1994).

⁸ Toxicity potentials are all expressed as kg reference substance per kg toxic substance, while emissions are expressed as kg toxic substance. This means that all impact scores are expressed as kg reference substance

In principle, human characteristics must be derived for the continental, moderate, arctic and tropic scale, separately. Although it is very well possible that human characteristics vary considerably between the four scales, it was not considered as a feasible option within the scope of this assessment to find reliable information for each of the four scales, separately. Here, the practical choice is made to use the same human characteristics on the continental scale as well on the global scale.

3.2 Substance-dependent input data

An extensive literature research is performed to find representative experimental substance-dependent input parameters and thereby to avoid as much as possible the QSAR estimation routines of USES 2.0 or worst-case default values. This is especially important for heavy metals and other inorganic chemicals, because the estimation routines are only valid for (non-ionic) organic chemicals. When several reported values for one parameter are considered to be valid, the geometric mean of these values is calculated and used in the assessment:

$$\bar{x}_g = \left(\prod_{i=1}^{i=n} x_i \right)^{1/n} \quad (19)$$

where, \bar{x}_g is the geometric mean; x_i are the individual values; and n is the number of values.

The geometric mean is considered as the most representative value, because it reflects the median of a lognormal uncertainty distribution. According to Slob (1994) and Seiler & Alvarez (1996), there are strong theoretical and empirical arguments to assume beforehand a lognormal uncertainty distribution for many physical parameters. If no experimental values for organic chemicals are found, estimation routines are applied in the model computations (see RIVM et al., 1998). As a first start, data research is performed for 181 substances (→ Appendix B).

Physico-chemical properties

Molecular weight, octanol-water partition coefficient, melting point, water solubility and vapour pressure are needed as input parameters in USES-LCA. Recommended values in the handbooks of Mackay et al. (1992a, b, 1993, 1995, 1997), reviews of McKone et al. (1995) and Staples et al. (1997) are used preferably. If chemicals are not listed in these references, the pesticide manual (Tomlin, 1994), handbooks of Howard (1989, 1991) and Verschueren (1996), RIVM documents (Slooff et al., 1989a, 1991a, 1993a, 1993b; Crommentuijn et al., 1997b), WHO documents (WHO, 1995b, 1997a) are used for physico-chemical information. If the above mentioned literature sources did not provide an answer, online databases on the internet (Environmental Science Center, 1998; Cambridgesoft Corporation, 1998, Spectrum Laboratories, 1998; USEPA, 1998a; Howard Hughes Medical Institute, 1998; University of Akron, 1998) and data from Guinée et al. (1996a) are used. This occurred sporadically. Finally, for metals recommendations given in Crommentuijn et al. (1997a) and RIVM et al. (1998) are followed. Very low values are used for vapour pressure and water solubility ($1 \cdot 10^{-30}$ Pa and $1 \cdot 10^{-13}$ mg.l⁻¹, respectively) in the calculations. For fine particulate matter

(PM10) the same recommendations as for metals are applied in the model calculations.

Partition coefficients

Henry's law constant is used to estimate the transfer of substances from the aqueous phase to the gas phase, while the solids-water partitioning for organic chemicals in the environment is estimated by means of the organic carbon partitioning coefficient. Experimental Henry's law constant are taken from McKone et al. (1995), Mackay et al (1993, 1995), Lide (1993), and Van de Plassche & Bockting (1993). Furthermore, Crommentuijn et al. (1997b), Bockting et al. (1993), Van de Plassche (1994), Slooff et al. (1991a, 1994a), WHO (1995b), Sabljic et al. (1995), McKone et al. (1995) and the handbooks of Mackay et al. (1992a, b, 1993, 1995, 1997) are used as sources for empirical organic carbon partitioning coefficients.

Based on Crommentuijn et al. (1997a), a scavenging ratio of 1.10^5 and a fraction of aerosol bounded substance of 0.95 is used for all metals, except for mercury and methyl-mercury. A scavenging ratio of 2.10^5 and aerosol bounded fraction of 0.05 is assumed for these two substances instead. Furthermore, for (methyl-)mercury another adaptation in the model is needed. Because mercury has a relatively high air-water partitioning coefficient in the air phase and a relatively low air-water partitioning coefficient in the water phase, USES-LCA is in principle not suited to model the intermedia transport of these two substances (Crommentuijn et al., 1997a). However, to make calculations possible, Crommentuijn et al. (1997a) suggest to set the air-water partitioning coefficient to a value of $1.3.10^{-5} \text{ mol.m}_{\text{air}}^{-3}/\text{mol.m}_{\text{water}}^{-3}$. This value is used here.⁹ For all other inorganic substances volatilisation is assumed to be negligible in the calculations. For PM10 the aerosol bound substance is set to a value of 1. Furthermore, for PM10 an aerosol collection efficiency of $3.5.10^5$ and an aerosol deposition rate of $1.5.10^{-3} \text{ m.s}^{-1}$ is implemented in the model calculations (D. van de Meent and F. de Leeuw, pers. comm.). Scavenging ratios of SO_2 ($3.0.10^5$) and NH_3 ($1.4.10^6$) are taken from Barrett & Berge (1996). In addition, for HCl a scavenging ratio equal to HNO_3 ($1.4.10^6$; Barrett & Berge, 1996), and for H_2S a scavenging ratio equal to SO_2 is assumed. Moreover, measured solids-water partition coefficients (K_p -values) for soil, sediment and particulate matter are needed for metals. Field-based K_p -values are preferred in the assessment. Whenever possible, field K_p -values for soils are taken from the De Groot et al. (1998). If field-based soil K_p -values are not available, metal-to-metal extrapolation methods, as applied by Bockting et al. (1992), and experimental soil K_p -values, taken from Crommentuijn et al. (1997a), are used. Field K_p -values for particulate matter are all taken from Crommentuijn et al. (1997a). Sediment K_p -values for metals, which are estimated on the basis of particulate matter K_p -values, are also taken from Crommentuijn et al. (1997a). Finally, for organo-metallic compounds K_p -values should be estimated on the basis of empirical data. In line with Crommentuijn et al. (1997a, b), K_p -values for methyl-mercury are set equal to mercury, and empirical K_{oc} -values are used to derive K_p -values for other organo-metallic compounds.

⁹ the Henry's law constant (25 °C) of (methyl-)mercury is estimated from the air-water partition coefficient given in Crommentuijn et al. (1997) using an environmental temperature of 12 °C. This value is used, after applying a scale-specific temperature correction, in the calculation of air-water partition coefficients on all geographical scales

Environmental degradation and transformation rates

Substance-specific degradation rates in air, water, soil, aerobic and anaerobic sediment are derived from numerous literature sources (see below), while for metals and PM10 extremely long half-lives (1.10^{40} days) for all compartments are used, since these substances are not degradable. Although substance-specific degradation rates are preferred in the model calculations, degradation data are most of the time lacking for one or more of the compartments. If this is the case, a worst-case scenario is avoided by extrapolating degradation rates from one compartment to the other. Furthermore, for five substances degradation rates are assumed equal to degradation rates of chemically related substances.¹⁰

For most substances the most effective elimination process in the troposphere is reaction with OH-radicals, although for some substances reaction with ozone or nitrate radicals, or direct photolysis in the air may be important (Howard et al., 1991). For 14 substances temperature dependent OH-radical reaction rates, based on Atkinson (1986a) and Brubaker & Hites (1997), are used in the calculations (\rightarrow Section 2.2.1). For the remaining substances the most important literature source for air degradation rates is Howard et al. (1991).¹¹ Additional literature sources are Atkinson (1985), McKone et al. (1995), Mackay et al. (1995, 1997), Howard (1989, 1990, 1991), Peijnenburg et al. (1991)¹², Barrett & Berge (1996) and Slooff et al. (1991a). However, these literature sources did not provide air degradation rates for about 50 of the selected substances. Air degradation rates for these substances are estimated with the atmospheric oxidation program of Syracuse Research Corporation (1993), based on QSAR-methods developed by Atkinson (1985, 1987, 1988). For the organo metallic compounds, such as fentin acetate and zineb, atmospheric degradation half-lives could be found nor estimated. Extremely long degradation half-lives in air (1.10^{40} d) are assumed for these compounds.

The most important literature sources for biodegradation rates in water, soil and sediment are Howard et al. (1991), together with Mackay et al. (1997) and Linders et al. (1994) for biodegradation rates of pesticides. McKone et al. (1995), Mackay et al. (1995), Van Rijn et al. (1995), Tomlin (1994), Slooff et al. (1991b), Peijnenburg et al. (1991)¹⁰, Howard (1989, 1990, 1991) and Slooff (1988b) are used as additional literature sources. Here, it is assumed that biodegradation rates in the literature are measured at 20 °C. However, for a considerable amount of substances, in particular for pesticides, biodegradation rates are lacking for one or more compartments. Assumptions are made to overcome these data gaps. First, if only the sediment biodegradation half-life of a substance is lacking, the estimation procedure listed in

¹⁰ degradation rates of 3-chloroaniline are assumed to be equivalent to 2-chloroaniline; degradation rates of 1,2,3-trichlorobenzene and 1,3,5-trichlorobenzene are assumed to be equivalent to 1,2,4-trichlorobenzene; degradation rates of 1,2,3,4-tetrachlorobenzene and 1,2,3,5-tetrachlorobenzene are assumed to be equivalent to 1,2,4,5-tetrachlorobenzene

¹¹ If degradation rates depend on the concentration of OH-radicals in the air, half-lives listed in Howard et al. (1991) are converted to half-lives related to the assumed OH-concentration of 5.10^{11} molecules.m⁻³ in USES-LCA. If Howard et al. (1991) consider direct photolysis as the most important degradation process in the air, the geometric mean of the expected high and low photolysis half-life is calculated.

¹² Peijnenburg et al. (1991) use the octanol-water partitioning coefficient to estimate degradation half-lives in air, water and soil of phthalates. This relationship is used to derive degradation half-lives in air, water and soil for dihexylphthalate, diisooctylphthalate and diisodecylphthalate

RIVM et al. (1998) is used to estimate the sediment biodegradation half-life from the soil biodegradation half-life of the substance. Furthermore, if no specific biodegradation half-life in water is found, and the biodegradation half-life in soil is below the 100 days, the substance is classified as 'inherently biodegradable'. According to Jager et al. (1997), the median half-life in the water compartment may be set to 30 days at 12 °C for this class of substances. Moreover, if for a substance no specific biodegradation half-lives in water, soil and sediment are found, the substance is either classified as 'inherently biodegradable' or 'not biodegradable, no information', dependent on the available qualitative information in the literature. Corresponding median half-lives for water, soil and aerobic sediment are taken from Jager et al. (1997). Finally, following Howard et al. (1991), if anaerobic sediment biodegradation half-lives are not found in the literature, anaerobic half-lives are assumed four times larger than for aerobic biodegradation in sediments.¹³

Hydrolysis may also be an important degradation process for some substances. Howard et al. (1991), Jeffers et al. (1996), Mackay et al. (1997), Tomlin (1994) and WHO (1995b) list hydrolysis rates for some substances in the aquatic environment. According to Howard et al. (1991), hydrolysis rates in the aquatic environment may also be used for defining abiotic degradation rates in the terrestrial and sediment compartment. This extrapolation may be valid for substances with relatively low Kp-values in these compartments. The following hydrolysis rate compartment-to-compartment extrapolation categories are distinguished (J. Struijs, pers. comm.):

- 1) if Kp-values $\leq 100 \text{ l.kg}^{-1}$, then $DT50_{\text{soil, sediment}} = DT50_{\text{water}}$
- 2) if $100 \text{ l.kg}^{-1} < \text{Kp-values} \leq 1000 \text{ l.kg}^{-1}$, then $DT50_{\text{soil, sediment}} = 10 * DT50_{\text{water}}$
- 3) if $1000 \text{ l.kg}^{-1} < \text{Kp-values} \leq 10000 \text{ l.kg}^{-1}$, then $DT50_{\text{soil, sediment}} = 100 * DT50_{\text{water}}$

Furthermore, pH-dependence of hydrolysis rates is taken into account in the assessment (\rightarrow Section 2.2.1). However, not all hydrolysis rates for pHs listed in Table 2 could be found in the literature. Therefore, hydrolysis rates at very low or high pHs are converted to hydrolysis rates at relevant pHs with help of the following formula (W. Peijnenburg, pers. comm.):

$$k_{\text{total}} = k_{\text{acid}} \times [H^+] + k_{\text{base}} \times [OH^-] + k_{\text{neutral}} \times 55.5 \quad (20)$$

where k_{total} is the overall hydrolysis rate (d^{-1}), k_{acid} is the acid rate constant ($\text{M}^{-1} \cdot \text{d}^{-1}$), k_{base} is the base rate constant ($\text{M}^{-1} \cdot \text{d}^{-1}$), and k_{neutral} is the neutral rate constant ($\text{M}^{-1} \cdot \text{d}^{-1}$). Finally, for the hydrolysis rates is also a temperature correction applied in the same way as done for the biodegradation rates.

Although for some substances photolysis in water and soil may be an important degradation route, photolysis rates may decrease up to 98% due to light absorbance by natural constituents (RIVM et al., 1998). Moreover, photolysis processes are normally restricted to the upper zones of water bodies. Therefore, it is assumed that photolysis in water and soil compartments can be neglected in the assessment.

¹³ The estimation procedure for anaerobic biodegradation half-lives of dihexyl-, diisodecyl-, and diisooctylphtalate is different. For these three substances the anaerobic biodegradation half-life is derived by multiplying the aerobic biodegradation half-life with the ratio of the anaerobic and aerobic biodegradation half-lives of di(n-octyl)phtalate, which is 18.3

Human exposure assessment

Experimental bioconcentration factors for fish, biotransfer factors for meat and milk, and biotransfer factors for plants are found in the handbooks of Mackay (1992a, b, 1993, 1995, 1997), various RIVM documents (Bockting et al., 1996; Cleven et al., 1993; Liem et al., 1993; Slooff et al., 1990a, b, 1992a, b, 1993, 1994, 1995; Van de Berg, 1995; Van de Plassche et al., 1992, 1994; Van de Plassche, 1994), articles published in scientific journals (Briggs et al., 1982; Devillers et al., 1996; Dowdy et al., 1996; Dowdy & McKone, 1997; Garten & Trabalka, 1983; Nendza, 1991; Ng, 1982; Paterson et al., 1991; Polder et al., 1995, 1998; Riederer, 1995; Sicbaldi et al., 1997; Staples et al., 1997; Tsuda et al., 1997), the AQUIRE database (Spectrum Research, 1992), McKone et al. (1995) and Guinée et al. (1996a). As mentioned above, if no experimental values for organic chemicals are found, QSAR estimation routines taken from USES 2.0 can be applied in the model computations. However, if for metals empirical values are lacking, these QSAR routines cannot be used.

The following estimation procedures are applied to fill in data gaps for metals:

- 1) for all metals fish bioconcentration factors are used for the estimation of bioconcentration factors for aquatic biota (needed in the calculation of the dissolved water concentration of a chemical);
- 2) fish bioconcentration factors for barium, molybdenum and tin are set to the average fish bioconcentration factor for other metals except mercury and organo-metallo compounds. This bioconcentration factor is 216 l.kg^{-1} ;
- 3) the milk biotransfer factor for methyl-mercury is derived from the milk biotransfer factor of mercury using the ratio of the fish bioconcentration factors of methyl-mercury and mercury as a conversion factor. A conversion factor of 7.2 is calculated;
- 4) meat biotransfer factors for 11 metals are estimated on the basis of the typical (geometrical average) ratio between meat and milk biotransfer factors for metals where both values are known. It is found that the typical meat biotransfer factor is 3.4 times larger than the typical milk biotransfer factor for metals;
- 5) the bioconcentration factor in respectively plant roots and leafs relative to antimony soil concentration are estimated on the basis of an estimation routine for metals given by Van de Berg (1995);¹⁴
- 6) For all metals bioconcentration factors in plant leafs relative to contaminant air or aerosol concentration are unknown. This plant uptake route of metals is disregarded.

Elimination of substances in plants by metabolism in plants or photodegradation on the surface of plants should also be taken into account in the the human exposure assessment. On the basis of literature data (Cabras et al., 1990; Komoßa et al., 1995; Mackay et al., 1997; Schwack et al., 1994; Schynowski & Schwack, 1996; Trapp & Matthies, 1995) it was possible to derive for 25 substances metabolic half-lives and for 3 substances photodegradation half-lives in/upon plants, assuming first-order degradation kinetics. However, caution must be taken with the implementation of metabolic half-lives together with experimentally derived air-plant partition coefficient

¹⁴ The estimation routine is: $\ln(\text{BCFr-s/l-s}) = 2.67 - 1.12 * \ln(\text{Kp}_{\text{soil}})$, where BCFr-s/l-s is the bioconcentration factor in roots and leafs relative to the soil concentration ($\text{kg}_{\text{dwt}} \cdot \text{kg}_{\text{dwt}}^{-1}$) and Kp_{soil} is the solids-water partitioning coefficient in soil (l.kg^{-1})

($K_{\text{leaf-air}}$) and soil-plant bioconcentration factors ($\text{BCF}_{\text{leaf-soil}}$), because it is likely that plant metabolism is already (implicitly) taken into account in the derivation of these experimental plant bioconcentration factors. Therefore, if an experimentally derived $K_{\text{leaf-air}}$ or $\text{BCF}_{\text{leaf-soil}}$ is available, metabolic half-lives in plants are not used for that particular uptake route of the chemical. For all other substances elimination rates are set to 0 d^{-1} .

As discussed in Section 2.2.2, a standard purification factor of 0.15 for all substances is used in the calculations, which means that it is expected that 85% of the dissolved concentration of a substance is removed from the surface water during drinking water purification processes.

Finally, bioavailability for inhalation and oral uptake should be assessed substance-dependently. For some organic chemicals and metals substance-specific inhalatory and oral bioavailability values are found in Owen (1990), WHO environmental health criteria reports (WHO, 1985a, 1989a, b, c, 1992a, b, 1993, 1994a, b, c, 1995a, b, 1996a, b; 1997a, b) and RIVM reports (Peijnenburg et al., 1991; RIVM & TNO, 1986; Slooff, 1988; Slooff et al., 1990a, 1991c, 1992a, c, 1993, 1995). If substance-specific values are not found, standard defaults within USES 2.0 for bioavailability for inhalation and oral uptake, which are respectively 0.75 and 1, are used.

Effects assessment

Effect factors for aquatic and terrestrial ecosystems, also called Predicted No Effect Concentrations (PNECs), are taken from RIZA (1999) and Huijbregts (1999), respectively. In both reports the Technical Guidance Document (TGD; EC, 1996) is used for the derivation of ecotoxicological effect factors. PNECs are derived from ecotoxicological data by applying statistical extrapolation, safety factors or the equilibrium partition method. The statistical extrapolation method is based on the assumption that the sensitivities of species in an ecosystem can be described by statistical distribution. The concentration corresponding with a protection level of 95% of all the species is considered as the effect factor. If, for a toxicant four or more chronic No Observed Effect Concentrations (NOECs) from different taxonomic groups are available, the statistical extrapolation method is in most cases preferred (Slooff, 1992; Aldenberg & Slob, 1993). If less than four NOECs are available, safety factors are applied to toxicity data. If no or hardly any experimental toxicological data for terrestrial ecosystems are available, the equilibrium-partitioning method may be used to derive the terrestrial PNEC. This assumes that bioavailability, bioaccumulation and toxicity are closely related to the soil porewater concentrations. Furthermore, it is assumed that (1) sensitivities of aquatic organisms are comparable with sensitivities of soil organisms and (2) an equilibrium between the chemical sorbed to soil particulates and porewater exists that can be described by a partition coefficient (Crommentuijn et al., 1997a). Sediment effect factors are all derived with the equilibrium partition method in this assessment.

Except for organotin-compounds, no distinction is made between PNECs for saltwater species and PNECs for freshwater species. For metals, the PNEC without the background concentrations are used as the toxic effect parameter for the aquatic and terrestrial environment. This is done because in LCA the potential effect caused by an anthropogenic addition of a toxic substance is of primary interest and not the risk

related to the total concentration of the toxicant in the environment. In LCA toxic emissions are per definition related to economic activities of a product system. The main goal of using toxicity potentials in LCA is to characterise the potential severity of these toxic emissions. Because background concentrations, which are an integral part of the PNEC for metals, are not caused by economic activities, it is not appropriate to characterise these toxic emissions with PNECs including background concentrations.¹⁵

¹⁶

After deriving PNECs for all compartment separately, PNECs for all compartments are (preferably) harmonised with each other in risk assessment (VROM, 1997). This means, for instance, that the PNEC_{aqua} will not result in an exceedance of the PNEC_{soil}. Moreover, for risk assessment purposes aquatic and terrestrial PNECs are adjusted for the possible effect of secondary poisoning on higher organisms, such as worm-eating and fish-eating predators. However, PNEC harmonisation and adjustment for secondary poisoning is not preferred in the calculation of toxicity potentials that are to be used in LCAs. Characterising the potential impact of a toxic emission for each specific impact categories *separately* is the primary goal, and not maintaining harmonised quality objectives or to account for the possible effect of secondary poisoning.¹⁷

For human effect assessment in USES-LCA oral and inhalatory human limit values (HLV_{oral} and HLV_{inh.}) are implemented. HLVs published by the WHO (FAO/WHO, 1993, 1998, 1999; JECFA, 1982, 1986, 1989; WHO, 1997a; WHO-EURO, 1987; WHO-EURO, 1996), various RIVM documents (Annema et al., 1996, Janus et al., 1994, Vermeire et al. 1991, Vermeire 1993, Rademaker et al., 1993; Rademaker & Van de Plassche, 1993, Janssen et al., 1998), the IRIS online internet database (USEPA, 1998b), the online internet database of the Environmental Defense Fund (1999), Tomlin (1994), and Guinée et al. (1996a) are consulted for oral and inhalatory HLVs. If either an experimental HLV_{oral} or a HLV_{inh.} for a substance is not available, route-to-route extrapolation on the basis of bioavailability for inhalation and oral uptake is performed (see RIVM et al., 1998). These literature sources are preferred in the following descending order:

- 1) HLVs derived by the WHO;
- 2) HLVs listed in RIVM documents;
- 3) HLVs derived by USEPA (1998b);
- 4) HLVs listed by the Environmental Defense Fund (1999);
- 5) HLVs listed in Guinée et al. (1996a);
- 6) HLVs listed in Tomlin (1994);
- 7) HLVs derived from NOAELs or LOAELs listed in Tomlin (1994) or Guinée et al. (1996a).
- 8) HLVs derived by route-to-route extrapolation on the basis of bioavailability for

¹⁵ The background concentration is the concentration of the chemical that is present in rural sites due to natural causes only. However, in the Netherlands it is impossible to find locations at which real background concentrations can be measured. Models are used to derive metal background concentrations in surface water and soils, although some of the model outcomes may be influenced by anthropogenic sources (Crommentuijn et al., 1997a)

¹⁶ In fact, this holds true for all substances with background concentrations in a particular environment

¹⁷ Fish-eating and worm-eating predators are considered as separate impact categories and not as parts of the aquatic and terrestrial ecosystem, respectively

inhalation and oral uptake (see RIVM et al., 1998).

For two substances an exception in the preference of literature sources is made. First, the Health Council of the Netherlands (1996) concluded that the HLV_{oral} for 2,3,7,8 TCDD derived by the WHO and RIVM was not appropriate. They derived an HLV_{oral} 10 times more conservative than the limit value derived by the WHO and RIVM. ($1 \text{ pg.kg bwt}^{-1}.\text{day}^{-1}$ instead of $1 \text{ ng.kg bwt}^{-1}.\text{day}^{-1}$). The other exception is the $HLV_{inh.}$ for PM_{10} . Annema et al. (1996) concluded that the current $HLV_{inh.}$ for PM_{10} in the Netherlands of $40 \text{ }\mu\text{g.m}^{-3}$ may not be conservative enough, while the WHO recommended an $HLV_{inh.}$ for PM_{10} of $70 \text{ }\mu\text{g.m}^{-3}$. Here, it is decided to use for both substances the most conservative HLV available.

For the substances 1,3-dichlorobenzene, dihexylphthalate and dimethylphthalate toxicity data for the derivation of the HLV_{oral} and $HLV_{inh.}$ were not found. For these substances, a default HLV_{oral} of $1 \cdot 10^{-9} \text{ kg.kg}_{bwt}^{-1}.\text{day}^{-1}$ and $HLV_{inh.}$ of $4.7 \cdot 10^{-9} \text{ kg.m}^{-3}$ are used in the assessment. RIVM et al. (1994) proposed to use these default values for non-genotoxic substances, if toxicity data are lacking for the derivation of HLVs.

As argued before, worst-case estimates are not preferred in the calculation of toxicity potentials. However, the use of safety factors in the derivation of HLVs¹⁸, and safety factors in the derivation of PNECs¹⁹ may be considered as worst-case approaches (ECETOC, 1995; Emans et al., 1993). Thus, in principle PNECs derived with help of safety factors, and all HLVs should be adjusted for the application of worst-case safety factors. However, there are also reasons for not using lower assessment factors (assuming that one gets lower typical values than the arbitrary factors of 10). One practical argument is that a substance may/should be 'punished' if toxicity data are scarce. Another argument is that (human) assessment factors may not be so conservative, if the ultimate aim is to protect the major part of the human population (Renwick & Lazarus, 1998; Watanabe et al., 1992). Here, it is not considered as a feasible task to adjust the default assessment factors in more likely estimates.

Carcinogenic PAHs

A specific difficulty is connected with the calculation of human toxicity potentials for carcinogenic PAHs. The problem is that the inhalatory HLV for carcinogenic PAHs is representative for the over-all group of carcinogenic PAHs and not for individual substances of this group (Slooff et al., 1989a). This means that it is not possible to calculate HTPs for individual carcinogenic PAHs. Therefore, it is decided to calculate the HTP for the total group of carcinogenic PAHs. Here, an inhalatory HLV of 1 ng.m^{-3} (Slooff et al., 1989; Janus et al., 1994) and an oral HLV of $6.3 \cdot 10^{-9} \text{ kg.kg}^{-1}.\text{day}^{-1}$ (Vermeire, 1993) are used. Vermeire (1993) calculated the oral HLV for the carcinogenic PAHs from the individual oral HLVs of carcinogenic PAHs by assuming the following typical composition of carcinogenic PAH occurrence: 0.20 fluoranthene; 0.18 chrysene; 0.09 benzo[a]anthracene; 0.31 benzo[k]fluoranthene; 0.06 benzop[a]lyrene; 0.08 benzo[ghi]perylene; and 0.08 indeno[1,2,3-cd]pyrene. This composition is derived from the occurrence of individual carcinogenic PAHs in

¹⁸ In human risk assessment safety factors may be applied to account for inter- and intraspecies variation, or extrapolation from sub-acute or sub-chronic effects to chronic effects

¹⁹ In ecotoxicological risk assessment safety factors may be applied to account for extrapolation of acute LC50 to chronic NOEC, inter-species differences, and extrapolation from lab results to ecosystems

industrial soils. One is still left with the problem, what kind of substance-specific input data, such as solubility and degradation rates, should be used in the fate analysis. Here, it is decided to use the above mentioned typical composition of carcinogenic PAHs to calculate weighted averaged input data for the fate analysis from the substance-specific data input of the individual carcinogenic PAHs. TETPs, AETPs and SETPs are calculated both for individual carcinogenic PAHs and for the the over-all group of carcinogenic PAHs, using the above mentioned typical composition of carcinogenic PAHs.

4. Results

4.1 Toxicity potentials

Table 7 lists the toxicity potentials for 181 evaluated substances related to the initial emission compartments and impact categories.

Table 7: Toxicity potentials of 181 substances related to the initial emission compartments and impact categories. AETP_{fresh} = fresh water Aquatic Ecotoxicity Potential; AETP_{marine} = marine Aquatic Ecotoxicity Potential; SETP_{fresh} = fresh water Sediment Ecotoxicity Potential; SETP_{marine} = marine Sediment Ecotoxicity Potential; TETP = Terrestrial Ecotoxicity Potential; HTP = Human Toxicity Potential; x = toxicity potential was not calculated.

Substance No.	Name	CAS No.	Type	Initial emission compartment				
				air	fresh water	sea water	agricult. soil	industrial soil
Metals								
1.	Antimony	7440-36-0	AETP _{fresh}	3.7	$2.0 \cdot 10^1$	$7.6 \cdot 10^{-21}$	$1.0 \cdot 10^1$	$1.0 \cdot 10^1$
			AETP _{marine}	$3.3 \cdot 10^4$	$2.7 \cdot 10^4$	$4.9 \cdot 10^4$	$1.4 \cdot 10^4$	$1.4 \cdot 10^4$
			SETP _{fresh}	9.1	$4.8 \cdot 10^1$	$1.8 \cdot 10^{-20}$	$2.4 \cdot 10^1$	$2.4 \cdot 10^1$
			SETP _{marine}	$3.1 \cdot 10^4$	$2.5 \cdot 10^4$	$4.6 \cdot 10^4$	$1.3 \cdot 10^4$	$1.3 \cdot 10^4$
			TETP	$6.1 \cdot 10^{-1}$	$1.7 \cdot 10^{-20}$	$3.0 \cdot 10^{-20}$	1.3	1.3
			HTP	$6.7 \cdot 10^3$	$5.1 \cdot 10^3$	$8.6 \cdot 10^3$	$8.9 \cdot 10^3$	$2.6 \cdot 10^3$
2.	Arsenic	7440-38-2	AETP _{fresh}	$5.0 \cdot 10^1$	$2.1 \cdot 10^2$	$3.8 \cdot 10^{-20}$	$1.3 \cdot 10^2$	$1.3 \cdot 10^2$
			AETP _{marine}	$2.3 \cdot 10^5$	$1.2 \cdot 10^5$	$3.4 \cdot 10^5$	$7.7 \cdot 10^4$	$7.7 \cdot 10^4$
			SETP _{fresh}	$1.3 \cdot 10^2$	$5.3 \cdot 10^2$	$9.8 \cdot 10^{-20}$	$3.4 \cdot 10^2$	$3.4 \cdot 10^2$
			SETP _{marine}	$2.3 \cdot 10^5$	$1.2 \cdot 10^5$	$3.4 \cdot 10^5$	$7.7 \cdot 10^4$	$7.7 \cdot 10^4$
			TETP	$1.6 \cdot 10^3$	$1.0 \cdot 10^{-17}$	$3.0 \cdot 10^{-17}$	$3.3 \cdot 10^3$	$3.3 \cdot 10^3$
			HTP	$3.5 \cdot 10^5$	$9.5 \cdot 10^2$	$2.4 \cdot 10^3$	$3.2 \cdot 10^4$	$1.0 \cdot 10^3$
3.	Barium	7440-39-3	AETP _{fresh}	$4.3 \cdot 10^1$	$2.3 \cdot 10^2$	$2.4 \cdot 10^{-19}$	$1.1 \cdot 10^2$	$1.1 \cdot 10^2$
			AETP _{marine}	$7.8 \cdot 10^5$	$8.3 \cdot 10^5$	$1.1 \cdot 10^6$	$4.2 \cdot 10^5$	$4.2 \cdot 10^5$
			SETP _{fresh}	$9.7 \cdot 10^1$	$5.1 \cdot 10^2$	$5.4 \cdot 10^{-19}$	$2.6 \cdot 10^2$	$2.6 \cdot 10^2$
			SETP _{marine}	$6.7 \cdot 10^5$	$7.1 \cdot 10^5$	$9.3 \cdot 10^5$	$3.6 \cdot 10^5$	$3.6 \cdot 10^5$
			TETP	4.9	$5.1 \cdot 10^{-19}$	$6.6 \cdot 10^{-19}$	$1.0 \cdot 10^1$	$1.0 \cdot 10^1$
			HTP	$7.6 \cdot 10^2$	$6.3 \cdot 10^2$	$8.0 \cdot 10^2$	$3.6 \cdot 10^2$	$3.2 \cdot 10^2$
4.	Beryllium	7440-41-7	AETP _{fresh}	$1.7 \cdot 10^4$	$9.1 \cdot 10^4$	$1.6 \cdot 10^{-16}$	$4.6 \cdot 10^4$	$4.6 \cdot 10^4$
			AETP _{marine}	$4.7 \cdot 10^8$	$5.4 \cdot 10^8$	$6.4 \cdot 10^8$	$2.7 \cdot 10^8$	$2.7 \cdot 10^8$
			SETP _{fresh}	$2.0 \cdot 10^4$	$1.1 \cdot 10^5$	$1.8 \cdot 10^{-16}$	$5.4 \cdot 10^4$	$5.4 \cdot 10^4$
			SETP _{marine}	$2.0 \cdot 10^8$	$2.3 \cdot 10^8$	$2.8 \cdot 10^8$	$1.2 \cdot 10^8$	$1.2 \cdot 10^8$
			TETP	$1.8 \cdot 10^3$	$3.3 \cdot 10^{-16}$	$3.9 \cdot 10^{-16}$	$3.6 \cdot 10^3$	$3.6 \cdot 10^3$
			HTP	$2.3 \cdot 10^5$	$1.4 \cdot 10^4$	$1.6 \cdot 10^4$	$1.3 \cdot 10^4$	$7.0 \cdot 10^3$
5.	Cadmium	7440-43-9	AETP _{fresh}	$2.9 \cdot 10^2$	$1.5 \cdot 10^3$	$2.5 \cdot 10^{-20}$	$7.8 \cdot 10^2$	$7.8 \cdot 10^2$
			AETP _{marine}	$1.1 \cdot 10^6$	$2.2 \cdot 10^5$	$1.8 \cdot 10^6$	$1.1 \cdot 10^5$	$1.1 \cdot 10^5$

SETP _{fresh}	$7.4 \cdot 10^2$	$3.9 \cdot 10^3$	$6.5 \cdot 10^{-20}$	$2.0 \cdot 10^3$	$2.0 \cdot 10^3$
SETP _{marine}	$1.1 \cdot 10^6$	$2.2 \cdot 10^5$	$1.9 \cdot 10^6$	$1.1 \cdot 10^5$	$1.1 \cdot 10^5$
TETP	$8.1 \cdot 10^1$	$1.4 \cdot 10^{-20}$	$1.1 \cdot 10^{-19}$	$1.7 \cdot 10^2$	$1.7 \cdot 10^2$
HTP	$1.5 \cdot 10^5$	$2.3 \cdot 10^1$	$1.0 \cdot 10^2$	$2.0 \cdot 10^4$	$6.7 \cdot 10^1$

Substance No.	Name	CAS No.	Type	Initial emission compartment				
				air	fresh water	sea water	agricult. soil	industrial soil
Metals								
6.	Chromium III	7440-47-3	AETP _{fresh}	1.9	6.9	$8.8 \cdot 10^{-23}$	5.3	5.3
			AETP _{marine}	$5.2 \cdot 10^3$	$8.6 \cdot 10^2$	$8.2 \cdot 10^3$	$6.5 \cdot 10^2$	$6.5 \cdot 10^2$
			SETP _{fresh}	4.9	$1.8 \cdot 10^1$	$2.3 \cdot 10^{-22}$	$1.3 \cdot 10^1$	$1.3 \cdot 10^1$
			SETP _{marine}	$5.3 \cdot 10^3$	$8.8 \cdot 10^2$	$8.4 \cdot 10^3$	$6.7 \cdot 10^2$	$6.7 \cdot 10^2$
			TETP	$3.0 \cdot 10^3$	$2.3 \cdot 10^{-19}$	$2.0 \cdot 10^{-18}$	$6.3 \cdot 10^3$	$6.3 \cdot 10^3$
			HTP	$6.5 \cdot 10^2$	2.1	$1.0 \cdot 10^1$	$5.1 \cdot 10^3$	$3.0 \cdot 10^2$
7.	Chromium VI	7440-47-3	AETP _{fresh}	7.7	$2.8 \cdot 10^1$	$3.5 \cdot 10^{-22}$	$2.1 \cdot 10^1$	$2.1 \cdot 10^1$
			AETP _{marine}	$2.1 \cdot 10^4$	$3.4 \cdot 10^3$	$3.3 \cdot 10^4$	$2.6 \cdot 10^3$	$2.6 \cdot 10^3$
			SETP _{fresh}	$2.0 \cdot 10^1$	$7.1 \cdot 10^1$	$9.1 \cdot 10^{-22}$	$5.4 \cdot 10^1$	$5.4 \cdot 10^1$
			SETP _{marine}	$2.1 \cdot 10^4$	$3.5 \cdot 10^3$	$3.4 \cdot 10^4$	$2.7 \cdot 10^3$	$2.7 \cdot 10^3$
			TETP	$3.0 \cdot 10^3$	$2.3 \cdot 10^{-19}$	$2.0 \cdot 10^{-18}$	$6.3 \cdot 10^3$	$6.3 \cdot 10^3$
			HTP	$3.4 \cdot 10^6$	3.4	$1.7 \cdot 10^1$	$8.5 \cdot 10^3$	$5.0 \cdot 10^2$
8.	Cobalt	7440-48-4	AETP _{fresh}	$6.4 \cdot 10^2$	$3.4 \cdot 10^3$	$1.2 \cdot 10^{-18}$	$1.7 \cdot 10^3$	$1.7 \cdot 10^3$
			AETP _{marine}	$5.4 \cdot 10^6$	$4.4 \cdot 10^6$	$8.0 \cdot 10^6$	$2.2 \cdot 10^6$	$2.2 \cdot 10^6$
			SETP _{fresh}	$1.1 \cdot 10^3$	$5.6 \cdot 10^3$	$2.0 \cdot 10^{-18}$	$2.8 \cdot 10^3$	$2.8 \cdot 10^3$
			SETP _{marine}	$3.5 \cdot 10^6$	$2.8 \cdot 10^6$	$5.2 \cdot 10^6$	$1.4 \cdot 10^6$	$1.4 \cdot 10^6$
			TETP	$1.1 \cdot 10^2$	$2.7 \cdot 10^{-18}$	$4.9 \cdot 10^{-18}$	$2.2 \cdot 10^2$	$2.2 \cdot 10^2$
			HTP	$1.7 \cdot 10^4$	$9.7 \cdot 10^1$	$6.0 \cdot 10^1$	$2.4 \cdot 10^3$	$5.9 \cdot 10^1$
9.	Copper	7440-50-8	AETP _{fresh}	$2.2 \cdot 10^2$	$1.2 \cdot 10^3$	$4.1 \cdot 10^{-20}$	$5.9 \cdot 10^2$	$5.9 \cdot 10^2$
			AETP _{marine}	$8.9 \cdot 10^5$	$2.3 \cdot 10^5$	$1.5 \cdot 10^6$	$1.2 \cdot 10^5$	$1.2 \cdot 10^5$
			SETP _{fresh}	$5.6 \cdot 10^2$	$2.9 \cdot 10^3$	$1.0 \cdot 10^{-19}$	$1.5 \cdot 10^3$	$1.5 \cdot 10^3$
			SETP _{marine}	$8.8 \cdot 10^5$	$2.3 \cdot 10^5$	$1.5 \cdot 10^6$	$1.2 \cdot 10^5$	$1.2 \cdot 10^5$
			TETP	7.0	$4.1 \cdot 10^{-21}$	$2.5 \cdot 10^{-20}$	$1.4 \cdot 10^1$	$1.4 \cdot 10^1$
			HTP	$4.3 \cdot 10^3$	1.3	5.9	$9.4 \cdot 10^1$	1.3
E.	Lead	7439-92-1	AETP _{fresh}	2.4	9.6	$5.6 \cdot 10^{-23}$	6.5	6.5
			AETP _{marine}	$7.0 \cdot 10^3$	$1.1 \cdot 10^3$	$1.1 \cdot 10^4$	$7.5 \cdot 10^2$	$7.5 \cdot 10^2$
			SETP _{fresh}	6.2	$2.5 \cdot 10^1$	$1.4 \cdot 10^{-22}$	$1.7 \cdot 10^1$	$1.7 \cdot 10^1$
			SETP _{marine}	$7.2 \cdot 10^3$	$1.1 \cdot 10^3$	$1.2 \cdot 10^4$	$7.8 \cdot 10^2$	$7.8 \cdot 10^2$
			TETP	$1.6 \cdot 10^1$	$4.8 \cdot 10^{-22}$	$4.6 \cdot 10^{-21}$	$3.3 \cdot 10^1$	$3.3 \cdot 10^1$
			HTP	$4.7 \cdot 10^2$	$1.2 \cdot 10^1$	$7.9 \cdot 10^1$	$3.3 \cdot 10^3$	$2.9 \cdot 10^2$
11.	Mercury	7439-97-6	AETP _{fresh}	$3.2 \cdot 10^2$	$1.7 \cdot 10^3$	6.8	$8.5 \cdot 10^2$	$8.5 \cdot 10^2$
			AETP _{marine}	$1.2 \cdot 10^6$	$2.1 \cdot 10^5$	$1.9 \cdot 10^6$	$1.7 \cdot 10^5$	$1.7 \cdot 10^5$
			SETP _{fresh}	$8.1 \cdot 10^2$	$4.4 \cdot 10^3$	$1.7 \cdot 10^1$	$2.2 \cdot 10^3$	$2.2 \cdot 10^3$
			SETP _{marine}	$1.2 \cdot 10^6$	$2.2 \cdot 10^5$	$1.9 \cdot 10^6$	$1.7 \cdot 10^5$	$1.7 \cdot 10^5$
			TETP	$2.8 \cdot 10^4$	$9.3 \cdot 10^2$	$7.6 \cdot 10^3$	$5.6 \cdot 10^4$	$5.6 \cdot 10^4$
			HTP	$6.0 \cdot 10^3$	$1.4 \cdot 10^3$	$8.2 \cdot 10^3$	$5.9 \cdot 10^3$	$1.1 \cdot 10^3$
12.	Methyl-mercury	22967-92-6	AETP _{fresh}	$7.3 \cdot 10^3$	$3.9 \cdot 10^4$	$1.6 \cdot 10^2$	$1.9 \cdot 10^4$	$1.9 \cdot 10^4$
			AETP _{marine}	$2.8 \cdot 10^7$	$4.9 \cdot 10^6$	$4.3 \cdot 10^7$	$3.8 \cdot 10^6$	$3.8 \cdot 10^6$
			SETP _{fresh}	$1.9 \cdot 10^4$	$1.0 \cdot 10^5$	$4.0 \cdot 10^2$	$5.0 \cdot 10^4$	$5.0 \cdot 10^4$
			SETP _{marine}	$2.8 \cdot 10^7$	$5.1 \cdot 10^6$	$4.4 \cdot 10^7$	$3.9 \cdot 10^6$	$3.9 \cdot 10^6$
			TETP	$2.8 \cdot 10^4$	$9.3 \cdot 10^2$	$7.6 \cdot 10^3$	$5.6 \cdot 10^4$	$5.6 \cdot 10^4$
			HTP	$5.8 \cdot 10^4$	$1.5 \cdot 10^4$	$8.8 \cdot 10^4$	$2.0 \cdot 10^4$	$1.1 \cdot 10^4$
13.	Molybdenum	7439-98-7	AETP _{fresh}	$9.7 \cdot 10^1$	$4.8 \cdot 10^2$	$6.6 \cdot 10^{-19}$	$2.6 \cdot 10^2$	$2.6 \cdot 10^2$
			AETP _{marine}	$1.9 \cdot 10^6$	$2.1 \cdot 10^6$	$2.6 \cdot 10^6$	$1.2 \cdot 10^6$	$1.2 \cdot 10^6$
			SETP _{fresh}	$2.1 \cdot 10^2$	$1.1 \cdot 10^3$	$1.5 \cdot 10^{-18}$	$5.8 \cdot 10^2$	$5.8 \cdot 10^2$
			SETP _{marine}	$1.6 \cdot 10^6$	$1.7 \cdot 10^6$	$2.2 \cdot 10^6$	$9.6 \cdot 10^5$	$9.6 \cdot 10^5$
			TETP	$1.8 \cdot 10^1$	$2.3 \cdot 10^{-18}$	$2.9 \cdot 10^{-18}$	$3.6 \cdot 10^1$	$3.6 \cdot 10^1$
			HTP	$5.4 \cdot 10^3$	$5.5 \cdot 10^3$	$6.8 \cdot 10^3$	$6.2 \cdot 10^3$	$3.1 \cdot 10^3$

Substance No.	Name	CAS No.	Type	Initial emission compartment				
				air	fresh water	sea water	agricult. soil	industrial soil
Metals								
14.	Nickel	7440-2-0	AETP _{fresh}	$6.3 \cdot 10^2$	$3.2 \cdot 10^3$	$6.1 \cdot 10^{-19}$	$1.7 \cdot 10^3$	$1.7 \cdot 10^3$
			AETP _{marine}	$3.8 \cdot 10^6$	$2.2 \cdot 10^6$	$5.8 \cdot 10^6$	$1.2 \cdot 10^6$	$1.2 \cdot 10^6$
			SETP _{fresh}	$1.6 \cdot 10^3$	$8.3 \cdot 10^3$	$1.6 \cdot 10^{-18}$	$4.3 \cdot 10^3$	$4.3 \cdot 10^3$
			SETP _{marine}	$3.7 \cdot 10^6$	$2.2 \cdot 10^6$	$5.7 \cdot 10^6$	$1.2 \cdot 10^6$	$1.2 \cdot 10^6$
			TETP	$1.2 \cdot 10^2$	$1.0 \cdot 10^{-18}$	$2.6 \cdot 10^{-18}$	$2.4 \cdot 10^2$	$2.4 \cdot 10^2$
			HTP	$3.5 \cdot 10^4$	$3.3 \cdot 10^2$	$7.5 \cdot 10^2$	$2.7 \cdot 10^3$	$2.0 \cdot 10^2$
15.	Selenium	7782-49-2	AETP _{fresh}	$5.5 \cdot 10^2$	$2.9 \cdot 10^3$	$7.4 \cdot 10^{-18}$	$1.5 \cdot 10^3$	$1.5 \cdot 10^3$
			AETP _{marine}	$2.1 \cdot 10^7$	$2.5 \cdot 10^7$	$2.9 \cdot 10^7$	$1.3 \cdot 10^7$	$1.3 \cdot 10^7$
			SETP _{fresh}	$6.4 \cdot 10^2$	$3.4 \cdot 10^3$	$8.6 \cdot 10^{-18}$	$1.7 \cdot 10^3$	$1.7 \cdot 10^3$
			SETP _{marine}	$9.0 \cdot 10^6$	$1.1 \cdot 10^7$	$1.2 \cdot 10^7$	$5.4 \cdot 10^6$	$5.4 \cdot 10^6$
			TETP	$5.3 \cdot 10^1$	$1.6 \cdot 10^{-17}$	$1.8 \cdot 10^{-17}$	$1.1 \cdot 10^2$	$1.1 \cdot 10^2$
			HTP	$4.8 \cdot 10^4$	$5.6 \cdot 10^4$	$6.3 \cdot 10^4$	$2.9 \cdot 10^4$	$2.8 \cdot 10^4$
16.	Thallium	7440-28-0	AETP _{fresh}	$1.6 \cdot 10^3$	$8.0 \cdot 10^3$	$7.9 \cdot 10^{-18}$	$4.2 \cdot 10^3$	$4.2 \cdot 10^3$
			AETP _{marine}	$2.6 \cdot 10^7$	$2.7 \cdot 10^7$	$3.6 \cdot 10^7$	$1.4 \cdot 10^7$	$1.4 \cdot 10^7$
			SETP _{fresh}	$3.9 \cdot 10^3$	$2.0 \cdot 10^4$	$2.0 \cdot 10^{-17}$	$1.1 \cdot 10^4$	$1.1 \cdot 10^4$
			SETP _{marine}	$2.4 \cdot 10^7$	$2.5 \cdot 10^7$	$3.4 \cdot 10^7$	$1.3 \cdot 10^7$	$1.3 \cdot 10^7$
			TETP	$3.4 \cdot 10^2$	$3.1 \cdot 10^{-17}$	$4.2 \cdot 10^{-17}$	$7.0 \cdot 10^2$	$7.0 \cdot 10^2$
			HTP	$4.3 \cdot 10^5$	$2.3 \cdot 10^5$	$2.9 \cdot 10^5$	$2.0 \cdot 10^6$	$1.2 \cdot 10^5$
17.	Tin	7440-31-5	AETP _{fresh}	2.5	$1.0 \cdot 10^1$	$9.5 \cdot 10^{-23}$	6.9	6.9
			AETP _{marine}	$7.5 \cdot 10^3$	$1.2 \cdot 10^3$	$1.2 \cdot 10^4$	$8.3 \cdot 10^2$	$8.3 \cdot 10^2$
			SETP _{fresh}	1.3	5.2	$4.8 \cdot 10^{-23}$	3.5	3.5
			SETP _{marine}	$1.5 \cdot 10^3$	$2.5 \cdot 10^2$	$2.5 \cdot 10^3$	$1.7 \cdot 10^2$	$1.7 \cdot 10^2$
			TETP	$1.4 \cdot 10^1$	$7.9 \cdot 10^{-22}$	$7.2 \cdot 10^{-21}$	$3.0 \cdot 10^1$	$3.0 \cdot 10^1$
			HTP	1.7	$1.7 \cdot 10^{-2}$	$1.1 \cdot 10^{-1}$	$1.3 \cdot 10^1$	$5.2 \cdot 10^{-1}$
18.	Vanadium	7440-62-2	AETP _{fresh}	$1.7 \cdot 10^3$	$9.0 \cdot 10^3$	$2.4 \cdot 10^{-18}$	$4.7 \cdot 10^3$	$4.7 \cdot 10^3$
			AETP _{marine}	$1.2 \cdot 10^7$	$8.6 \cdot 10^6$	$1.8 \cdot 10^7$	$4.5 \cdot 10^6$	$4.5 \cdot 10^6$
			SETP _{fresh}	$4.1 \cdot 10^3$	$2.1 \cdot 10^4$	$5.7 \cdot 10^{-18}$	$1.1 \cdot 10^4$	$1.1 \cdot 10^4$
			SETP _{marine}	$1.1 \cdot 10^7$	$7.9 \cdot 10^6$	$1.7 \cdot 10^7$	$4.1 \cdot 10^6$	$4.1 \cdot 10^6$
			TETP	$6.7 \cdot 10^2$	$1.0 \cdot 10^{-17}$	$2.2 \cdot 10^{-17}$	$1.4 \cdot 10^3$	$1.4 \cdot 10^3$
			HTP	$6.2 \cdot 10^3$	$3.2 \cdot 10^3$	$6.2 \cdot 10^3$	$1.9 \cdot 10^4$	$1.7 \cdot 10^3$
19.	Zinc	7440-66-6	AETP _{fresh}	$1.8 \cdot 10^1$	$9.2 \cdot 10^1$	$1.8 \cdot 10^{-21}$	$4.8 \cdot 10^1$	$4.8 \cdot 10^1$
			AETP _{marine}	$6.7 \cdot 10^4$	$1.4 \cdot 10^4$	$1.1 \cdot 10^5$	$7.2 \cdot 10^3$	$7.2 \cdot 10^3$
			SETP _{fresh}	$4.6 \cdot 10^1$	$2.4 \cdot 10^2$	$4.5 \cdot 10^{-21}$	$1.2 \cdot 10^2$	$1.2 \cdot 10^2$
			SETP _{marine}	$6.8 \cdot 10^4$	$1.4 \cdot 10^4$	$1.1 \cdot 10^5$	$7.3 \cdot 10^3$	$7.3 \cdot 10^3$
			TETP	$1.2 \cdot 10^1$	$2.5 \cdot 10^{-21}$	$1.9 \cdot 10^{-20}$	$2.5 \cdot 10^1$	$2.5 \cdot 10^1$
			HTP	$1.0 \cdot 10^2$	$5.8 \cdot 10^{-1}$	3.2	$6.4 \cdot 10^1$	$4.2 \cdot 10^{-1}$
Inorganics								
20.	Ammonia	7664-41-7	AETP _{fresh}	x	x	x	x	x
			AETP _{marine}	x	x	x	x	x
			SETP _{fresh}	x	x	x	x	x
			SETP _{marine}	x	x	x	x	x
			TETP	x	x	x	x	x
			HTP	$1.0 \cdot 10^{-1}$	x	x	x	x
21.	Hydrogen sulphide	10102-44-0	AETP _{fresh}	x	x	x	x	x
			AETP _{marine}	x	x	x	x	x
			SETP _{fresh}	x	x	x	x	x
			SETP _{marine}	x	x	x	x	x
			TETP	x	x	x	x	x
			HTP	$2.2 \cdot 10^{-1}$	x	x	x	x

Substance No.	Name	CAS No.	Type	Initial emission compartment				
				air	fresh water	sea water	agricult. soil	industrial soil
Inorganics								
22.	Hydrogen chloride	7446-9-5	AETP _{fresh}	x	x	x	x	x
			AETP _{marine}	x	x	x	x	x
			SETP _{fresh}	x	x	x	x	x
			SETP _{marine}	x	x	x	x	x
			TETP	x	x	x	x	x
			HTP	5.0·10 ⁻¹	x	x	x	x
23.	Nitrogen dioxide	7783-6-4	AETP _{fresh}	x	x	x	x	x
			AETP _{marine}	x	x	x	x	x
			SETP _{fresh}	x	x	x	x	x
			SETP _{marine}	x	x	x	x	x
			TETP	x	x	x	x	x
			HTP	1.2	x	x	x	x
24.	Sulphur dioxide	7647-1-0	AETP _{fresh}	x	x	x	x	x
			AETP _{marine}	x	x	x	x	x
			SETP _{fresh}	x	x	x	x	x
			SETP _{marine}	x	x	x	x	x
			TETP	x	x	x	x	x
			HTP	3.1·10 ⁻¹	x	x	x	x
25.	PM10		AETP _{fresh}	x	x	x	x	x
			AETP _{marine}	x	x	x	x	x
			SETP _{fresh}	x	x	x	x	x
			SETP _{marine}	x	x	x	x	x
			TETP	x	x	x	x	x
			HTP	9.6·10 ⁻²	x	x	x	x
Non-aromatics								
26.	Acrylonitrile	107-13-1	AETP _{fresh}	4.1·10 ⁻¹	7.9·10 ¹	6.0·10 ⁻³	6.5	8.1
			AETP _{marine}	9.1·10 ⁻¹	5.4·10 ⁻¹	3.1	2.1·10 ⁻¹	2.7·10 ⁻¹
			SETP _{fresh}	2.7·10 ⁻¹	5.2·10 ¹	3.9·10 ⁻³	4.2	5.3
			SETP _{marine}	7.7·10 ⁻¹	5.1·10 ⁻¹	4.0	1.9·10 ⁻¹	2.3·10 ⁻¹
			TETP	8.0·10 ⁻³	3.9·10 ⁻³	1.2·10 ⁻⁴	2.5	2.1
			HTP	3.4·10 ³	7.1·10 ³	5.1·10 ¹	4.9·10 ⁵	1.5·10 ³
27.	Acrolein	107-2-8	AETP _{fresh}	5.2·10 ²	2.5·10 ⁵	5.0	4.5·10 ⁴	4.5·10 ⁴
			AETP _{marine}	5.7·10 ²	1.1·10 ³	8.9·10 ³	2.5·10 ²	2.5·10 ²
			SETP _{fresh}	3.9·10 ²	1.9·10 ⁵	3.7	3.4·10 ⁴	3.4·10 ⁴
			SETP _{marine}	7.5·10 ²	1.6·10 ³	1.3·10 ⁴	3.6·10 ²	3.6·10 ²
			TETP	1.6·10 ¹	5.8	1.6·10 ⁻¹	7.0·10 ³	7.0·10 ³
			HTP	5.7·10 ¹	5.9·10 ¹	8.0·10 ⁻¹	2.3·10 ²	1.7·10 ¹
28.	1,3-Butadiene	75-15-0	AETP _{fresh}	3.3·10 ⁻⁷	3.0	5.6·10 ⁻⁸	5.7·10 ⁻⁵	5.7·10 ⁻⁵
			AETP _{marine}	2.7·10 ⁻⁶	8.7·10 ⁻³	7.3·10 ⁻¹	2.9·10 ⁻⁶	2.9·10 ⁻⁶
			SETP _{fresh}	2.2·10 ⁻⁷	2.0	3.8·10 ⁻⁸	3.8·10 ⁻⁵	3.8·10 ⁻⁵
			SETP _{marine}	3.0·10 ⁻⁶	9.9·10 ⁻³	8.3·10 ⁻¹	3.2·10 ⁻⁶	3.2·10 ⁻⁶
			TETP	2.3·10 ⁻⁸	2.1·10 ⁻⁸	4.0·10 ⁻⁹	3.1·10 ⁻⁴	3.1·10 ⁻⁴
			HTP	2.2·10 ³	7.0·10 ³	4.5·10 ²	3.1·10 ³	2.2·10 ³
29.	Carbon disulfide	106-99-0	AETP _{fresh}	3.3·10 ⁻²	1.1·10 ²	6.5·10 ⁻³	3.4·10 ⁻¹	3.4·10 ⁻¹
			AETP _{marine}	1.5	1.8	3.0·10 ¹	1.4	1.4
			SETP _{fresh}	2.7·10 ⁻²	8.6·10 ¹	5.4·10 ⁻³	2.8·10 ⁻¹	2.8·10 ⁻¹
			SETP _{marine}	8.6·10 ⁻¹	1.4	4.5·10 ¹	7.9·10 ⁻¹	7.9·10 ⁻¹
			TETP	5.1·10 ⁻³	4.8·10 ⁻³	1.0·10 ⁻³	1.6	1.6
			HTP	2.4	2.4	4.8·10 ⁻¹	3.6	2.2

Substance No.	Name	CAS No.	Type	Initial emission compartment				
				air	fresh water	sea water	agricult. soil	industrial soil
Non-aromatics								
30.	Ethylene	74-85-1	AETP _{fresh}	1.4·10 ⁻¹¹	2.2·10 ⁻²	1.0·10 ⁻¹²	1.1·10 ⁻⁹	1.1·10 ⁻⁹
			AETP _{marine}	7.9·10 ⁻¹¹	2.8·10 ⁻⁵	2.6·10 ⁻³	7.8·10 ⁻¹¹	7.8·10 ⁻¹¹
			SETP _{fresh}	9.0·10 ⁻¹²	1.4·10 ⁻²	6.6·10 ⁻¹³	7.1·10 ⁻¹⁰	7.1·10 ⁻¹⁰
			SETP _{marine}	7.1·10 ⁻¹¹	3.4·10 ⁻⁵	3.2·10 ⁻³	7.1·10 ⁻¹¹	7.1·10 ⁻¹¹
			TETP	1.3·10 ⁻¹²	1.1·10 ⁻¹²	9.9·10 ⁻¹⁴	2.3·10 ⁻⁹	2.3·10 ⁻⁹
			HTP	6.4·10 ⁻¹	6.5·10 ⁻¹	4.7·10 ⁻²	7.8·10 ⁻¹	6.2·10 ⁻¹
31.	Formaldehyde	50-00-0	AETP _{fresh}	8.3	2.8·10 ²	2.1·10 ⁻⁴	1.5·10 ¹	4.4·10 ¹
			AETP _{marine}	1.6	1.9·10 ⁻¹	5.6	1.8·10 ⁻²	5.5·10 ⁻²
			SETP _{fresh}	4.5	1.5·10 ²	1.2·10 ⁻⁴	7.9	2.4·10 ¹
			SETP _{marine}	1.5	2.0·10 ⁻¹	6.0	1.8·10 ⁻²	5.5·10 ⁻²
			TETP	9.4·10 ⁻¹	1.6·10 ⁻³	2.4·10 ⁻⁵	5.8	4.4
			HTP	8.3·10 ⁻¹	3.7·10 ⁻²	2.8·10 ⁻⁵	2.3	1.9·10 ⁻²
32.	Propylene oxide	75-56-9	AETP _{fresh}	3.7·10 ⁻²	4.0	4.4·10 ⁻⁴	4.2·10 ⁻¹	4.8·10 ⁻¹
			AETP _{marine}	1.4·10 ⁻¹	6.4·10 ⁻²	1.5·10 ⁻¹	3.3·10 ⁻²	3.7·10 ⁻²
			SETP _{fresh}	2.0·10 ⁻²	2.1	2.4·10 ⁻⁴	2.3·10 ⁻¹	2.5·10 ⁻¹
			SETP _{marine}	6.6·10 ⁻²	3.4·10 ⁻²	1.5·10 ⁻¹	1.6·10 ⁻²	1.8·10 ⁻²
			TETP	1.5·10 ⁻³	6.5·10 ⁻⁴	1.8·10 ⁻⁵	1.4·10 ⁻¹	1.2·10 ⁻¹
			HTP	1.3·10 ³	2.6·10 ³	1.6·10 ¹	2.2·10 ⁵	5.9·10 ²
Aromatics								
33.	Benzene	71-43-2	AETP _{fresh}	8.4·10 ⁻⁵	9.1·10 ⁻²	9.2·10 ⁻⁶	7.2·10 ⁻⁴	7.2·10 ⁻⁴
			AETP _{marine}	2.8·10 ⁻³	2.7·10 ⁻³	1.5·10 ⁻²	2.4·10 ⁻³	2.4·10 ⁻³
			SETP _{fresh}	6.4·10 ⁻⁵	7.0·10 ⁻²	7.0·10 ⁻⁶	5.4·10 ⁻⁴	5.4·10 ⁻⁴
			SETP _{marine}	1.3·10 ⁻³	1.4·10 ⁻³	2.1·10 ⁻²	1.1·10 ⁻³	1.1·10 ⁻³
			TETP	1.6·10 ⁻⁵	1.4·10 ⁻⁵	1.7·10 ⁻⁶	3.4·10 ⁻³	3.4·10 ⁻³
			HTP	1.9·10 ³	1.8·10 ³	2.1·10 ²	1.5·10 ⁴	1.6·10 ³
34.	Toluene	108-88-3	AETP _{fresh}	7.0·10 ⁻⁵	2.9·10 ⁻¹	8.3·10 ⁻⁶	1.1·10 ⁻³	1.1·10 ⁻³
			AETP _{marine}	7.0·10 ⁻⁴	1.2·10 ⁻³	5.1·10 ⁻²	4.5·10 ⁻⁴	4.5·10 ⁻⁴
			SETP _{fresh}	5.0·10 ⁻⁵	2.1·10 ⁻¹	5.9·10 ⁻⁶	7.5·10 ⁻⁴	7.5·10 ⁻⁴
			SETP _{marine}	5.8·10 ⁻⁴	1.3·10 ⁻³	6.3·10 ⁻²	3.7·10 ⁻⁴	3.7·10 ⁻⁴
			TETP	1.6·10 ⁻⁵	1.4·10 ⁻⁵	1.9·10 ⁻⁶	1.9·10 ⁻²	1.9·10 ⁻²
			HTP	3.3·10 ⁻¹	3.0·10 ⁻¹	3.9·10 ⁻²	3.5·10 ⁻¹	2.1·10 ⁻¹
35.	Styrene	100-42-5	AETP _{fresh}	5.1·10 ⁻⁵	4.4·10 ⁻¹	1.0·10 ⁻⁵	1.5·10 ⁻³	2.6·10 ⁻³
			AETP _{marine}	5.1·10 ⁻⁴	2.2·10 ⁻³	1.2·10 ⁻¹	1.1·10 ⁻⁴	1.8·10 ⁻⁴
			SETP _{fresh}	3.5·10 ⁻⁵	3.0·10 ⁻¹	7.0·10 ⁻⁶	1.1·10 ⁻³	1.8·10 ⁻³
			SETP _{marine}	3.6·10 ⁻⁴	1.6·10 ⁻³	9.3·10 ⁻²	7.6·10 ⁻⁵	1.3·10 ⁻⁴
			TETP	1.4·10 ⁻⁷	1.3·10 ⁻⁷	2.7·10 ⁻⁸	1.4·10 ⁻³	1.2·10 ⁻³
			HTP	4.7·10 ⁻²	8.5·10 ⁻²	1.0·10 ⁻²	4.8·10 ⁻¹	1.8·10 ⁻²
36.	Phenol	108-95-2	AETP _{fresh}	1.5	2.4·10 ²	1.7·10 ⁻⁵	3.5	1.3·10 ¹
			AETP _{marine}	5.5·10 ⁻¹	5.6·10 ⁻²	4.7	1.7·10 ⁻³	6.1·10 ⁻³
			SETP _{fresh}	5.6·10 ⁻¹	8.8·10 ¹	6.4·10 ⁻⁶	1.3	4.7
			SETP _{marine}	3.6·10 ⁻¹	3.8·10 ⁻²	3.2	1.1·10 ⁻³	4.0·10 ⁻³
			TETP	3.3·10 ⁻³	2.5·10 ⁻⁶	3.8·10 ⁻⁸	4.5·10 ⁻²	4.1·10 ⁻²
			HTP	5.2·10 ⁻¹	4.9·10 ⁻²	8.0·10 ⁻⁵	1.9	6.0·10 ⁻³
37.	Ethylbenzene	100-41-4	AETP _{fresh}	1.3·10 ⁻⁴	5.5·10 ⁻¹	9.4·10 ⁻⁶	1.8·10 ⁻³	1.8·10 ⁻³
			AETP _{marine}	8.0·10 ⁻⁴	1.4·10 ⁻³	6.2·10 ⁻²	4.1·10 ⁻⁴	4.1·10 ⁻⁴
			SETP _{fresh}	8.7·10 ⁻⁵	3.6·10 ⁻¹	6.3·10 ⁻⁶	1.2·10 ⁻³	1.2·10 ⁻³
			SETP _{marine}	6.1·10 ⁻⁴	1.3·10 ⁻³	6.7·10 ⁻²	3.2·10 ⁻⁴	3.2·10 ⁻⁴
			TETP	1.4·10 ⁻⁶	1.2·10 ⁻⁶	1.0·10 ⁻⁷	1.9·10 ⁻³	1.9·10 ⁻³
			HTP	9.7·10 ⁻¹	8.3·10 ⁻¹	7.0·10 ⁻²	7.5·10 ⁻¹	5.0·10 ⁻¹

Substance No.	Name	CAS No.	Type	Initial emission compartment				
				air	fresh water	sea water	agricult. soil	industrial soil
Aromatics								
38.	m-Xylene	108-38-3	AETP _{fresh}	4.4·10 ⁻⁵	6.0·10 ⁻¹	7.2·10 ⁻⁶	1.9·10 ⁻³	1.9·10 ⁻³
			AETP _{marine}	3.9·10 ⁻⁴	2.1·10 ⁻³	1.4·10 ⁻¹	2.5·10 ⁻⁴	2.5·10 ⁻⁴
			SETP _{fresh}	2.8·10 ⁻⁵	3.9·10 ⁻¹	4.7·10 ⁻⁶	1.2·10 ⁻³	1.2·10 ⁻³
			SETP _{marine}	3.5·10 ⁻⁴	2.1·10 ⁻³	1.4·10 ⁻¹	2.3·10 ⁻⁴	2.3·10 ⁻⁴
			TETP	6.5·10 ⁻⁷	6.0·10 ⁻⁷	1.1·10 ⁻⁷	3.0·10 ⁻³	3.0·10 ⁻³
			HTP	2.7·10 ⁻²	3.4·10 ⁻¹	1.0·10 ⁻²	3.8	1.9·10 ⁻²
39.	o-Xylene	95-47-6	AETP _{fresh}	9.3·10 ⁻⁵	5.6·10 ⁻¹	1.5·10 ⁻⁵	2.5·10 ⁻³	2.5·10 ⁻³
			AETP _{marine}	9.1·10 ⁻⁴	2.5·10 ⁻³	1.3·10 ⁻¹	5.5·10 ⁻⁴	5.5·10 ⁻⁴
			SETP _{fresh}	7.4·10 ⁻⁵	4.5·10 ⁻¹	1.2·10 ⁻⁵	2.0·10 ⁻³	2.0·10 ⁻³
			SETP _{marine}	9.9·10 ⁻⁴	3.1·10 ⁻³	1.7·10 ⁻¹	6.0·10 ⁻⁴	6.0·10 ⁻⁴
			TETP	1.3·10 ⁻⁶	1.2·10 ⁻⁶	2.1·10 ⁻⁷	3.4·10 ⁻³	3.4·10 ⁻³
			HTP	1.2·10 ⁻¹	4.2·10 ⁻¹	2.6·10 ⁻²	5.0	7.6·10 ⁻²
40.	p-Xylene	106-42-3	AETP _{fresh}	6.1·10 ⁻⁵	5.5·10 ⁻¹	1.0·10 ⁻⁵	1.4·10 ⁻³	1.4·10 ⁻³
			AETP _{marine}	6.1·10 ⁻⁴	2.2·10 ⁻³	1.3·10 ⁻¹	3.2·10 ⁻⁴	3.2·10 ⁻⁴
			SETP _{fresh}	3.7·10 ⁻⁵	3.3·10 ⁻¹	6.1·10 ⁻⁶	8.6·10 ⁻⁴	8.7·10 ⁻⁴
			SETP _{marine}	3.8·10 ⁻⁴	1.6·10 ⁻³	9.7·10 ⁻²	2.0·10 ⁻⁴	2.0·10 ⁻⁴
			TETP	5.3·10 ⁻⁷	4.9·10 ⁻⁷	8.9·10 ⁻⁸	1.5·10 ⁻³	1.5·10 ⁻³
			HTP	4.3·10 ⁻²	3.5·10 ⁻¹	1.3·10 ⁻²	3.0	2.5·10 ⁻²
41.	Butylbenzylphtalate	85-68-7	AETP _{fresh}	4.0·10 ⁻¹	7.6·10 ¹	3.2·10 ⁻⁵	2.5·10 ⁻²	1.0·10 ⁻¹
			AETP _{marine}	3.2·10 ⁻¹	5.3·10 ⁻²	1.6	2.9·10 ⁻⁵	1.2·10 ⁻⁴
			SETP _{fresh}	1.3·10 ⁻¹	2.5·10 ¹	1.0·10 ⁻⁵	8.2·10 ⁻³	3.3·10 ⁻²
			SETP _{marine}	7.1·10 ⁻²	1.3·10 ⁻²	4.0·10 ⁻¹	7.1·10 ⁻⁶	2.8·10 ⁻⁵
			TETP	1.3·10 ⁻³	6.6·10 ⁻⁶	1.0·10 ⁻⁷	1.0·10 ⁻²	1.0·10 ⁻²
			HTP	1.0·10 ¹	8.6·10 ⁻²	8.5·10 ⁻⁴	3.1·10 ⁻¹	1.8·10 ⁻³
42	Di(2ethylhexyl)phtalate	117-81-7	AETP _{fresh}	3.5·10 ⁻¹	7.9·10 ¹	1.6·10 ⁻³	1.5·10 ⁻³	6.0·10 ⁻³
			AETP _{marine}	2.4	3.7·10 ⁻¹	1.5·10 ¹	1.6·10 ⁻⁵	6.2·10 ⁻⁵
			SETP _{fresh}	4.7·10 ⁻¹	1.0·10 ²	2.1·10 ⁻³	2.0·10 ⁻³	7.9·10 ⁻³
			SETP _{marine}	1.7	2.7·10 ⁻¹	1.1·10 ¹	1.1·10 ⁻⁵	4.4·10 ⁻⁵
			TETP	2.2·10 ⁻⁴	6.6·10 ⁻⁶	9.6·10 ⁻⁷	1.4·10 ⁻³	1.4·10 ⁻³
			HTP	2.6	9.1·10 ⁻¹	4.0·10 ⁻²	1.8	5.2·10 ⁻³
43.	Dibutylphtalate	84-74-2	AETP _{fresh}	5.6·10 ⁻¹	7.9·10 ¹	2.9·10 ⁻⁵	7.9·10 ⁻²	3.1·10 ⁻¹
			AETP _{marine}	4.4·10 ⁻¹	7.7·10 ⁻²	1.7	1.2·10 ⁻⁴	4.8·10 ⁻⁴
			SETP _{fresh}	7.3·10 ⁻²	1.0·10 ¹	3.8·10 ⁻⁶	1.0·10 ⁻²	4.1·10 ⁻²
			SETP _{marine}	3.8·10 ⁻²	7.5·10 ⁻³	1.6·10 ⁻¹	1.1·10 ⁻⁵	4.5·10 ⁻⁵
			TETP	3.9·10 ⁻³	1.3·10 ⁻⁵	2.1·10 ⁻⁷	2.3·10 ⁻²	2.3·10 ⁻²
			HTP	2.5·10 ¹	5.4·10 ⁻¹	3.0·10 ⁻³	1.3	1.3·10 ⁻²
44.	Diethylphtalate	84-66-2	AETP _{fresh}	4.2·10 ⁻¹	3.4·10 ¹	7.9·10 ⁻⁵	1.6·10 ⁻¹	6.3·10 ⁻¹
			AETP _{marine}	3.4·10 ⁻¹	1.1·10 ⁻¹	8.0·10 ⁻¹	7.1·10 ⁻⁴	2.8·10 ⁻³
			SETP _{fresh}	2.8·10 ⁻¹	2.2·10 ¹	5.2·10 ⁻⁵	1.1·10 ⁻¹	4.1·10 ⁻¹
			SETP _{marine}	2.3·10 ⁻¹	9.4·10 ⁻²	6.5·10 ⁻¹	5.6·10 ⁻⁴	2.2·10 ⁻³
			TETP	5.3·10 ⁻¹	5.6·10 ⁻³	1.0·10 ⁻⁴	2.1	2.1
			HTP	3.2·10 ⁻¹	1.4·10 ⁻¹	5.7·10 ⁻⁴	5.7·10 ⁻²	3.3·10 ⁻³
45.	Dihexylphtalate	84-75-3	AETP _{fresh}	5.0·10 ⁻¹	1.1·10 ²	1.1·10 ⁻²	1.8·10 ⁻²	7.4·10 ⁻²
			AETP _{marine}	1.7	1.2	9.7	4.3·10 ⁻⁴	1.7·10 ⁻³
			SETP _{fresh}	1.2	2.6·10 ²	2.6·10 ⁻²	4.4·10 ⁻²	1.8·10 ⁻¹
			SETP _{marine}	3.2	2.3	2.0·10 ¹	8.0·10 ⁻⁴	3.2·10 ⁻³
			TETP	7.8·10 ⁻⁴	2.6·10 ⁻⁴	1.7·10 ⁻⁵	7.3·10 ⁻³	7.3·10 ⁻³
			HTP	7.0·10 ³	1.4·10 ⁴	3.7·10 ²	1.2·10 ³	1.4·10 ¹

Substance No.	Name	CAS No.	Type	Initial emission compartment				
				air	fresh water	sea water	agricult. soil	industrial soil
Aromatics								
46.	Diisooctylphthalate	27554-26-3	AETP _{fresh}	1.2·10 ⁻¹	2.1·10 ¹	3.9·10 ⁻³	6.2·10 ⁻⁴	2.5·10 ⁻³
			AETP _{marine}	3.6	4.3·10 ⁻¹	1.6·10 ¹	6.5·10 ⁻⁵	2.6·10 ⁻⁴
			SETP _{fresh}	2.8·10 ⁻¹	4.7·10 ¹	8.7·10 ⁻³	1.4·10 ⁻³	5.5·10 ⁻³
			SETP _{marine}	5.6	7.2·10 ⁻¹	2.8·10 ¹	1.0·10 ⁻⁴	4.1·10 ⁻⁴
			TETP	1.1·10 ⁻⁴	6.4·10 ⁻⁶	3.5·10 ⁻⁶	5.5·10 ⁻⁴	5.5·10 ⁻⁴
			HTP	3.1·10 ²	1.8·10 ¹	9.7	3.2·10 ¹	5.2·10 ⁻²
47.	Diisodecylphthalate	26761-40-0	AETP _{fresh}	5.6·10 ⁻¹	8.6·10 ¹	3.8·10 ⁻²	4.6·10 ⁻³	1.8·10 ⁻²
			AETP _{marine}	4.7	2.3	1.9·10 ¹	8.6·10 ⁻⁴	3.4·10 ⁻³
			SETP _{fresh}	1.2	1.9·10 ²	8.5·10 ⁻²	1.0·10 ⁻²	4.1·10 ⁻²
			SETP _{marine}	7.5	3.8	3.4·10 ¹	1.4·10 ⁻³	5.4·10 ⁻³
			TETP	9.2·10 ⁻⁴	3.8·10 ⁻⁴	6.4·10 ⁻⁵	4.0·10 ⁻³	4.0·10 ⁻³
			HTP	4.6·10 ¹	1.9·10 ¹	3.2	1.1·10 ²	3.8·10 ⁻²
48.	Dimethylphthalate	133-11-3	AETP _{fresh}	5.2·10 ⁻²	3.1	3.8·10 ⁻⁷	7.4·10 ⁻³	2.9·10 ⁻²
			AETP _{marine}	2.7·10 ⁻²	1.7·10 ⁻³	5.2·10 ⁻²	9.7·10 ⁻⁶	3.8·10 ⁻⁵
			SETP _{fresh}	1.3·10 ⁻²	7.9·10 ⁻¹	9.8·10 ⁻⁸	1.9·10 ⁻³	7.5·10 ⁻³
			SETP _{marine}	6.2·10 ⁻³	4.3·10 ⁻⁴	1.3·10 ⁻²	2.3·10 ⁻⁶	9.1·10 ⁻⁶
			TETP	6.4·10 ⁻¹	3.7·10 ⁻⁴	4.7·10 ⁻⁶	1.4	1.4
			HTP	2.1·10 ²	7.2	8.4·10 ⁻³	2.8·10 ¹	2.7·10 ⁻¹
49.	Diocetylphthalate	117-84-0	AETP _{fresh}	1.6·10 ⁻²	2.8	1.4·10 ⁻⁴	4.2·10 ⁻⁵	1.7·10 ⁻⁴
			AETP _{marine}	5.4·10 ⁻¹	3.5·10 ⁻²	2.5	1.3·10 ⁻⁶	5.2·10 ⁻⁶
			SETP _{fresh}	2.7·10 ⁻²	4.7	2.4·10 ⁻⁴	7.1·10 ⁻⁵	2.8·10 ⁻⁴
			SETP _{marine}	5.2·10 ⁻¹	3.6·10 ⁻²	2.6	1.3·10 ⁻⁶	5.1·10 ⁻⁶
			TETP	9.8·10 ⁻⁶	1.3·10 ⁻⁷	8.8·10 ⁻⁸	4.8·10 ⁻⁵	4.8·10 ⁻⁵
			HTP	1.9·10 ¹	6.3	1.3	8.6	8.8·10 ⁻³
50.	Phthalic anhydride	85-44-9	AETP _{fresh}	8.2·10 ⁻³	5.5·10 ⁻¹	4.6·10 ⁻¹¹	4.8·10 ⁻⁵	3.1·10 ⁻⁵
			AETP _{marine}	8.5·10 ⁻³	4.1·10 ⁻⁶	1.7·10 ⁻²	1.8·10 ⁻⁸	1.2·10 ⁻⁸
			SETP _{fresh}	1.7·10 ⁻⁵	1.1·10 ⁻³	9.4·10 ⁻¹⁴	9.8·10 ⁻⁸	6.3·10 ⁻⁸
			SETP _{marine}	4.9·10 ⁻⁵	2.4·10 ⁻⁸	9.9·10 ⁻⁵	1.1·10 ⁻¹⁰	6.8·10 ⁻¹¹
			TETP	5.1·10 ⁻⁴	1.2·10 ⁻¹⁰	2.8·10 ⁻¹²	2.6·10 ⁻³	4.2·10 ⁻⁴
			HTP	4.1·10 ⁻¹	1.1·10 ⁻⁴	1.0·10 ⁻⁷	1.0·10 ⁻²	6.6·10 ⁻⁷
Polycyclic aromatics								
51.	Naphthalene	91-20-3	AETP _{fresh}	5.0·10 ⁻¹	6.6·10 ²	1.1·10 ⁻²	3.8	1.2·10 ¹
			AETP _{marine}	9.1·10 ⁻¹	1.1	3.3·10 ¹	5.7·10 ⁻²	1.9·10 ⁻¹
			SETP _{fresh}	1.9·10 ⁻¹	2.6·10 ²	4.5·10 ⁻³	1.5	4.9
			SETP _{marine}	3.2·10 ⁻¹	3.8·10 ⁻¹	1.2·10 ¹	2.0·10 ⁻²	6.7·10 ⁻²
			TETP	8.2·10 ⁻⁴	4.9·10 ⁻⁴	1.9·10 ⁻⁵	3.1	2.6
			HTP	8.1	5.6	1.9·10 ⁻¹	4.8	1.6
52.	Anthracene	120-12-7	AETP _{fresh}	1.4·10 ²	5.7·10 ⁴	1.7·10 ¹	8.2·10 ¹	3.2·10 ²
			AETP _{marine}	1.7·10 ³	3.0·10 ³	1.8·10 ⁴	6.2	2.5·10 ¹
			SETP _{fresh}	1.9·10 ²	8.0·10 ⁴	2.3·10 ¹	1.1·10 ²	4.5·10 ²
			SETP _{marine}	2.1·10 ³	4.1·10 ³	2.5·10 ⁴	8.2	3.2·10 ¹
			TETP	3.2·10 ⁻²	2.0·10 ⁻²	4.0·10 ⁻³	8.9	8.8
			HTP	5.2·10 ⁻¹	2.1	1.6·10 ⁻¹	5.1·10 ⁻¹	2.0·10 ⁻²
53.	Phenanthrene	85-1-8	AETP _{fresh}	1.3	5.2·10 ²	5.8·10 ⁻²	2.9·10 ⁻¹	1.2
			AETP _{marine}	7.3	1.0·10 ¹	7.4·10 ¹	8.7·10 ⁻³	3.5·10 ⁻²
			SETP _{fresh}	1.4	5.6·10 ²	6.3·10 ⁻²	3.2·10 ⁻¹	1.3
			SETP _{marine}	5.4	8.6	6.4·10 ¹	7.0·10 ⁻³	2.8·10 ⁻²
			TETP	1.4·10 ⁻⁴	6.0·10 ⁻⁵	6.3·10 ⁻⁶	3.7·10 ⁻²	3.7·10 ⁻²
			HTP	x	x	x	x	x

No.	Substance Name	CAS No.	Type	Initial emission compartment				
				air	fresh water	sea water	agricult. soil	industrial soil
Polycyclic aromatics								
54.	Fluoranthrene	206-44-0	AETP _{fresh}	1.8·10 ¹	1.3·10 ⁴	8.7·10 ⁻¹	1.9·10 ¹	7.6·10 ¹
			AETP _{marine}	2.0·10 ²	8.7·10 ²	4.2·10 ³	1.3	5.3
			SETP _{fresh}	5.3·10 ¹	3.9·10 ⁴	2.6	5.7·10 ¹	2.3·10 ²
			SETP _{marine}	6.1·10 ²	2.8·10 ³	1.4·10 ⁴	4.3	1.7·10 ¹
			TETP	1.8·10 ⁻²	4.9·10 ⁻³	9.6·10 ⁻⁴	2.3	2.3
			HTP	x	x	x	x	x
55.	Benzo[a]anthracene	56-55-3	AETP _{fresh}	4.2·10 ¹	1.1·10 ⁵	1.1	6.2·10 ¹	2.5·10 ²
			AETP _{marine}	1.0·10 ³	8.3·10 ³	8.5·10 ⁴	4.5	1.8·10 ¹
			SETP _{fresh}	1.3·10 ²	3.5·10 ⁵	3.2	1.9·10 ²	7.4·10 ²
			SETP _{marine}	3.4·10 ³	2.8·10 ⁴	2.8·10 ⁵	1.5·10 ¹	6.0·10 ¹
			TETP	2.3·10 ⁻¹	1.4·10 ⁻²	6.2·10 ⁻³	3.1·10 ¹	3.1·10 ¹
			HTP	x	x	x	x	x
56.	Chrysene	218-1-9	AETP _{fresh}	3.9·10 ¹	1.9·10 ⁴	2.6·10 ⁻¹	7.4·10 ¹	2.9·10 ²
			AETP _{marine}	4.1·10 ²	3.0·10 ³	7.6·10 ³	1.2·10 ¹	4.7·10 ¹
			SETP _{fresh}	1.3·10 ²	5.9·10 ⁴	8.3·10 ⁻¹	2.4·10 ²	9.3·10 ²
			SETP _{marine}	1.4·10 ³	1.0·10 ⁴	2.6·10 ⁴	4.0·10 ¹	1.6·10 ²
			TETP	2.2·10 ⁻¹	8.4·10 ⁻³	1.6·10 ⁻³	4.6	4.5
			HTP	x	x	x	x	x
57.	Benzo[k]fluoranthrene	207-8-9	AETP _{fresh}	3.9·10 ³	1.2·10 ⁶	9.1	5.2·10 ³	2.0·10 ⁴
			AETP _{marine}	1.2·10 ⁵	4.4·10 ⁵	1.5·10 ⁶	2.0·10 ³	7.8·10 ³
			SETP _{fresh}	1.3·10 ⁴	3.9·10 ⁶	3.0·10 ¹	1.7·10 ⁴	6.8·10 ⁴
			SETP _{marine}	3.5·10 ⁵	1.3·10 ⁶	4.4·10 ⁶	5.9·10 ³	2.3·10 ⁴
			TETP	3.0·10 ¹	2.1·10 ⁻¹	8.8·10 ⁻²	3.9·10 ²	3.9·10 ²
			HTP	x	x	x	x	x
58.	Benzo[a]pyrene	50-32-8	AETP _{fresh}	8.8·10 ¹	2.5·10 ⁵	2.8·10 ⁻¹	1.3·10 ²	5.3·10 ²
			AETP _{marine}	1.4·10 ³	1.2·10 ⁴	1.2·10 ⁵	6.5	2.6·10 ¹
			SETP _{fresh}	2.5·10 ²	7.2·10 ⁵	8.0·10 ⁻¹	3.8·10 ²	1.5·10 ³
			SETP _{marine}	4.1·10 ³	3.6·10 ⁴	3.7·10 ⁵	1.9·10 ¹	7.7·10 ¹
			TETP	2.4·10 ⁻¹	2.5·10 ⁻³	8.0·10 ⁻⁴	2.3·10 ¹	2.3·10 ¹
			HTP	x	x	x	x	x
59.	Benzo[ghi]perylene	191-24-2	AETP _{fresh}	4.4·10 ¹	5.2·10 ⁴	4.9·10 ⁻²	6.1·10 ¹	2.4·10 ²
			AETP _{marine}	1.7·10 ³	9.1·10 ³	6.5·10 ⁴	1.1·10 ¹	4.3·10 ¹
			SETP _{fresh}	1.4·10 ²	1.7·10 ⁵	1.6·10 ⁻¹	2.0·10 ²	7.8·10 ²
			SETP _{marine}	5.7·10 ³	3.2·10 ⁴	2.3·10 ⁵	3.7·10 ¹	1.5·10 ²
			TETP	2.0·10 ⁻¹	4.3·10 ⁻⁴	2.5·10 ⁻⁴	8.3	8.3
			HTP	x	x	x	x	x
60.	Indeno[1,2,3-cd]pyrene	193-39-5	AETP _{fresh}	1.7·10 ²	7.7·10 ⁴	7.4·10 ⁻⁴	9.0·10 ¹	3.6·10 ²
			AETP _{marine}	7.3·10 ³	1.5·10 ⁴	1.1·10 ⁵	1.7·10 ¹	6.8·10 ¹
			SETP _{fresh}	5.3·10 ²	2.5·10 ⁵	2.4·10 ⁻³	2.9·10 ²	1.2·10 ³
			SETP _{marine}	2.5·10 ⁴	5.0·10 ⁴	3.8·10 ⁵	5.9·10 ¹	2.4·10 ²
			TETP	8.0·10 ⁻¹	6.2·10 ⁻⁶	4.1·10 ⁻⁶	1.3·10 ¹	1.3·10 ¹
			HTP	x	x	x	x	x
61.	Carcinogenic PAHs		AETP _{fresh}	1.7·10 ²	2.8·10 ⁴	1.2·10 ⁻¹	5.8·10 ¹	2.3·10 ²
			AETP _{marine}	4.3·10 ³	5.5·10 ³	2.4·10 ⁴	1.2·10 ¹	4.8·10 ¹
			SETP _{fresh}	5.6·10 ²	8.9·10 ⁴	3.8·10 ⁻¹	1.9·10 ²	7.5·10 ²
			SETP _{marine}	1.4·10 ⁴	1.8·10 ⁴	8.0·10 ⁴	4.1·10 ¹	1.6·10 ²
			TETP	1.0	2.1·10 ⁻³	8.1·10 ⁻⁴	6.3	6.3
			HTP	5.7·10 ⁵	2.8·10 ⁵	2.9·10 ⁴	7.1·10 ⁴	2.7·10 ³

Substance No. Name	CAS No.	Type	Initial emission compartment					
			air	fresh water	sea water	agricult. soil	industrial soil	
Halogenated non-aromatics								
62. Dichloromethane	75-9-2	AETP _{fresh}	$3.3 \cdot 10^{-5}$	$1.2 \cdot 10^{-2}$	$5.0 \cdot 10^{-6}$	$1.6 \cdot 10^{-4}$	$1.6 \cdot 10^{-4}$	
		AETP _{marine}	$3.8 \cdot 10^{-3}$	$3.5 \cdot 10^{-3}$	$3.2 \cdot 10^{-3}$	$2.5 \cdot 10^{-3}$	$2.5 \cdot 10^{-3}$	
		SETP _{fresh}	$2.4 \cdot 10^{-5}$	$8.8 \cdot 10^{-3}$	$3.6 \cdot 10^{-6}$	$1.1 \cdot 10^{-4}$	$1.1 \cdot 10^{-4}$	
		SETP _{marine}	$1.4 \cdot 10^{-3}$	$1.3 \cdot 10^{-3}$	$3.8 \cdot 10^{-3}$	$9.2 \cdot 10^{-4}$	$9.2 \cdot 10^{-4}$	
		TETP	$4.3 \cdot 10^{-6}$	$3.9 \cdot 10^{-6}$	$6.5 \cdot 10^{-7}$	$2.5 \cdot 10^{-4}$	$2.5 \cdot 10^{-4}$	
		HTP	2.0	1.8	$3.0 \cdot 10^{-1}$	2.4	1.3	
63. Trichloromethane	67-66-3	AETP _{fresh}	$9.5 \cdot 10^{-5}$	$4.2 \cdot 10^{-2}$	$4.5 \cdot 10^{-5}$	$4.7 \cdot 10^{-4}$	$4.7 \cdot 10^{-4}$	
		AETP _{marine}	$5.9 \cdot 10^{-2}$	$5.8 \cdot 10^{-2}$	$5.6 \cdot 10^{-2}$	$4.7 \cdot 10^{-2}$	$4.7 \cdot 10^{-2}$	
		SETP _{fresh}	$4.9 \cdot 10^{-5}$	$2.2 \cdot 10^{-2}$	$2.3 \cdot 10^{-5}$	$2.4 \cdot 10^{-4}$	$2.4 \cdot 10^{-4}$	
		SETP _{marine}	$1.6 \cdot 10^{-2}$	$1.6 \cdot 10^{-2}$	$3.3 \cdot 10^{-2}$	$1.3 \cdot 10^{-2}$	$1.3 \cdot 10^{-2}$	
		TETP	$4.0 \cdot 10^{-5}$	$3.9 \cdot 10^{-5}$	$1.9 \cdot 10^{-5}$	$1.6 \cdot 10^{-3}$	$1.6 \cdot 10^{-3}$	
		HTP	$1.3 \cdot 10^1$	$1.3 \cdot 10^1$	6.0	$1.4 \cdot 10^1$	$1.0 \cdot 10^1$	
64. Tetrachloromethane	56-23-5	AETP _{fresh}	$2.5 \cdot 10^{-4}$	$2.1 \cdot 10^{-1}$	$1.9 \cdot 10^{-4}$	$5.6 \cdot 10^{-4}$	$5.6 \cdot 10^{-4}$	
		AETP _{marine}	1.2	1.1	1.1	1.1	1.1	
		SETP _{fresh}	$1.4 \cdot 10^{-4}$	$1.2 \cdot 10^{-1}$	$1.1 \cdot 10^{-4}$	$3.2 \cdot 10^{-4}$	$3.2 \cdot 10^{-4}$	
		SETP _{marine}	$3.1 \cdot 10^{-1}$	$3.1 \cdot 10^{-1}$	$4.6 \cdot 10^{-1}$	$3.0 \cdot 10^{-1}$	$3.0 \cdot 10^{-1}$	
		TETP	$4.7 \cdot 10^{-4}$	$4.7 \cdot 10^{-4}$	$3.6 \cdot 10^{-4}$	$2.1 \cdot 10^{-3}$	$2.1 \cdot 10^{-3}$	
		HTP	$2.2 \cdot 10^2$	$2.2 \cdot 10^2$	$1.7 \cdot 10^2$	$2.2 \cdot 10^2$	$2.2 \cdot 10^2$	
65. 1,2-Dichloroethane	107-6-2	AETP _{fresh}	$1.2 \cdot 10^{-4}$	$2.3 \cdot 10^{-2}$	$8.8 \cdot 10^{-5}$	$7.5 \cdot 10^{-4}$	$7.5 \cdot 10^{-4}$	
		AETP _{marine}	$8.2 \cdot 10^{-2}$	$8.1 \cdot 10^{-2}$	$9.1 \cdot 10^{-2}$	$5.9 \cdot 10^{-2}$	$5.9 \cdot 10^{-2}$	
		SETP _{fresh}	$1.0 \cdot 10^{-4}$	$1.9 \cdot 10^{-2}$	$7.4 \cdot 10^{-5}$	$6.3 \cdot 10^{-4}$	$6.3 \cdot 10^{-4}$	
		SETP _{marine}	$3.1 \cdot 10^{-2}$	$3.1 \cdot 10^{-2}$	$6.1 \cdot 10^{-2}$	$2.2 \cdot 10^{-2}$	$2.2 \cdot 10^{-2}$	
		TETP	$2.6 \cdot 10^{-5}$	$2.6 \cdot 10^{-5}$	$2.0 \cdot 10^{-5}$	$1.7 \cdot 10^{-3}$	$1.7 \cdot 10^{-3}$	
		HTP	6.8	$2.8 \cdot 10^1$	5.5	$1.3 \cdot 10^3$	5.7	
66. 1,1,1-Trichloroethane	71-55-6	AETP _{fresh}	$1.2 \cdot 10^{-4}$	$1.1 \cdot 10^{-1}$	$7.2 \cdot 10^{-5}$	$3.7 \cdot 10^{-4}$	$3.7 \cdot 10^{-4}$	
		AETP _{marine}	$3.3 \cdot 10^{-1}$	$3.2 \cdot 10^{-1}$	$2.8 \cdot 10^{-1}$	$3.1 \cdot 10^{-1}$	$3.1 \cdot 10^{-1}$	
		SETP _{fresh}	$1.0 \cdot 10^{-4}$	$9.0 \cdot 10^{-2}$	$5.9 \cdot 10^{-5}$	$3.1 \cdot 10^{-4}$	$3.1 \cdot 10^{-4}$	
		SETP _{marine}	$1.1 \cdot 10^{-1}$	$1.1 \cdot 10^{-1}$	$1.9 \cdot 10^{-1}$	$1.0 \cdot 10^{-1}$	$1.0 \cdot 10^{-1}$	
		TETP	$1.8 \cdot 10^{-4}$	$1.8 \cdot 10^{-4}$	$1.1 \cdot 10^{-4}$	$1.5 \cdot 10^{-3}$	$1.5 \cdot 10^{-3}$	
		HTP	$1.7 \cdot 10^1$	$1.7 \cdot 10^1$	9.9	$1.6 \cdot 10^1$	$1.6 \cdot 10^1$	
67. Trichloroethylene	79-1-6	AETP _{fresh}	$3.8 \cdot 10^{-5}$	$9.7 \cdot 10^{-2}$	$1.6 \cdot 10^{-5}$	$4.6 \cdot 10^{-4}$	$4.6 \cdot 10^{-4}$	
		AETP _{marine}	$2.7 \cdot 10^{-3}$	$3.3 \cdot 10^{-3}$	$5.7 \cdot 10^{-2}$	$2.5 \cdot 10^{-3}$	$2.5 \cdot 10^{-3}$	
		SETP _{fresh}	$3.2 \cdot 10^{-5}$	$8.2 \cdot 10^{-2}$	$1.3 \cdot 10^{-5}$	$3.9 \cdot 10^{-4}$	$3.9 \cdot 10^{-4}$	
		SETP _{marine}	$1.7 \cdot 10^{-3}$	$2.7 \cdot 10^{-3}$	$8.1 \cdot 10^{-2}$	$1.5 \cdot 10^{-3}$	$1.5 \cdot 10^{-3}$	
		TETP	$4.7 \cdot 10^{-6}$	$4.6 \cdot 10^{-6}$	$1.9 \cdot 10^{-6}$	$2.1 \cdot 10^{-3}$	$2.1 \cdot 10^{-3}$	
		HTP	$3.4 \cdot 10^1$	$3.3 \cdot 10^1$	$1.4 \cdot 10^1$	$3.2 \cdot 10^1$	$3.2 \cdot 10^1$	
68. Tetrachloroethylene	127-18-4	AETP _{fresh}	$4.1 \cdot 10^{-4}$	$7.0 \cdot 10^{-1}$	$2.0 \cdot 10^{-4}$	$2.2 \cdot 10^{-3}$	$2.2 \cdot 10^{-3}$	
		AETP _{marine}	$3.4 \cdot 10^{-1}$	$3.4 \cdot 10^{-1}$	$6.5 \cdot 10^{-1}$	$3.1 \cdot 10^{-1}$	$3.1 \cdot 10^{-1}$	
		SETP _{fresh}	$3.9 \cdot 10^{-4}$	$6.7 \cdot 10^{-1}$	$1.9 \cdot 10^{-4}$	$2.1 \cdot 10^{-3}$	$2.1 \cdot 10^{-3}$	
		SETP _{marine}	$1.2 \cdot 10^{-1}$	$1.3 \cdot 10^{-1}$	$7.8 \cdot 10^{-1}$	$1.1 \cdot 10^{-1}$	$1.1 \cdot 10^{-1}$	
		TETP	$8.1 \cdot 10^{-3}$	$7.9 \cdot 10^{-3}$	$4.0 \cdot 10^{-3}$	$3.0 \cdot 10^{-1}$	$3.0 \cdot 10^{-1}$	
		HTP	5.5	5.7	2.8	6.4	5.2	
69. Vinylchloride	75-1-4	AETP _{fresh}	$2.9 \cdot 10^{-6}$	$2.8 \cdot 10^{-2}$	$1.4 \cdot 10^{-6}$	$6.4 \cdot 10^{-5}$	$6.4 \cdot 10^{-5}$	
		AETP _{marine}	$1.3 \cdot 10^{-4}$	$3.8 \cdot 10^{-4}$	$2.0 \cdot 10^{-2}$	$1.3 \cdot 10^{-4}$	$1.3 \cdot 10^{-4}$	
		SETP _{fresh}	$2.3 \cdot 10^{-6}$	$2.3 \cdot 10^{-2}$	$1.1 \cdot 10^{-6}$	$5.2 \cdot 10^{-5}$	$5.2 \cdot 10^{-5}$	
		SETP _{marine}	$1.2 \cdot 10^{-4}$	$4.9 \cdot 10^{-4}$	$2.9 \cdot 10^{-2}$	$1.2 \cdot 10^{-4}$	$1.2 \cdot 10^{-4}$	
		TETP	$2.6 \cdot 10^{-7}$	$2.6 \cdot 10^{-7}$	$1.3 \cdot 10^{-7}$	$3.1 \cdot 10^{-4}$	$3.1 \cdot 10^{-4}$	
		HTP	$8.4 \cdot 10^1$	$1.4 \cdot 10^2$	$4.3 \cdot 10^1$	$5.2 \cdot 10^2$	$8.3 \cdot 10^1$	

Substance No.	Name	CAS No.	Type	Initial emission compartment				
				air	fresh water	sea water	agricult. soil	industria l soil
Halogenated non-aromatics								
70.	Hexachloro-1,3-butadiene	87-68-3	AETP _{fresh}	4.6·10 ¹	4.5·10 ⁴	2.3·10 ¹	7.0·10 ¹	8.4·10 ¹
			AETP _{marine}	7.7·10 ⁴	7.5·10 ⁴	7.0·10 ⁴	2.8·10 ⁴	3.4·10 ⁴
			SETP _{fresh}	5.4·10 ¹	5.2·10 ⁴	2.6·10 ¹	8.0·10 ¹	9.7·10 ¹
			SETP _{marine}	2.9·10 ⁴	2.8·10 ⁴	4.7·10 ⁴	1.1·10 ⁴	1.3·10 ⁴
			TETP	4.2	4.0	2.1	5.3·10 ¹	4.7·10 ¹
			HTP	7.9·10 ⁴	8.0·10 ⁴	3.9·10 ⁴	3.0·10 ⁴	3.5·10 ⁴
Halogenated aromatics								
71.	Chlorobenzene	108-90-7	AETP _{fresh}	4.7·10 ⁻⁴	3.6·10 ⁻¹	2.6·10 ⁻⁴	3.2·10 ⁻³	3.2·10 ⁻³
			AETP _{marine}	1.1·10 ⁻¹	1.1·10 ⁻¹	3.5·10 ⁻¹	8.3·10 ⁻²	8.3·10 ⁻²
			SETP _{fresh}	4.4·10 ⁻⁴	3.4·10 ⁻¹	2.4·10 ⁻⁴	3.0·10 ⁻³	3.0·10 ⁻³
			SETP _{marine}	5.0·10 ⁻²	5.5·10 ⁻²	4.5·10 ⁻¹	3.7·10 ⁻²	3.7·10 ⁻²
			TETP	7.3·10 ⁻⁴	7.2·10 ⁻⁴	4.1·10 ⁻⁴	1.2·10 ⁻¹	1.2·10 ⁻¹
			HTP	9.2	9.1	5.2	7.1	6.8
72.	1,2-Dichlorobenzene	95-50-1	AETP _{fresh}	2.9·10 ⁻³	1.0	1.3·10 ⁻³	1.9·10 ⁻²	1.9·10 ⁻²
			AETP _{marine}	6.7·10 ⁻¹	6.6·10 ⁻¹	9.5·10 ⁻¹	5.1·10 ⁻¹	5.1·10 ⁻¹
			SETP _{fresh}	2.7·10 ⁻³	9.5·10 ⁻¹	1.2·10 ⁻³	1.8·10 ⁻²	1.8·10 ⁻²
			SETP _{marine}	2.8·10 ⁻¹	2.8·10 ⁻¹	1.0	2.1·10 ⁻¹	2.1·10 ⁻¹
			TETP	5.3·10 ⁻⁴	5.2·10 ⁻⁴	2.4·10 ⁻⁴	5.4·10 ⁻²	5.4·10 ⁻²
			HTP	9.1	8.9	4.1	7.3	6.9
73.	1,3-Dichlorobenzene	541-73-1	AETP _{fresh}	2.4·10 ⁻³	1.2	1.1·10 ⁻³	1.8·10 ⁻²	1.8·10 ⁻²
			AETP _{marine}	4.6·10 ⁻¹	4.6·10 ⁻¹	1.0	3.7·10 ⁻¹	3.7·10 ⁻¹
			SETP _{fresh}	2.2·10 ⁻³	1.2	1.0·10 ⁻³	1.6·10 ⁻²	1.6·10 ⁻²
			SETP _{marine}	2.0·10 ⁻¹	2.1·10 ⁻¹	1.2	1.6·10 ⁻¹	1.6·10 ⁻¹
			TETP	4.4·10 ⁻⁴	4.2·10 ⁻⁴	2.0·10 ⁻⁴	6.2·10 ⁻²	6.2·10 ⁻²
			HTP	6.2·10 ¹	7.4·10 ¹	3.0·10 ¹	2.5·10 ²	5.0·10 ¹
74.	1,4-Dichlorobenzene	106-46-7	AETP _{fresh}	2.4·10 ⁻³	1.0	1.1·10 ⁻³	1.4·10 ⁻²	1.4·10 ⁻²
			AETP _{marine}	7.4·10 ⁻¹	7.3·10 ⁻¹	1.0	5.5·10 ⁻¹	5.5·10 ⁻¹
			SETP _{fresh}	2.4·10 ⁻³	1.0	1.1·10 ⁻³	1.4·10 ⁻²	1.4·10 ⁻²
			SETP _{marine}	2.9·10 ⁻¹	2.9·10 ⁻¹	1.0	2.1·10 ⁻¹	2.1·10 ⁻¹
			TETP	1.2·10 ⁻²	1.2·10 ⁻²	5.7·10 ⁻³	1.0	1.0
			HTP	1.0	1.1	4.7·10 ⁻¹	2.9	7.4·10 ⁻¹
75.	1,2,3-Trichlorobenzene	87-61-6	AETP _{fresh}	8.5·10 ⁻³	4.0	3.9·10 ⁻³	2.3·10 ⁻²	3.0·10 ⁻²
			AETP _{marine}	2.1	2.1	3.6	6.5·10 ⁻¹	8.6·10 ⁻¹
			SETP _{fresh}	9.3·10 ⁻³	4.4	4.3·10 ⁻³	2.5·10 ⁻²	3.3·10 ⁻²
			SETP _{marine}	8.5·10 ⁻¹	8.7·10 ⁻¹	3.5	2.6·10 ⁻¹	3.5·10 ⁻¹
			TETP	7.5·10 ⁻²	7.3·10 ⁻²	3.5·10 ⁻²	9.3	8.0
			HTP	1.3·10 ²	1.3·10 ²	6.2·10 ¹	5.6·10 ¹	5.4·10 ¹
76.	1,2,4-Trichlorobenzene	120-82-1	AETP _{fresh}	9.9·10 ⁻³	3.5	4.4·10 ⁻³	2.0·10 ⁻²	3.2·10 ⁻²
			AETP _{marine}	2.0	2.0	3.1	4.3·10 ⁻¹	7.1·10 ⁻¹
			SETP _{fresh}	1.1·10 ⁻²	3.8	4.8·10 ⁻³	2.2·10 ⁻²	3.6·10 ⁻²
			SETP _{marine}	8.4·10 ⁻¹	8.6·10 ⁻¹	2.9	1.8·10 ⁻¹	3.0·10 ⁻¹
			TETP	8.8·10 ⁻³	8.5·10 ⁻³	4.0·10 ⁻³	1.2	9.9·10 ⁻¹
			HTP	1.2·10 ²	1.2·10 ²	5.6·10 ¹	4.2·10 ¹	4.3·10 ¹
77.	1,3,5-Trichlorobenzene	108-70-3	AETP _{fresh}	1.6·10 ⁻²	5.0	7.0·10 ⁻³	5.4·10 ⁻²	6.6·10 ⁻²
			AETP _{marine}	3.0	3.0	4.5	1.1	1.3
			SETP _{fresh}	1.7·10 ⁻²	5.2	7.2·10 ⁻³	5.6·10 ⁻²	6.9·10 ⁻²
			SETP _{marine}	1.3	1.3	4.5	4.5·10 ⁻¹	5.5·10 ⁻¹
			TETP	1.9·10 ⁻³	1.8·10 ⁻³	8.3·10 ⁻⁴	2.5·10 ⁻¹	2.2·10 ⁻¹
			HTP	1.2·10 ²	1.2·10 ²	5.4·10 ¹	6.9·10 ¹	5.2·10 ¹

Substance No.	Name	CAS No.	Type	Initial emission compartment				
				air	fresh water	sea water	agricult. soil	industria l soil
Halogenated aromatics								
78.	1,2,3,4-Tetrachlorobenzene	634-66-2	AETP _{fresh}	1.0·10 ⁻¹	1.6·10 ¹	3.8·10 ⁻²	2.8·10 ⁻²	1.0·10 ⁻¹
			AETP _{marine}	1.7·10 ¹	1.6·10 ¹	1.5·10 ¹	3.9·10 ⁻¹	1.5
			SETP _{fresh}	1.2·10 ⁻¹	1.9·10 ¹	4.5·10 ⁻²	3.2·10 ⁻²	1.2·10 ⁻¹
			SETP _{marine}	6.9	6.7	1.2·10 ¹	1.6·10 ⁻¹	6.0·10 ⁻¹
			TETP	9.9·10 ⁻³	9.3·10 ⁻³	3.7·10 ⁻³	8.3·10 ⁻¹	7.7·10 ⁻¹
			HTP	5.0·10 ¹	1.6·10 ²	3.0·10 ¹	8.0·10 ¹	5.2
79.	1,2,3,5-Tetrachlorobenzene	634-90-2	AETP _{fresh}	7.3·10 ⁻²	1.4·10 ¹	3.0·10 ⁻²	8.3·10 ⁻²	1.9·10 ⁻¹
			AETP _{marine}	1.8·10 ¹	1.7·10 ¹	1.6·10 ¹	2.3	5.1
			SETP _{fresh}	8.1·10 ⁻²	1.6·10 ¹	3.3·10 ⁻²	9.3·10 ⁻²	2.1·10 ⁻¹
			SETP _{marine}	7.0	7.0	1.3·10 ¹	9.0·10 ⁻¹	2.0
			TETP	1.8·10 ⁻¹	1.7·10 ⁻¹	7.4·10 ⁻²	1.5·10 ¹	1.2·10 ¹
			HTP	4.6·10 ¹	9.2·10 ¹	2.5·10 ¹	1.8·10 ²	1.4·10 ¹
80.	1,2,4,5-Tetrachlorobenzene	95-94-3	AETP _{fresh}	7.3·10 ⁻²	1.3·10 ¹	2.9·10 ⁻²	2.5·10 ⁻²	9.0·10 ⁻²
			AETP _{marine}	1.5·10 ¹	1.4·10 ¹	1.3·10 ¹	5.1·10 ⁻¹	1.8
			SETP _{fresh}	8.5·10 ⁻²	1.5·10 ¹	3.3·10 ⁻²	2.9·10 ⁻²	1.0·10 ⁻¹
			SETP _{marine}	6.1	5.9	1.0·10 ¹	2.1·10 ⁻¹	7.4·10 ⁻¹
			TETP	2.4·10 ⁻¹	2.3·10 ⁻¹	9.5·10 ⁻²	1.9·10 ¹	1.7·10 ¹
			HTP	3.5·10 ¹	1.8·10 ²	3.0·10 ¹	8.4·10 ¹	5.4
81.	Pentachlorobenzene	608-93-5	AETP _{fresh}	3.7·10 ⁻¹	5.1·10 ¹	2.4·10 ⁻¹	5.9·10 ⁻¹	1.1
			AETP _{marine}	1.7·10 ²	1.7·10 ²	1.7·10 ²	2.8·10 ¹	5.4·10 ¹
			SETP _{fresh}	5.2·10 ⁻¹	7.2·10 ¹	3.3·10 ⁻¹	8.3·10 ⁻¹	1.6
			SETP _{marine}	8.7·10 ¹	8.7·10 ¹	1.4·10 ²	1.4·10 ¹	2.7·10 ¹
			TETP	3.9·10 ⁻²	3.8·10 ⁻²	2.6·10 ⁻²	2.1	1.7
			HTP	4.1·10 ²	1.2·10 ³	4.1·10 ²	4.5·10 ³	1.4·10 ²
82.	Hexachlorobenzene	118-74-1	AETP _{fresh}	1.3	1.5·10 ²	1.1	3.2	4.3
			AETP _{marine}	2.4·10 ³	2.4·10 ³	2.4·10 ³	7.2·10 ²	9.6·10 ²
			SETP _{fresh}	4.3	4.9·10 ²	3.6	1.0·10 ¹	1.4·10 ¹
			SETP _{marine}	2.8·10 ³	2.7·10 ³	3.4·10 ³	8.3·10 ²	1.1·10 ³
			TETP	2.6·10 ⁻¹	2.6·10 ⁻¹	2.4·10 ⁻¹	3.5	3.0
			HTP	3.2·10 ⁶	5.6·10 ⁶	3.4·10 ⁶	3.3·10 ⁷	1.3·10 ⁶
83.	2-Chlorophenol	95-57-8	AETP _{fresh}	1.3·10 ¹	1.6·10 ³	6.7·10 ⁻³	7.9	3.1·10 ¹
			AETP _{marine}	1.2·10 ¹	1.3·10 ¹	4.6·10 ¹	6.8·10 ⁻²	2.6·10 ⁻¹
			SETP _{fresh}	1.0·10 ¹	1.3·10 ³	5.3·10 ⁻³	6.3	2.4·10 ¹
			SETP _{marine}	1.3·10 ¹	1.7·10 ¹	6.1·10 ¹	9.0·10 ⁻²	3.5·10 ⁻¹
			TETP	5.3·10 ⁻²	1.3·10 ⁻³	2.7·10 ⁻⁵	3.8·10 ⁻¹	3.7·10 ⁻¹
			HTP	2.2·10 ¹	7.0·10 ¹	3.5·10 ⁻¹	8.3	1.4
84.	2,4-Dichlorophenol	120-83-2	AETP _{fresh}	1.4	1.7·10 ²	2.9·10 ⁻⁴	2.5	9.2
			AETP _{marine}	1.3	2.5·10 ⁻¹	3.7	7.0·10 ⁻³	2.7·10 ⁻²
			SETP _{fresh}	5.5·10 ⁻¹	6.8·10 ¹	1.1·10 ⁻⁴	1.0	3.6
			SETP _{marine}	5.2·10 ⁻¹	1.3·10 ⁻¹	2.0	3.2·10 ⁻³	1.2·10 ⁻²
			TETP	3.0·10 ⁻²	9.6·10 ⁻⁴	6.2·10 ⁻⁶	5.9·10 ⁻¹	5.4·10 ⁻¹
			HTP	9.5·10 ¹	1.6·10 ¹	6.5·10 ⁻²	7.4·10 ²	1.9
85.	2,4,5-Trichlorophenol	95-95-4	AETP _{fresh}	1.5·10 ¹	1.6·10 ³	5.4·10 ⁻²	2.8·10 ¹	9.9·10 ¹
			AETP _{marine}	5.3·10 ¹	6.4·10 ¹	1.2·10 ²	1.3	4.6
			SETP _{fresh}	1.7·10 ¹	1.9·10 ³	6.4·10 ⁻²	3.3·10 ¹	1.2·10 ²
			SETP _{marine}	4.8·10 ¹	8.1·10 ¹	1.6·10 ²	1.6	5.7
			TETP	2.4·10 ⁻¹	6.1·10 ⁻²	9.1·10 ⁻⁴	4.4	3.9

HTP 8.3 $4.5 \cdot 10^1$ $6.1 \cdot 10^{-1}$ 5.3 2.9

Substance No. Name	CAS No.	Type	Initial emission compartment				
			air	fresh water	sea water	agricult. soil	industria l soil
Halogenated aromatics							
86. 2,4,6-Trichlorophenol	88-6-2	AETP _{fresh}	5.9	2.9·10 ²	2.4·10 ⁻⁴	1.2	4.8
		AETP _{marine}	3.9	1.6	7.6	8.2·10 ⁻³	3.2·10 ⁻²
		SETP _{fresh}	5.7	2.9·10 ²	2.3·10 ⁻⁴	1.2	4.7
		SETP _{marine}	4.3	1.9	8.9	9.5·10 ⁻³	3.7·10 ⁻²
		TETP	3.2·10 ⁻¹	6.7·10 ⁻⁴	1.3·10 ⁻⁵	7.0·10 ⁻¹	6.8·10 ⁻¹
		HTP	1.4·10 ⁴	9.1·10 ³	4.7·10 ¹	1.8·10 ³	1.7·10 ²
87. 2,3,4,6-Tetrachlorophenol	58-90-2	AETP _{fresh}	8.0·10 ¹	5.2·10 ³	1.3·10 ⁻³	3.2·10 ¹	1.2·10 ²
		AETP _{marine}	1.3·10 ²	9.1·10 ¹	2.2·10 ²	6.2·10 ⁻¹	2.5
		SETP _{fresh}	8.7·10 ¹	5.7·10 ³	1.4·10 ⁻³	3.5·10 ¹	1.3·10 ²
		SETP _{marine}	1.1·10 ²	1.0·10 ²	2.5·10 ²	6.8·10 ⁻¹	2.7
		TETP	3.1·10 ⁻¹	1.7·10 ⁻³	5.2·10 ⁻⁶	1.0	9.7·10 ⁻¹
		HTP	2.9·10 ²	3.5·10 ¹	2.6·10 ⁻¹	3.1·10 ¹	1.6
88. Pentachlorophenol	87-86-5	AETP _{fresh}	1.1·10 ¹	7.1·10 ²	1.2·10 ⁻⁵	3.3·10 ⁻¹	1.3
		AETP _{marine}	4.0·10 ¹	1.2·10 ¹	7.8·10 ¹	5.9·10 ⁻³	2.7·10 ⁻²
		SETP _{fresh}	2.4·10 ¹	1.6·10 ³	2.7·10 ⁻⁵	7.4·10 ⁻¹	3.0
		SETP _{marine}	6.9·10 ¹	2.2·10 ¹	1.4·10 ²	1.1·10 ⁻²	4.9·10 ⁻²
		TETP	2.3	3.2·10 ⁻⁴	2.6·10 ⁻⁶	4.8	4.8
		HTP	5.1	7.2	1.4·10 ⁻¹	1.5·10 ⁻¹	3.9·10 ⁻²
89. Benzylchloride	100-44-7	AETP _{fresh}	7.6·10 ⁻¹	2.0·10 ²	1.1·10 ⁻²	9.2·10 ⁻¹	3.2
		AETP _{marine}	2.1	1.2	7.8	8.2·10 ⁻²	2.9·10 ⁻¹
		SETP _{fresh}	1.1·10 ⁻¹	2.9·10 ¹	1.7·10 ⁻³	1.3·10 ⁻¹	4.7·10 ⁻¹
		SETP _{marine}	3.3·10 ⁻¹	1.9·10 ⁻¹	1.9	1.3·10 ⁻²	4.5·10 ⁻²
		TETP	1.7·10 ⁻³	8.3·10 ⁻⁴	2.5·10 ⁻⁵	8.0·10 ⁻¹	7.1·10 ⁻¹
		HTP	3.5·10 ³	2.4·10 ³	5.5·10 ¹	5.5·10 ³	4.9·10 ²
90. 3-Chloroaniline	108-42-9	AETP _{fresh}	1.0·10 ²	2.5·10 ³	3.7·10 ⁻⁶	7.4·10 ¹	2.5·10 ²
		AETP _{marine}	2.3·10 ¹	1.1·10 ¹	5.9·10 ¹	3.2·10 ⁻¹	1.2
		SETP _{fresh}	9.3·10 ¹	2.3·10 ³	3.4·10 ⁻⁶	6.8·10 ¹	2.3·10 ²
		SETP _{marine}	3.2·10 ¹	1.5·10 ¹	8.2·10 ¹	4.5·10 ⁻¹	1.6
		TETP	4.7·10 ⁻¹	9.4·10 ⁻⁶	1.7·10 ⁻⁸	1.4	1.2
		HTP	1.7·10 ⁴	3.5·10 ³	2.1	3.0·10 ⁴	4.6·10 ²
91. 4-Chloroaniline	106-47-8	AETP _{fresh}	2.0	3.1·10 ³	1.1·10 ⁻²	1.7·10 ²	4.9·10 ²
		AETP _{marine}	1.7	1.4·10 ¹	9.6·10 ¹	7.7·10 ⁻¹	2.2
		SETP _{fresh}	1.8	2.7·10 ³	9.7·10 ⁻³	1.5·10 ²	4.2·10 ²
		SETP _{marine}	2.3	2.0·10 ¹	1.4·10 ²	1.1	3.3
		TETP	1.6·10 ⁻²	3.6·10 ⁻³	8.6·10 ⁻⁵	1.6·10 ¹	1.1·10 ¹
		HTP	2.6·10 ²	2.9·10 ³	4.0	3.5·10 ⁴	5.1·10 ²
92. 3,4-Dichloroaniline	95-76-1	AETP _{fresh}	1.7·10 ³	1.9·10 ⁴	1.2·10 ⁻³	1.8·10 ³	4.0·10 ³
		AETP _{marine}	1.7·10 ³	2.8·10 ³	3.3·10 ³	2.7·10 ²	6.0·10 ²
		SETP _{fresh}	2.1·10 ³	2.4·10 ⁴	1.5·10 ⁻³	2.3·10 ³	5.0·10 ³
		SETP _{marine}	2.1·10 ³	3.5·10 ³	4.1·10 ³	3.3·10 ²	7.4·10 ²
		TETP	8.7	7.6·10 ⁻⁴	6.7·10 ⁻⁶	2.6·10 ¹	1.8·10 ¹
		HTP	2.2·10 ²	1.3·10 ²	1.5	1.7·10 ³	3.1·10 ¹
93. 1-Chloro-4-nitrobenzene	100-00-5	AETP _{fresh}	1.1·10 ¹	8.6·10 ²	1.9	1.5·10 ²	1.5·10 ²
		AETP _{marine}	3.9·10 ²	3.7·10 ²	3.7·10 ²	1.2·10 ²	1.2·10 ²
		SETP _{fresh}	1.0·10 ¹	7.7·10 ²	1.7	1.3·10 ²	1.3·10 ²
		SETP _{marine}	2.4·10 ²	2.6·10 ²	4.4·10 ²	7.9·10 ¹	7.9·10 ¹
		TETP	5.4·10 ⁻¹	4.4·10 ⁻¹	9.6·10 ⁻²	1.7·10 ¹	1.7·10 ¹
		HTP	1.2·10 ³	1.7·10 ³	2.2·10 ²	2.2·10 ⁴	4.6·10 ²

Substance No. Name	CAS No.	Type	Initial emission compartment				
			air	fresh water	sea water	agricult. soil	industria l soil
Halogenated aromatics							
94. Pentachloronitrobenzene	82-68-8	AETP _{fresh}	4.7·10 ¹	4.0·10 ³	1.1·10 ¹	1.5·10 ¹	5.810 ¹
		AETP _{marine}	6.0·10 ³	2.8·10 ³	5.6·10 ³	3.0·10 ¹	1.210 ²
		SETP _{fresh}	1.3·10 ¹	1.1·10 ³	3.1	4.3	1.710 ¹
		SETP _{marine}	4.4·10 ²	2.2·10 ²	5.5·10 ²	2.3	8.8
		TETP	1.2·10 ⁻¹	5.0·10 ⁻²	2.9·10 ⁻²	2.7	2.6
		HTP	1.9·10 ²	9.1·10 ¹	4.6·10 ¹	7.2·10 ¹	4.3
95. 2,3,7,8-TCDD	1746-1-6	AETP _{fresh}	2.1·10 ⁶	1.7·10 ⁸	1.3·10 ⁵	1.2·10 ⁵	4.9·10 ⁵
		AETP _{marine}	3.0·10 ⁸	4.5·10 ⁷	5.0·10 ⁸	4.5·10 ⁴	1.8·10 ⁵
		SETP _{fresh}	6.8·10 ⁶	5.6·10 ⁸	4.3·10 ⁵	4.0·10 ⁵	1.6·10 ⁶
		SETP _{marine}	8.1·10 ⁸	1.5·10 ⁸	1.9·10 ⁹	1.4·10 ⁵	5.7·10 ⁵
		TETP	1.2·10 ⁴	5.9·10 ²	8.3·10 ²	2.7·10 ⁴	2.7·10 ⁴
		HTP	1.9·10 ⁹	8.6·10 ⁸	4.2·10 ⁸	1.3·10 ⁹	1.0·10 ⁷
Pesticides							
96. Acephate	30560-19-1	AETP _{fresh}	7.9·10 ¹	1.1·10 ³	6.0·10 ⁻⁸	5.1·10 ¹	1.6·10 ²
		AETP _{marine}	1.9·10 ¹	1.5·10 ¹	3.7·10 ¹	6.7·10 ⁻¹	2.1
		SETP _{fresh}	4.0·10 ¹	5.6·10 ²	3.1·10 ⁻⁸	2.6·10 ¹	8.1·10 ¹
		SETP _{marine}	1.8·10 ¹	1.4·10 ¹	3.5·10 ¹	6.4·10 ⁻¹	2.0
		TETP	6.9·10 ⁻¹	2.2·10 ⁻⁸	5.310 ⁻¹⁰	1.7	1.3
		HTP	3.1	2.1	5.1·10 ⁻⁴	2.2·10 ¹	3.1·10 ⁻¹
26. Acrylonitrile	107-13-1	AETP _{fresh}	see non-aromatics				
		AETP _{marine}	see non-aromatics				
		SETP _{fresh}	see non-aromatics				
		SETP _{marine}	see non-aromatics				
		TETP	see non-aromatics				
		HTP	see non-aromatics				
27. Acrolein	107-2-8	AETP _{fresh}	see non-aromatics				
		AETP _{marine}	see non-aromatics				
		SETP _{fresh}	see non-aromatics				
		SETP _{marine}	see non-aromatics				
		TETP	see non-aromatics				
		HTP	see non-aromatics				
97. Aldicarb	116-6-3	AETP _{fresh}	5.1·10 ⁴	4.4·10 ⁵	1.2·10 ⁻¹	9.6·10 ⁴	9.6·10 ⁴
		AETP _{marine}	8.2·10 ³	7.4·10 ³	1.5·10 ⁴	1.6·10 ³	1.6·10 ³
		SETP _{fresh}	4.1·10 ⁴	3.5·10 ⁵	9.8·10 ⁻²	7.6·10 ⁴	7.6·10 ⁴
		SETP _{marine}	1.2·10 ⁴	1.1·10 ⁴	2.2·10 ⁴	2.4·10 ³	2.4·10 ³
		TETP	2.0·10 ³	1.9·10 ⁻¹	4.8·10 ⁻³	4.2·10 ³	4.2·10 ³
		HTP	7.2·10 ¹	6.1·10 ¹	2.4·10 ⁻¹	5.1·10 ²	1.3·10 ¹
98. Aldrin	309-00-2	AETP _{fresh}	2.7	1.2·10 ⁴	1.3	2.8·10 ²	2.9·10 ²
		AETP _{marine}	6.1·10 ¹	2.1·10 ²	8.0·10 ³	3.2·10 ¹	3.3·10 ¹
		SETP _{fresh}	2.4·10 ⁻¹	1.0·10 ³	1.1·10 ⁻¹	2.4·10 ¹	2.5·10 ¹
		SETP _{marine}	5.4	1.9·10 ¹	7.4·10 ²	2.9	3.0
		TETP	1.4·10 ⁻²	1.4·10 ⁻²	6.7·10 ⁻³	2.0·10 ¹	2.0·10 ¹
		HTP	1.9·10 ¹	6.0·10 ³	7.8·10 ²	4.7·10 ³	1.6·10 ²
99. Anilazine	101-5-3	AETP _{fresh}	1.4·10 ¹	1.1·10 ³	1.1·10 ⁻⁷	2.1·10 ⁻¹	8.6·10 ⁻¹
		AETP _{marine}	8.3	2.5·10 ⁻¹	2.0·10 ¹	5.0·10 ⁻⁵	2.0·10 ⁻⁴
		SETP _{fresh}	8.8·10 ⁻¹	7.0·10 ¹	6.8·10 ⁻⁹	1.4·10 ⁻²	5.5·10 ⁻²
		SETP _{marine}	3.4·10 ⁻¹	1.0·10 ⁻²	8.3·10 ⁻¹	2.1·10 ⁻⁶	8.5·10 ⁻⁶
		TETP	9.2·10 ⁻²	5.0·10 ⁻⁸	7.0·10 ⁻¹⁰	2.3·10 ⁻¹	2.3·10 ⁻¹
		HTP	7.2·10 ⁻²	2.4·10 ⁻¹	8.2·10 ⁻⁴	8.0·10 ⁻²	3.0·10 ⁻⁴

Substance No. Name	CAS No.	Type	Initial emission compartment				
			air	fresh water	sea water	agricult. soil	industria l soil
Pesticides							
100. Atrazine	1912-24-9	AETP _{fresh}	3.6·10 ²	5.0·10 ³	8.3·10 ⁻³	3.4·10 ²	9.3·10 ²
		AETP _{marine}	2.8·10 ²	4.9·10 ²	6.1·10 ²	3.4·10 ¹	9.3·10 ¹
		SETP _{fresh}	3.1·10 ²	4.3·10 ³	7.2·10 ⁻³	3.0·10 ²	8.0·10 ²
		SETP _{marine}	3.1·10 ²	5.4·10 ²	6.7·10 ²	3.8·10 ¹	1.0·10 ²
		TETP	2.0	7.6·10 ⁻⁴	5.0·10 ⁻⁵	6.6	4.4
		HTP	4.5	4.6	1.8·10 ⁻²	2.1·10 ¹	8.8·10 ⁻¹
101. Azinphos-ethyl	2642-71-9	AETP _{fresh}	2.9·10 ²	2.7·10 ⁵	4.1·10 ⁻²	2.8·10 ³	3.7·10 ³
		AETP _{marine}	1.6·10 ²	1.0·10 ³	5.9·10 ³	1.1·10 ¹	1.4·10 ¹
		SETP _{fresh}	2.1·10 ²	2.0·10 ⁵	3.0·10 ⁻²	2.0·10 ³	2.7·10 ³
		SETP _{marine}	1.3·10 ²	7.9·10 ²	4.7·10 ³	8.4	1.1·10 ¹
		TETP	2.4	2.1·10 ⁻²	3.4·10 ⁻⁴	2.2·10 ²	7.2·10 ¹
		HTP	2.0·10 ²	4.6·10 ²	1.6	7.6·10 ²	6.9
102. Azinphos-methyl	86-50-0	AETP _{fresh}	4.2·10 ²	5.2·10 ⁴	1.1·10 ⁻⁴	1.9·10 ²	8.0·10 ²
		AETP _{marine}	2.0·10 ²	3.5·10 ¹	1.0·10 ³	1.4·10 ⁻¹	5.8·10 ⁻¹
		SETP _{fresh}	2.2·10 ²	2.7·10 ⁴	5.6·10 ⁻⁵	1.0·10 ²	4.1·10 ²
		SETP _{marine}	5.7·10 ¹	1.0·10 ¹	2.9·10 ²	4.1·10 ⁻²	1.7·10 ⁻¹
		TETP	1.9·10 ⁻¹	3.3·10 ⁻⁶	4.9·10 ⁻⁸	9.7·10 ⁻¹	1.0
		HTP	1.4·10 ¹	2.5	5.7·10 ⁻³	3.9·10 ¹	9.9·10 ⁻²
103. Benomyl	17804-35-2	AETP _{fresh}	3.0·10 ¹	6.8·10 ³	8.9·10 ⁻⁸	4.6	1.8·10 ¹
		AETP _{marine}	2.1·10 ¹	8.6	1.5·10 ²	5.8·10 ⁻³	2.3·10 ⁻²
		SETP _{fresh}	3.9	8.8·10 ²	1.1·10 ⁻⁸	5.9·10 ⁻¹	2.4
		SETP _{marine}	1.8	7.5·10 ⁻¹	1.3·10 ¹	5.0·10 ⁻⁴	2.0·10 ⁻³
		TETP	4.7·10 ⁻¹	8.2·10 ⁻⁸	1.4·10 ⁻⁹	3.5	3.5
		HTP	2.1·10 ⁻²	1.4·10 ⁻¹	2.4·10 ⁻⁴	4.3·10 ⁻¹	1.1·10 ⁻³
104. Bentazone	25057-89-0	AETP _{fresh}	5.6	5.1·10 ¹	7.4·10 ⁻⁹	8.3	1.1·10 ¹
		AETP _{marine}	6.2·10 ⁻¹	2.2·10 ⁻¹	1.2	3.6·10 ⁻²	4.8·10 ⁻²
		SETP _{fresh}	4.5	4.1·10 ¹	6.0·10 ⁻⁹	6.7	8.8
		SETP _{marine}	9.4·10 ⁻¹	3.3·10 ⁻¹	1.8	5.5·10 ⁻²	7.2·10 ⁻²
		TETP	2.5·10 ⁻¹	1.8·10 ⁻⁷	3.3·10 ⁻¹⁰	5.9·10 ⁻¹	5.0·10 ⁻¹
		HTP	2.1	7.3·10 ⁻¹	2.2·10 ⁻³	1.5·10 ¹	1.6·10 ⁻¹
105. Bifenthrin	82657-4-3	AETP _{fresh}	8.2·10 ²	2.4·10 ⁵	5.5·10 ⁻²	1.0·10 ²	4.1·10 ²
		AETP _{marine}	1.0·10 ³	2.1·10 ²	8.9·10 ³	1.1·10 ⁻¹	4.5·10 ⁻¹
		SETP _{fresh}	2.4·10 ³	7.2·10 ⁵	1.6·10 ⁻¹	3.1·10 ²	1.2·10 ³
		SETP _{marine}	3.7·10 ³	8.1·10 ²	3.4·10 ⁴	4.3·10 ⁻¹	1.7
		TETP	8.8	2.1·10 ⁻²	5.9·10 ⁻⁴	8.3·10 ¹	8.3·10 ¹
		HTP	1.9·10 ¹	9.8·10 ¹	7.5·10 ⁻¹	2.9·10 ¹	3.0·10 ⁻¹
106. Captafol	2425-6-1	AETP _{fresh}	2.0·10 ⁴	5.4·10 ⁵	5.0·10 ⁻⁵	2.7·10 ⁴	8.3·10 ⁴
		AETP _{marine}	2.7·10 ⁴	8.0·10 ⁴	9.4·10 ⁴	4.0·10 ³	1.2·10 ⁴
		SETP _{fresh}	3.0·10 ⁴	7.7·10 ⁵	7.3·10 ⁻⁵	3.9·10 ⁴	1.2·10 ⁵
		SETP _{marine}	3.9·10 ⁴	1.2·10 ⁵	1.4·10 ⁵	5.8·10 ³	1.8·10 ⁴
		TETP	5.9	1.9·10 ⁻⁷	1.6·10 ⁻⁸	2.8·10 ¹	2.2·10 ¹
		HTP	8.7·10 ¹	5.0·10 ²	9.7	9.6·10 ²	7.9·10 ¹
107. Captan	133-06-2	AETP _{fresh}	1.6·10 ¹	2.1·10 ³	6.5·10 ⁻⁷	4.0·10 ⁻¹	4.7
		AETP _{marine}	1.0·10 ¹	1.0·10 ⁻¹	4.0·10 ¹	6.9·10 ⁻⁵	8.1·10 ⁻⁴
		SETP _{fresh}	1.4·10 ⁻¹	1.8·10 ¹	5.7·10 ⁻⁹	3.5·10 ⁻³	4.1·10 ⁻²
		SETP _{marine}	1.2·10 ⁻¹	1.3·10 ⁻³	5.0·10 ⁻¹	8.4·10 ⁻⁷	9.9·10 ⁻⁶
		TETP	2.4·10 ⁻²	6.2·10 ⁻⁸	9.4·10 ⁻¹⁰	4.1·10 ⁻²	1.2·10 ⁻¹
		HTP	5.9·10 ⁻¹	5.3·10 ⁻³	5.4·10 ⁻⁶	9.7·10 ⁻²	1.1·10 ⁻⁴

Substance No. Name	CAS No.	Type	Initial emission compartment				
			air	fresh water	sea water	agricult. soil	industria l soil
Pesticides							
108. Carbaryl	63-25-2	AETP _{fresh}	1.1·10 ²	4.5·10 ³	1.9·10 ⁻⁶	2.3·10 ¹	1.2·10 ²
		AETP _{marine}	1.2·10 ¹	1.4	2.4·10 ¹	7.4·10 ⁻³	4.0·10 ⁻²
		SETP _{fresh}	3.2·10 ¹	1.3·10 ³	5.5·10 ⁻⁷	6.7	3.6·10 ¹
		SETP _{marine}	1.0	1.3·10 ⁻¹	2.1	6.5·10 ⁻⁴	3.5·10 ⁻³
		TETP	6.3·10 ⁻²	2.6·10 ⁻⁷	1.1·10 ⁻⁹	1.1·10 ⁻¹	1.4·10 ⁻¹
		HTP	3.2	4.7	1.9·10 ⁻³	2.1·10 ¹	1.5·10 ⁻¹
109. Carbendazim	10605-21-7	AETP _{fresh}	3.0·10 ³	3.8·10 ⁴	2.4·10 ⁻⁸	2.0·10 ³	6.1·10 ³
		AETP _{marine}	7.2·10 ²	5.8·10 ²	1.3·10 ³	3.0·10 ¹	9.3·10 ¹
		SETP _{fresh}	3.0·10 ³	3.9·10 ⁴	2.4·10 ⁻⁸	2.0·10 ³	6.2·10 ³
		SETP _{marine}	1.1·10 ³	8.6·10 ²	2.0·10 ³	4.5·10 ¹	1.4·10 ²
		TETP	2.0·10 ¹	6.3·10 ⁻⁸	1.6·10 ⁻¹⁰	4.9·10 ¹	3.8·10 ¹
		HTP	1.9·10 ¹	2.5	2.0·10 ⁻³	1.4·10 ²	4.3·10 ⁻¹
110. Carbofuran	1563-66-2	AETP _{fresh}	9.0·10 ²	1.3·10 ⁴	1.8·10 ⁻⁴	5.8·10 ²	1.8·10 ³
		AETP _{marine}	1.5·10 ²	4.4·10 ¹	3.0·10 ²	2.0	6.2
		SETP _{fresh}	5.2·10 ²	7.6·10 ³	1.1·10 ⁻⁴	3.4·10 ²	1.1·10 ³
		SETP _{marine}	1.6·10 ²	4.6·10 ¹	3.1·10 ²	2.1	6.6
		TETP	3.0	3.5·10 ⁻⁵	6.1·10 ⁻⁷	7.5	5.9
		HTP	2.0·10 ²	5.6·10 ¹	2.1·10 ⁻¹	1.4·10 ³	8.0
29. Carbon disulfide	75-15-0	AETP _{fresh}	see non-aromatics				
		AETP _{marine}					
		SETP _{fresh}					
		SETP _{marine}					
		TETP					
		HTP					
111. Chlordane	57-74-9	AETP _{fresh}	2.7·10 ²	9.0·10 ⁴	3.1·10 ¹	9.4·10 ¹	3.7·10 ²
		AETP _{marine}	6.1·10 ⁴	8.9·10 ³	4.7·10 ⁵	3.0·10 ¹	1.2·10 ²
		SETP _{fresh}	2.7·10 ¹	9.1·10 ³	3.2	9.5	3.8·10 ¹
		SETP _{marine}	1.6·10 ³	2.7·10 ²	1.5·10 ⁴	8.4·10 ⁻¹	3.3
		TETP	2.2	9.7·10 ⁻²	2.8·10 ⁻¹	7.4·10 ¹	7.3·10 ¹
		HTP	6.7·10 ³	7.4·10 ²	1.2·10 ³	2.8·10 ³	2.7·10 ¹
112. Chlorfenvinphos	470-90-6	AETP _{fresh}	3.2·10 ¹	1.1·10 ³	5.6·10 ⁻⁵	1.6·10 ¹	5.9·10 ¹
		AETP _{marine}	1.1·10 ¹	5.7	2.8·10 ¹	8.5·10 ⁻²	3.1·10 ⁻¹
		SETP _{fresh}	2.7·10 ¹	9.4·10 ²	4.8·10 ⁻⁵	1.4·10 ¹	5.0·10 ¹
		SETP _{marine}	1.3·10 ¹	6.7	3.3·10 ¹	1.0·10 ⁻¹	3.7·10 ⁻¹
		TETP	4.9·10 ⁻¹	4.6·10 ⁻⁵	8.6·10 ⁻⁷	1.3	1.2
		HTP	2.7·10 ²	8.1·10 ²	3.8	1.2·10 ³	4.4·10 ¹
113. Chloridazon	1698-60-8	AETP _{fresh}	2.6·10 ⁻²	3.1·10 ¹	3.5·10 ⁻³	1.8	3.9
		AETP _{marine}	2.2·10 ⁻¹	1.2	8.0	8.1·10 ⁻²	1.8·10 ⁻¹
		SETP _{fresh}	2.0·10 ⁻²	2.5·10 ¹	2.7·10 ⁻³	1.4	3.1
		SETP _{marine}	2.6·10 ⁻¹	1.5	1.0·10 ¹	1.0·10 ⁻¹	2.2·10 ⁻¹
		TETP	4.6·10 ⁻⁴	3.8·10 ⁻⁴	6.4·10 ⁻⁵	9.0·10 ⁻¹	6.8·10 ⁻¹
		HTP	1.3·10 ⁻²	1.4·10 ⁻¹	2.1·10 ⁻³	2.2	2.0·10 ⁻²
114. Chlorothalonil	1897-45-6	AETP _{fresh}	2.5	3.7·10 ²	1.4·10 ⁻¹	1.0	3.7
		AETP _{marine}	5.1·10 ¹	4.0·10 ¹	3.6·10 ¹	1.7	6.0
		SETP _{fresh}	1.8	2.6·10 ²	9.5·10 ⁻²	7.3·10 ⁻¹	2.6
		SETP _{marine}	1.5·10 ¹	1.2·10 ¹	2.3·10 ¹	4.7·10 ⁻¹	1.7
		TETP	7.1·10 ⁻³	5.5·10 ⁻³	3.8·10 ⁻⁴	6.8·10 ⁻¹	6.1·10 ⁻¹
		HTP	8.4	6.7	4.5·10 ⁻¹	9.4·10 ⁻¹	1.0

Substance No. Name	CAS No.	Type	Initial emission compartment				
			air	fresh water	sea water	agricult. soil	industria l soil
Pesticides							
115. Chlorpropham	101-21-3	AETP _{fresh}	2.3	8.3·10 ¹	2.8·10 ⁻⁵	1.8	6.4
		AETP _{marine}	6.4·10 ⁻¹	3.5·10 ⁻¹	2.0	8.4·10 ⁻³	3.0·10 ⁻²
		SETP _{fresh}	2.0	7.1·10 ¹	2.4·10 ⁻⁵	1.6	5.5
		SETP _{marine}	8.1·10 ⁻¹	4.5·10 ⁻¹	2.5	1.1·10 ⁻²	3.8·10 ⁻²
		TETP	3.7·10 ⁻²	2.5·10 ⁻⁵	4.5·10 ⁻⁷	1.3·10 ⁻¹	1.2·10 ⁻¹
		HTP	3.4·10 ⁻¹	1.0	4.3·10 ⁻³	2.1	8.1·10 ⁻²
116. Chlorpyriphos	2921-88-2	AETP _{fresh}	5.2·10 ²	6.4·10 ⁵	2.3·10 ⁻¹	3.6·10 ²	1.4·10 ³
		AETP _{marine}	6.2·10 ¹	2.4·10 ²	2.2·10 ³	1.4·10 ⁻¹	5.8·10 ⁻¹
		SETP _{fresh}	3.3·10 ²	4.1·10 ⁵	1.5·10 ⁻¹	2.3·10 ²	9.3·10 ²
		SETP _{marine}	6.0	2.4·10 ¹	2.2·10 ²	1.4·10 ⁻²	5.8·10 ⁻²
		TETP	1.3·10 ⁻¹	2.1·10 ⁻²	5.7·10 ⁻⁵	1.7·10 ¹	1.7·10 ¹
		HTP	2.1·10 ¹	4.4·10 ¹	3.8·10 ⁻²	1.4·10 ¹	1.4·10 ⁻¹
117. Coumaphos	56-72-4	AETP _{fresh}	2.4·10 ⁵	2.0·10 ⁷	1.1·10 ²	1.0·10 ⁶	3.1·10 ⁶
		AETP _{marine}	3.4·10 ⁵	3.0·10 ⁶	3.6·10 ⁶	1.5·10 ⁵	4.6·10 ⁵
		SETP _{fresh}	3.5·10 ⁵	2.9·10 ⁷	1.5·10 ²	1.5·10 ⁶	4.4·10 ⁶
		SETP _{marine}	4.8·10 ⁵	4.4·10 ⁶	5.2·10 ⁶	2.2·10 ⁵	6.7·10 ⁵
		TETP	1.0·10 ³	6.0	5.0·10 ⁻¹	1.6·10 ⁴	1.2·10 ⁴
		HTP	7.8·10 ²	1.0·10 ⁴	2.2·10 ²	1.1·10 ⁴	1.6·10 ³
118. Cyanazine	21725-46-2	AETP _{fresh}	1.9·10 ³	5.4·10 ⁴	2.5·10 ⁻⁶	8.1·10 ²	3.0·10 ³
		AETP _{marine}	6.3·10 ²	1.9·10 ²	1.3·10 ³	2.8	1.0·10 ¹
		SETP _{fresh}	1.5·10 ³	4.3·10 ⁴	1.9·10 ⁻⁶	6.3·10 ²	2.3·10 ³
		SETP _{marine}	8.1·10 ²	2.5·10 ²	1.6·10 ³	3.7	1.4·10 ¹
		TETP	3.1·10 ¹	2.2·10 ⁻⁶	4.0·10 ⁻⁸	6.9·10 ¹	6.3·10 ¹
		HTP	3.5	6.0	9.6·10 ⁻³	2.4·10 ¹	3.5·10 ⁻¹
119. Cypermethrin	52315-7-8	AETP _{fresh}	8.4·10 ⁴	7.9·10 ⁶	2.4	2.0·10 ⁵	6.9·10 ⁵
		AETP _{marine}	1.9·10 ⁴	1.0·10 ⁴	1.6·10 ⁵	3.0·10 ²	1.0·10 ³
		SETP _{fresh}	1.5·10 ⁵	1.4·10 ⁷	4.3	3.6·10 ⁵	1.3·10 ⁶
		SETP _{marine}	4.9·10 ⁴	2.7·10 ⁴	4.5·10 ⁵	8.0·10 ²	2.8·10 ³
		TETP	8.9·10 ³	1.6·10 ¹	2.5·10 ⁻¹	9.0·10 ⁴	7.8·10 ⁴
		HTP	1.7·10 ²	5.5	2.6·10 ⁻²	5.2·10 ³	1.8
120. Cyromazine	66215-27-8	AETP _{fresh}	3.5·10 ³	2.6·10 ⁴	8.1·10 ⁻⁷	6.5·10 ³	6.5·10 ³
		AETP _{marine}	9.2·10 ²	1.0·10 ³	1.6·10 ³	2.5·10 ²	2.5·10 ²
		SETP _{fresh}	2.8·10 ³	2.1·10 ⁴	6.5·10 ⁻⁷	5.2·10 ³	5.2·10 ³
		SETP _{marine}	1.3·10 ³	1.4·10 ³	2.2·10 ³	3.5·10 ²	3.5·10 ²
		TETP	3.1·10 ²	1.9·10 ⁻⁶	7.3·10 ⁻⁸	6.3·10 ²	6.3·10 ²
		HTP	3.8·10 ¹	5.4	2.6·10 ⁻³	2.8·10 ²	1.3
121. 2,4-D	94-75-7	AETP _{fresh}	3.9·10 ¹	4.0·10 ²	1.1·10 ⁻¹⁰	2.9·10 ¹	8.2·10 ¹
		AETP _{marine}	5.3	2.3	1.0·10 ¹	1.7·10 ⁻¹	4.6·10 ⁻¹
		SETP _{fresh}	2.9·10 ¹	3.0·10 ²	8.5·10 ⁻¹¹	2.2·10 ¹	6.1·10 ¹
		SETP _{marine}	7.3	3.1	1.4·10 ¹	2.3·10 ⁻¹	6.4·10 ⁻¹
		TETP	6.0·10 ⁻¹	9.3·10 ⁻¹⁰	1.8·10 ⁻¹²	1.6	1.1
		HTP	6.6	3.5	6.7·10 ⁻⁵	4.7·10 ¹	7.2·10 ⁻¹
122. DDT	50-29-3	AETP _{fresh}	3.2·10 ²	2.9·10 ⁴	1.5·10 ¹	8.7·10 ¹	3.4·10 ²
		AETP _{marine}	8.6·10 ⁴	4.4·10 ³	1.9·10 ⁵	4.3·10 ¹	1.7·10 ²
		SETP _{fresh}	3.5·10 ²	3.1·10 ⁴	1.6·10 ¹	9.4·10 ¹	3.7·10 ²
		SETP _{marine}	2.5·10 ⁴	1.6·10 ³	7.1·10 ⁴	1.4·10 ¹	5.3·10 ¹
		TETP	1.9·10 ¹	3.1·10 ⁻¹	9.6·10 ⁻¹	6.0·10 ¹	5.9·10 ¹
		HTP	1.1·10 ²	3.7·10 ¹	3.4·10 ¹	2.7·10 ²	1.8

Substance No. Name	CAS No.	Type	Initial emission compartment				
			air	fresh water	sea water	agricult. soil	industria l soil
Pesticides							
123. Deltamethrin	52918-63-5	AETP _{fresh}	1.8·10 ³	6.5·10 ⁵	3.2	2.4·10 ¹	9.6·10 ¹
		AETP _{marine}	3.5·10 ³	9.8·10 ²	3.6·10 ⁴	6.0·10 ⁻²	2.4·10 ⁻¹
		SETP _{fresh}	2.7·10 ³	9.8·10 ⁵	4.8	3.6·10 ¹	1.5·10 ²
		SETP _{marine}	6.8·10 ³	2.0·10 ³	7.2·10 ⁴	1.2·10 ⁻¹	4.7·10 ⁻¹
		TETP	7.6·10 ⁻¹	3.2·10 ⁻²	1.4·10 ⁻³	8.5	8.5
		HTP	1.6	2.8	3.3·10 ⁻²	1.6·10 ⁻¹	3.0·10 ⁻²
124. Demeton	8065-48-3	AETP _{fresh}	2.3·10 ¹	2.2·10 ⁴	1.7·10 ⁻²	8.0·10 ²	2.6·10 ³
		AETP _{marine}	9.1	9.6·10 ¹	5.5·10 ²	3.5	1.1·10 ¹
		SETP _{fresh}	1.6·10 ¹	1.6·10 ⁴	1.2·10 ⁻²	5.7·10 ²	1.8·10 ³
		SETP _{marine}	1.1·10 ¹	1.2·10 ²	7.0·10 ²	4.5	1.5·10 ¹
		TETP	3.0·10 ⁻¹	1.2·10 ⁻²	2.3·10 ⁻⁴	6.0·10 ¹	4.9·10 ¹
		HTP	7.1·10 ¹	7.2·10 ²	3.0·10 ⁻¹	5.7·10 ³	8.9·10 ¹
125. Desmetryn	1014-69-3	AETP _{fresh}	6.8	1.9·10 ²	4.1·10 ⁻⁶	3.0	1.1·10 ¹
		AETP _{marine}	2.6	1.5	5.4	2.4·10 ⁻²	8.8·10 ⁻²
		SETP _{fresh}	4.1	1.2·10 ²	2.4·10 ⁻⁶	1.8	6.6
		SETP _{marine}	2.6	1.6	5.5	2.4·10 ⁻²	8.8·10 ⁻²
		TETP	1.2	3.6·10 ⁻⁵	7.5·10 ⁻⁷	2.9	2.6
		HTP	9.5·10 ¹	5.0·10 ¹	1.2·10 ⁻¹	6.5·10 ²	2.9
126. Diazinon	333-41-5	AETP _{fresh}	2.3·10 ²	1.1·10 ⁵	6.4·10 ⁻²	1.3·10 ³	4.6·10 ³
		AETP _{marine}	1.2·10 ²	6.4·10 ²	2.8·10 ³	7.8	2.7·10 ¹
		SETP _{fresh}	1.6·10 ²	7.7·10 ⁴	4.6·10 ⁻²	9.3·10 ²	3.3·10 ³
		SETP _{marine}	1.1·10 ²	6.1·10 ²	2.7·10 ³	7.5	2.6·10 ¹
		TETP	2.9·10 ⁻¹	4.1·10 ⁻³	8.2·10 ⁻⁵	1.2·10 ¹	1.0·10 ¹
		HTP	5.9·10 ¹	6.6·10 ¹	2.7·10 ⁻¹	1.2·10 ²	3.2
127. Dichlorprop	7547-66-2	AETP _{fresh}	9.9·10 ⁻²	5.3	1.6·10 ⁻¹²	1.3·10 ⁻²	5.1·10 ⁻²
		AETP _{marine}	6.2·10 ⁻²	1.5·10 ⁻²	1.2·10 ⁻¹	3.6·10 ⁻⁵	1.4·10 ⁻⁴
		SETP _{fresh}	5.3·10 ⁻²	2.8	8.3·10 ⁻¹³	6.9·10 ⁻³	2.7·10 ⁻²
		SETP _{marine}	3.2·10 ⁻²	7.7·10 ⁻³	6.4·10 ⁻²	1.9·10 ⁻⁵	7.4·10 ⁻⁵
		TETP	6.8·10 ⁻⁴	6.11·10 ⁻¹²	1.1·10 ⁻¹⁴	1.4·10 ⁻³	1.4·10 ⁻³
		HTP	1.1	2.4·10 ¹	9.7·10 ⁻²	4.5	2.6·10 ⁻¹
128. Dichlorvos	62-73-7	AETP _{fresh}	5.1·10 ²	1.2·10 ⁵	1.1·10 ⁻²	7.4·10 ¹	3.0·10 ²
		AETP _{marine}	4.1·10 ²	1.2·10 ¹	2.4·10 ³	4.1·10 ⁻²	1.6·10 ⁻¹
		SETP _{fresh}	2.3·10 ¹	5.5·10 ³	5.1·10 ⁻⁴	3.3	1.3·10 ¹
		SETP _{marine}	2.7·10 ¹	9.1·10 ⁻¹	1.8·10 ²	2.7·10 ⁻³	1.1·10 ⁻²
		TETP	9.8	1.4·10 ⁻²	2.2·10 ⁻⁴	2.0·10 ²	2.0·10 ²
		HTP	1.0·10 ²	3.4·10 ⁻¹	2.3·10 ⁻³	9.7·10 ⁻¹	3.6·10 ⁻²
129. Dieldrin	60-57-1	AETP _{fresh}	2.0·10 ²	7.9·10 ⁴	1.6·10 ¹	6.0·10 ²	2.3·10 ³
		AETP _{marine}	5.2·10 ³	9.0·10 ³	5.9·10 ⁴	8.1·10 ¹	3.1·10 ²
		SETP _{fresh}	2.0·10 ¹	8.2·10 ³	1.7	6.3·10 ¹	2.4·10 ²
		SETP _{marine}	1.7·10 ²	3.2·10 ²	2.1·10 ³	2.8	1.1·10 ¹
		TETP	1.1	2.6·10 ⁻¹	1.0·10 ⁻¹	1.1·10 ²	1.0·10 ²
		HTP	1.3·10 ⁴	4.5·10 ⁴	5.5·10 ³	7.6·10 ³	1.5·10 ³
130. Dimethoate	60-51-5	AETP _{fresh}	1.3·10 ¹	1.7·10 ²	7.4·10 ⁻⁶	8.9	2.8·10 ¹
		AETP _{marine}	1.6	7.5·10 ⁻¹	3.4	3.9·10 ⁻²	1.2·10 ⁻¹
		SETP _{fresh}	9.3	1.3·10 ²	5.5·10 ⁻⁶	6.6	2.0·10 ¹
		SETP _{marine}	2.0	9.1·10 ⁻¹	4.1	4.8·10 ⁻²	1.5·10 ⁻¹
		TETP	3.0·10 ⁻¹	1.2·10 ⁻⁵	1.8·10 ⁻⁷	8.0·10 ⁻¹	6.2·10 ⁻¹
		HTP	4.4·10 ¹	1.8·10 ¹	3.3·10 ⁻³	3.2·10 ²	3.0

Substance No. Name	CAS No.	Type	Initial emission compartment				
			air	fresh water	sea water	agricult. soil	industria l soil
Pesticides							
48. Dimethylphtalate	133-11-3	AETP _{fresh} AETP _{marine} SETP _{fresh} SETP _{marine} TETP HTP			see aromatics		
131. Dinoseb	88-85-7	AETP _{fresh} AETP _{marine} SETP _{fresh} SETP _{marine} TETP HTP	$1.0 \cdot 10^4$ $4.6 \cdot 10^3$ $2.9 \cdot 10^3$ $1.5 \cdot 10^3$ $9.7 \cdot 10^1$ $3.6 \cdot 10^3$	$3.2 \cdot 10^5$ $5.9 \cdot 10^3$ $8.8 \cdot 10^4$ $2.2 \cdot 10^3$ $3.4 \cdot 10^{-1}$ $1.6 \cdot 10^2$	$1.1 \cdot 10^{-1}$ $1.3 \cdot 10^4$ $2.9 \cdot 10^{-2}$ $5.0 \cdot 10^3$ $1.0 \cdot 10^{-3}$ $6.3 \cdot 10^{-1}$	$2.0 \cdot 10^4$ $3.9 \cdot 10^2$ $5.6 \cdot 10^3$ $1.5 \cdot 10^2$ $5.9 \cdot 10^2$ $5.6 \cdot 10^2$	$5.8 \cdot 10^4$ $1.1 \cdot 10^3$ $1.6 \cdot 10^4$ $4.3 \cdot 10^2$ $4.2 \cdot 10^2$ $9.7 \cdot 10^1$
132. Dinoterb	1420-7-1	AETP _{fresh} AETP _{marine} SETP _{fresh} SETP _{marine} TETP HTP	$2.9 \cdot 10^3$ $7.3 \cdot 10^3$ $1.3 \cdot 10^3$ $2.1 \cdot 10^3$ 3.4 $1.7 \cdot 10^2$	$2.3 \cdot 10^5$ $5.4 \cdot 10^3$ $1.0 \cdot 10^5$ $2.0 \cdot 10^3$ $1.3 \cdot 10^{-2}$ 2.5	$4.2 \cdot 10^{-2}$ $1.2 \cdot 10^4$ $1.9 \cdot 10^{-2}$ $4.5 \cdot 10^3$ $5.1 \cdot 10^{-5}$ $2.9 \cdot 10^{-3}$	$3.3 \cdot 10^2$ 8.7 $1.5 \cdot 10^2$ 3.1 9.9 $3.6 \cdot 10^{-1}$	$1.3 \cdot 10^3$ $3.6 \cdot 10^1$ $5.9 \cdot 10^2$ $1.3 \cdot 10^1$ 9.9 $1.2 \cdot 10^{-1}$
133. Disulfothon	298-4-4	AETP _{fresh} AETP _{marine} SETP _{fresh} SETP _{marine} TETP HTP	$2.7 \cdot 10^1$ $2.0 \cdot 10^1$ 9.2 5.7 $4.3 \cdot 10^{-2}$ $2.9 \cdot 10^2$	$6.4 \cdot 10^4$ $1.2 \cdot 10^2$ $2.2 \cdot 10^4$ $3.5 \cdot 10^1$ $1.2 \cdot 10^{-3}$ $3.4 \cdot 10^2$	$1.3 \cdot 10^{-2}$ $1.5 \cdot 10^3$ $4.6 \cdot 10^{-3}$ $4.2 \cdot 10^2$ $2.1 \cdot 10^{-5}$ 1.5	$7.2 \cdot 10^1$ $1.4 \cdot 10^{-1}$ $2.5 \cdot 10^1$ $4.0 \cdot 10^{-2}$ $1.1 \cdot 10^1$ $1.7 \cdot 10^2$	$2.9 \cdot 10^2$ $5.6 \cdot 10^{-1}$ $9.9 \cdot 10^1$ $1.6 \cdot 10^{-1}$ $1.1 \cdot 10^1$ 2.0
134. Diuron	330-54-1	AETP _{fresh} AETP _{marine} SETP _{fresh} SETP _{marine} TETP HTP	$5.3 \cdot 10^2$ $1.1 \cdot 10^2$ $5.0 \cdot 10^2$ $1.6 \cdot 10^2$ 8.7 $2.1 \cdot 10^2$	$9.4 \cdot 10^3$ $5.5 \cdot 10^1$ $8.9 \cdot 10^3$ $7.8 \cdot 10^1$ $1.7 \cdot 10^{-3}$ $5.3 \cdot 10^1$	$1.9 \cdot 10^{-3}$ $2.4 \cdot 10^2$ $1.8 \cdot 10^{-3}$ $3.4 \cdot 10^2$ $3.2 \cdot 10^{-5}$ $1.9 \cdot 10^{-1}$	$3.5 \cdot 10^2$ 2.1 $3.3 \cdot 10^2$ 3.0 $2.3 \cdot 10^1$ $1.3 \cdot 10^3$	$1.1 \cdot 10^3$ 6.8 $1.1 \cdot 10^3$ 9.8 $1.9 \cdot 10^1$ 7.2
135. DNOC	534-51-1	AETP _{fresh} AETP _{marine} SETP _{fresh} SETP _{marine} TETP HTP	3.4 1.3 $5.7 \cdot 10^{-1}$ $3.0 \cdot 10^{-1}$ $2.4 \cdot 10^{-1}$ $1.6 \cdot 10^2$	$1.1 \cdot 10^2$ $3.4 \cdot 10^{-1}$ $1.9 \cdot 10^1$ $8.0 \cdot 10^{-2}$ $8.5 \cdot 10^{-7}$ $5.9 \cdot 10^1$	$2.1 \cdot 10^{-8}$ 2.6 $3.6 \cdot 10^{-9}$ $6.1 \cdot 10^{-1}$ $1.5 \cdot 10^{-9}$ $1.5 \cdot 10^{-3}$	1.2 $3.6 \cdot 10^{-3}$ $2.0 \cdot 10^{-1}$ $8.5 \cdot 10^{-4}$ $5.2 \cdot 10^{-1}$ $2.8 \cdot 10^2$	4.5 $1.4 \cdot 10^{-2}$ $7.5 \cdot 10^{-1}$ $3.3 \cdot 10^{-3}$ $4.9 \cdot 10^{-1}$ 2.8
136. Endosulfan	115-29-7	AETP _{fresh} AETP _{marine} SETP _{fresh} SETP _{marine} TETP HTP	$4.5 \cdot 10^1$ $1.9 \cdot 10^1$ 9.8 1.2 $3.6 \cdot 10^{-2}$ 6.7	$2.8 \cdot 10^4$ $1.1 \cdot 10^1$ $6.0 \cdot 10^3$ $7.7 \cdot 10^{-1}$ $1.8 \cdot 10^{-3}$ $1.7 \cdot 10^1$	$2.1 \cdot 10^{-2}$ $3.2 \cdot 10^2$ $4.5 \cdot 10^{-3}$ $2.2 \cdot 10^1$ $1.6 \cdot 10^{-5}$ $4.2 \cdot 10^{-2}$	2.2 $1.4 \cdot 10^{-3}$ $4.8 \cdot 10^{-1}$ $9.0 \cdot 10^{-5}$ 2.7 $2.6 \cdot 10^{-1}$	9.0 $5.5 \cdot 10^{-3}$ 1.9 $3.6 \cdot 10^{-4}$ 2.8 $1.6 \cdot 10^{-2}$
137. Endrin	72-20-8	AETP _{fresh} AETP _{marine} SETP _{fresh} SETP _{marine} TETP HTP	$1.1 \cdot 10^3$ $4.9 \cdot 10^4$ $3.4 \cdot 10^2$ $3.5 \cdot 10^3$ $4.9 \cdot 10^1$ $1.2 \cdot 10^3$	$7.0 \cdot 10^5$ $3.4 \cdot 10^5$ $2.1 \cdot 10^5$ $2.5 \cdot 10^4$ $3.5 \cdot 10^{-1}$ $6.0 \cdot 10^3$	6.1 $2.7 \cdot 10^6$ 1.9 $2.0 \cdot 10^5$ $3.8 \cdot 10^{-1}$ $1.6 \cdot 10^3$	$2.1 \cdot 10^4$ $1.0 \cdot 10^4$ $6.4 \cdot 10^3$ $7.5 \cdot 10^2$ $4.2 \cdot 10^3$ $8.4 \cdot 10^3$	$7.1 \cdot 10^4$ $3.5 \cdot 10^4$ $2.2 \cdot 10^4$ $2.5 \cdot 10^3$ $3.6 \cdot 10^3$ $7.5 \cdot 10^2$

Substance No. Name	CAS No.	Type	Initial emission compartment				
			air	fresh water	sea water	agricult. soil	industria l soil
Pesticides							
138. Ethoprophos	13194-48-4	AETP _{fresh}	2.4·10 ³	1.5·10 ⁵	1.0	1.1·10 ⁴	3.0·10 ⁴
		AETP _{marine}	7.1·10 ²	3.5·10 ³	6.6·10 ³	2.6·10 ²	7.2·10 ²
		SETP _{fresh}	1.9·10 ³	1.2·10 ⁵	7.9·10 ⁻¹	8.8·10 ³	2.4·10 ⁴
		SETP _{marine}	9.3·10 ²	4.8·10 ³	8.9·10 ³	3.6·10 ²	9.7·10 ²
		TETP	1.7·10 ¹	2.4·10 ⁻¹	7.2·10 ⁻³	2.7·10 ²	1.9·10 ²
		HTP	1.1·10 ³	1.8·10 ³	1.3·10 ¹	5.7·10 ³	3.8·10 ²
139. Fenitrothion	122-14-5	AETP _{fresh}	2.5·10 ³	2.4·10 ⁵	9.9·10 ⁻³	7.6·10 ²	3.0·10 ³
		AETP _{marine}	1.5·10 ³	6.7·10 ²	5.6·10 ³	2.3	8.9
		SETP _{fresh}	1.4·10 ³	1.4·10 ⁵	5.5·10 ⁻³	4.2·10 ²	1.7·10 ³
		SETP _{marine}	7.5·10 ²	3.4·10 ²	2.9·10 ³	1.1	4.5
		TETP	2.1·10 ¹	4.7·10 ⁻³	8.4·10 ⁻⁵	8.3·10 ¹	8.1·10 ¹
		HTP	5.9	2.2·10 ¹	9.0·10 ⁻²	1.2·10 ¹	3.2·10 ⁻¹
140. Fentin acetate	900-95-8	AETP _{fresh}	4.3·10 ³	2.7·10 ⁵	8.7·10 ⁻²	3.8·10 ²	1.5·10 ³
		AETP _{marine}	2.1·10 ⁴	3.2·10 ³	4.0·10 ⁴	6.8	2.7·10 ¹
		SETP _{fresh}	6.9·10 ³	4.3·10 ⁵	1.4·10 ⁻¹	6.2·10 ²	2.5·10 ³
		SETP _{marine}	5.3·10 ⁴	8.7·10 ³	1.1·10 ⁵	1.8·10 ¹	7.2·10 ¹
		TETP	5.3	6.1·10 ⁻³	1.1·10 ⁻⁴	1.2·10 ¹	1.1·10 ¹
		HTP	2.2·10 ³	8.8·10 ²	4.1	7.2·10 ¹	9.2
141. Fentin chloride	639-58-7	AETP _{fresh}	1.8·10 ³	1.7·10 ⁵	1.8·10 ¹	2.5·10 ²	9.9·10 ²
		AETP _{marine}	4.7·10 ⁴	1.9·10 ⁴	4.0·10 ⁴	9.5·10 ¹	3.7·10 ²
		SETP _{fresh}	3.0·10 ³	2.8·10 ⁵	2.9·10 ¹	4.1·10 ²	1.6·10 ³
		SETP _{marine}	5.7·10 ⁴	2.6·10 ⁴	1.1·10 ⁵	1.2·10 ²	4.7·10 ²
		TETP	2.6·10 ⁻¹	9.2·10 ⁻²	2.5·10 ⁻³	1.2·10 ¹	1.1·10 ¹
		HTP	8.4·10 ²	8.6·10 ²	1.2·10 ¹	1.3·10 ²	1.3·10 ¹
142. Fentin hydroxide	76-87-9	AETP _{fresh}	4.2·10 ³	2.7·10 ⁵	2.9·10 ⁻²	3.8·10 ²	1.5·10 ³
		AETP _{marine}	2.0·10 ⁴	3.1·10 ³	4.0·10 ⁴	6.1	2.4·10 ¹
		SETP _{fresh}	6.8·10 ³	4.3·10 ⁵	4.7·10 ⁻²	6.2·10 ²	2.5·10 ³
		SETP _{marine}	5.1·10 ⁴	8.6·10 ³	1.1·10 ⁵	1.6·10 ¹	6.5·10 ¹
		TETP	5.5	2.1·10 ⁻³	3.8·10 ⁻⁵	1.2·10 ¹	1.1·10 ¹
		HTP	8.5·10 ²	8.7·10 ²	4.1	8.8·10 ¹	8.5
143. Fenthion	55-38-9	AETP _{fresh}	2.5·10 ³	9.1·10 ⁵	2.6·10 ⁻¹	3.5·10 ³	1.4·10 ⁴
		AETP _{marine}	1.6·10 ³	3.6·10 ³	2.3·10 ⁴	1.5·10 ¹	5.7·10 ¹
		SETP _{fresh}	1.8·10 ³	6.6·10 ⁵	1.9·10 ⁻¹	2.5·10 ³	9.9·10 ³
		SETP _{marine}	1.1·10 ³	2.5·10 ³	1.5·10 ⁴	9.9	3.9·10 ¹
		TETP	1.6·10 ¹	8.8·10 ⁻²	1.7·10 ⁻³	2.9·10 ²	2.8·10 ²
		HTP	6.3·10 ¹	9.3·10 ¹	4.6·10 ⁻¹	3.0·10 ¹	1.5
144. Folpet	133-7-3	AETP _{fresh}	4.1·10 ²	8.2·10 ⁴	1.6·10 ¹	4.5·10 ³	1.3·10 ⁴
		AETP _{marine}	2.3·10 ³	1.2·10 ⁴	2.1·10 ⁴	7.1·10 ²	2.1·10 ³
		SETP _{fresh}	5.6·10 ²	1.1·10 ⁵	2.2·10 ¹	6.2·10 ³	1.8·10 ⁴
		SETP _{marine}	2.7·10 ³	1.6·10 ⁴	2.8·10 ⁴	9.3·10 ²	2.7·10 ³
		TETP	1.7	6.0·10 ⁻¹	7.4·10 ⁻²	1.1·10 ²	7.8·10 ¹
		HTP	2.0	8.6	3.1·10 ⁻¹	1.3·10 ¹	1.5
31. Formaldehyde		AETP _{fresh}	see non-aromatics				
		AETP _{marine}					
		SETP _{fresh}					
		SETP _{marine}					
		TETP					
		HTP					

Substance No. Name	CAS No.	Type	Initial emission compartment				
			air	fresh water	sea water	agricult. soil	industria l soil
Pesticides							
145. Glyphosate	1071-83-6	AETP _{fresh}	2.2·10 ¹	1.4·10 ³	2.1·10 ⁻¹¹	9.2·10 ⁻¹	3.7
		AETP _{marine}	1.7·10 ¹	4.2	3.3·10 ¹	2.8·10 ⁻³	1.1·10 ⁻²
		SETP _{fresh}	2.1·10 ¹	1.3·10 ³	2.0·10 ⁻¹¹	9.0·10 ⁻¹	3.6
		SETP _{marine}	1.5·10 ¹	3.7	3.0·10 ¹	2.5·10 ⁻³	9.9·10 ⁻³
		TETP	4.7·10 ⁻²	2.2·10 ⁻¹¹	4.4·10 ⁻¹⁴	9.6·10 ⁻²	9.6·10 ⁻²
		HTP	3.1·10 ⁻³	6.6·10 ⁻²	1.5·10 ⁻⁵	1.5·10 ⁻²	6.5·10 ⁻⁴
146. Heptachlor	76-44-8	AETP _{fresh}	1.4	1.8·10 ⁴	3.9·10 ⁻²	2.3	8.9
		AETP _{marine}	2.9	1.2·10 ¹	1.1·10 ³	2.4·10 ⁻²	9.5·10 ⁻²
		SETP _{fresh}	2.0	2.6·10 ⁴	5.5·10 ⁻²	3.2	1.3·10 ¹
		SETP _{marine}	2.4	1.0·10 ¹	9.2·10 ²	2.0·10 ⁻²	7.9·10 ⁻²
		TETP	8.8·10 ⁻⁴	5.3·10 ⁻⁴	2.4·10 ⁻⁵	5.5	5.3
		HTP	4.0·10 ¹	3.4·10 ³	4.3·10 ¹	6.7·10 ²	4.4
147. Heptenophos	23560-59-0	AETP _{fresh}	1.2·10 ²	2.2·10 ⁴	1.3·10 ⁻³	3.1·10 ¹	1.2·10 ²
		AETP _{marine}	7.8·10 ¹	1.1·10 ¹	4.5·10 ²	2.6·10 ⁻²	1.0·10 ⁻¹
		SETP _{fresh}	1.5·10 ¹	2.8·10 ³	1.7·10 ⁻⁴	3.8	1.5·10 ¹
		SETP _{marine}	1.5·10 ¹	2.3	9.1·10 ¹	5.1·10 ⁻³	2.0·10 ⁻²
		TETP	2.2	1.6·10 ⁻³	2.4·10 ⁻⁵	1.6·10 ¹	1.6·10 ¹
		HTP	2.3·10 ¹	1.3	2.3·10 ⁻³	3.4	2.0·10 ⁻²
81. Hexachlorobenzene	118-74-1	AETP _{fresh}	see halogenated aromatics				
		AETP _{marine}					
		SETP _{fresh}					
		SETP _{marine}					
		TETP					
		HTP					
148. Iprodione	36734-19-7	AETP _{fresh}	2.8	1.6·10 ²	3.8·10 ⁻⁹	2.3·10 ⁻¹	1.9
		AETP _{marine}	3.2·10 ⁻¹	1.5·10 ⁻²	7.2·10 ⁻¹	2.2·10 ⁻⁵	1.8·10 ⁻⁴
		SETP _{fresh}	2.3·10 ⁻¹	1.3·10 ¹	3.1·10 ⁻¹⁰	1.9·10 ⁻²	1.6·10 ⁻¹
		SETP _{marine}	5.2·10 ⁻³	2.4·10 ⁻⁴	1.2·10 ⁻²	3.5·10 ⁻⁷	2.9·10 ⁻⁶
		TETP	1.1·10 ⁻¹	4.4·10 ⁻⁸	1.5·10 ⁻¹⁰	1.4·10 ⁻¹	3.0·10 ⁻¹
		HTP	2.8·10 ⁻¹	1.8·10 ⁻¹	1.2·10 ⁻⁴	1.8	3.2·10 ⁻³
149. Isoproturon	34123-59-6	AETP _{fresh}	1.9·10 ²	1.9·10 ³	2.9·10 ⁻⁵	1.7·10 ²	4.0·10 ²
		AETP _{marine}	3.2·10 ¹	2.0·10 ¹	5.9·10 ¹	1.8	4.2
		SETP _{fresh}	7.1·10 ¹	7.1·10 ²	1.1·10 ⁻⁵	6.3·10 ¹	1.5·10 ²
		SETP _{marine}	2.0·10 ¹	1.3·10 ¹	3.7·10 ¹	1.1	2.7
		TETP	2.5	1.6·10 ⁻⁵	3.8·10 ⁻⁷	6.4	4.6
		HTP	1.3·10 ²	1.3·10 ¹	2.9·10 ⁻²	9.6·10 ²	2.8
150. Lindane	58-89-9	AETP _{fresh}	5.2·10 ¹	6.5·10 ³	1.1·10 ⁻¹	9.7·10 ¹	3.7·10 ²
		AETP _{marine}	5.2·10 ¹	8.8·10 ¹	2.3·10 ²	1.4	5.3
		SETP _{fresh}	1.4·10 ¹	1.7·10 ³	3.0·10 ⁻²	2.5·10 ¹	9.7·10 ¹
		SETP _{marine}	9.2	1.8·10 ¹	4.8·10 ¹	2.9·10 ⁻¹	1.1
		TETP	1.8	1.6·10 ⁻¹	3.9·10 ⁻³	2.3·10 ¹	2.2·10 ¹
		HTP	6.1·10 ²	8.3·10 ²	6.1	4.9·10 ²	5.2·10 ¹
151. Linuron	330-55-2	AETP _{fresh}	4.0·10 ¹	3.1·10 ⁴	6.0·10 ⁻²	6.9·10 ²	2.4·10 ³
		AETP _{marine}	2.7·10 ¹	5.6·10 ²	1.3·10 ³	1.2·10 ¹	4.4·10 ¹
		SETP _{fresh}	3.9·10 ¹	3.1·10 ⁴	6.0·10 ⁻²	6.9·10 ²	2.4·10 ³
		SETP _{marine}	3.5·10 ¹	7.3·10 ²	1.7·10 ³	1.6·10 ¹	5.7·10 ¹
		TETP	2.0·10 ⁻¹	1.1·10 ⁻²	3.1·10 ⁻⁴	2.1·10 ¹	1.8·10 ¹
		HTP	1.4·10 ¹	1.1·10 ²	6.5·10 ⁻¹	1.7·10 ²	9.4

Substance No. Name	CAS No.	Type	Initial emission compartment				
			air	fresh water	sea water	agricult. soil	industria l soil
Pesticides							
152. Malathion	121-74-6	AETP _{fresh}	$1.8 \cdot 10^3$	$2.1 \cdot 10^5$	$1.8 \cdot 10^{-2}$	$1.6 \cdot 10^2$	$6.5 \cdot 10^2$
		AETP _{marine}	$1.4 \cdot 10^3$	$7.7 \cdot 10^2$	$5.1 \cdot 10^3$	$6.6 \cdot 10^{-1}$	2.6
		SETP _{fresh}	$1.1 \cdot 10^3$	$1.2 \cdot 10^5$	$1.1 \cdot 10^{-2}$	$9.5 \cdot 10^1$	$3.8 \cdot 10^2$
		SETP _{marine}	$7.8 \cdot 10^2$	$4.3 \cdot 10^2$	$2.8 \cdot 10^3$	$3.7 \cdot 10^{-1}$	1.5
		TETP	$2.0 \cdot 10^{-2}$	$1.1 \cdot 10^{-5}$	$2.0 \cdot 10^{-7}$	$7.6 \cdot 10^{-2}$	$7.5 \cdot 10^{-2}$
		HTP	$3.5 \cdot 10^{-2}$	$2.4 \cdot 10^{-1}$	$8.4 \cdot 10^{-4}$	$2.6 \cdot 10^{-2}$	$9.5 \cdot 10^{-4}$
153. MCPA	94-74-6	AETP _{fresh}	1.1	$2.7 \cdot 10^1$	$5.3 \cdot 10^{-13}$	$4.6 \cdot 10^{-1}$	1.7
		AETP _{marine}	$2.8 \cdot 10^{-1}$	$3.6 \cdot 10^{-2}$	$5.6 \cdot 10^{-1}$	$6.2 \cdot 10^{-4}$	$2.2 \cdot 10^{-3}$
		SETP _{fresh}	$7.0 \cdot 10^{-1}$	$1.8 \cdot 10^1$	$3.6 \cdot 10^{-13}$	$3.1 \cdot 10^{-1}$	1.1
		SETP _{marine}	$3.5 \cdot 10^{-1}$	$4.4 \cdot 10^{-2}$	$6.9 \cdot 10^{-1}$	$7.6 \cdot 10^{-4}$	$2.7 \cdot 10^{-3}$
		TETP	$4.3 \cdot 10^{-2}$	$1.4 \cdot 10^{-11}$	$2.2 \cdot 10^{-14}$	$9.4 \cdot 10^{-2}$	$8.6 \cdot 10^{-2}$
		HTP	$1.5 \cdot 10^1$	$1.5 \cdot 10^1$	$3.7 \cdot 10^{-2}$	$1.0 \cdot 10^2$	$9.7 \cdot 10^{-1}$
154. Mecoprop	7085-19-0	AETP _{fresh}	$3.7 \cdot 10^1$	$3.8 \cdot 10^2$	$3.8 \cdot 10^{-10}$	$3.0 \cdot 10^1$	$7.8 \cdot 10^1$
		AETP _{marine}	4.1	$6.7 \cdot 10^{-1}$	8.0	$5.3 \cdot 10^{-2}$	$1.4 \cdot 10^{-1}$
		SETP _{fresh}	$2.5 \cdot 10^1$	$2.5 \cdot 10^2$	$2.5 \cdot 10^{-10}$	$2.0 \cdot 10^1$	$5.3 \cdot 10^1$
		SETP _{marine}	5.3	$8.7 \cdot 10^{-1}$	$1.1 \cdot 10^1$	$6.9 \cdot 10^{-2}$	$1.8 \cdot 10^{-1}$
		TETP	1.8	$1.1 \cdot 10^{-8}$	$1.8 \cdot 10^{-11}$	4.7	3.3
		HTP	$1.2 \cdot 10^2$	$2.0 \cdot 10^2$	$8.4 \cdot 10^{-1}$	$7.4 \cdot 10^2$	$4.2 \cdot 10^1$
155. Metamitron	41394-5-2	AETP _{fresh}	$9.3 \cdot 10^{-1}$	$2.3 \cdot 10^1$	$6.8 \cdot 10^{-10}$	$4.1 \cdot 10^{-1}$	1.5
		AETP _{marine}	$2.5 \cdot 10^{-1}$	$6.3 \cdot 10^{-2}$	$4.9 \cdot 10^{-1}$	$1.1 \cdot 10^{-3}$	$4.1 \cdot 10^{-3}$
		SETP _{fresh}	$4.9 \cdot 10^{-1}$	$1.2 \cdot 10^1$	$3.5 \cdot 10^{-10}$	$2.2 \cdot 10^{-1}$	$7.9 \cdot 10^{-1}$
		SETP _{marine}	$1.9 \cdot 10^{-1}$	$5.0 \cdot 10^{-2}$	$3.8 \cdot 10^{-1}$	$8.9 \cdot 10^{-4}$	$3.2 \cdot 10^{-3}$
		TETP	$1.9 \cdot 10^{-2}$	$8.5 \cdot 10^{-10}$	$1.4 \cdot 10^{-11}$	$4.2 \cdot 10^{-2}$	$3.8 \cdot 10^{-2}$
		HTP	$8.8 \cdot 10^{-1}$	$1.6 \cdot 10^{-1}$	$3.2 \cdot 10^{-5}$	6.5	$1.2 \cdot 10^{-2}$
156. Metazachlor	67129-8-2	AETP _{fresh}	7.4	$1.5 \cdot 10^2$	$3.0 \cdot 10^{-6}$	3.9	$1.4 \cdot 10^1$
		AETP _{marine}	2.2	1.3	4.4	$3.3 \cdot 10^{-2}$	$1.1 \cdot 10^{-1}$
		SETP _{fresh}	5.3	$1.1 \cdot 10^2$	$2.2 \cdot 10^{-6}$	2.8	9.8
		SETP _{marine}	2.6	1.5	5.2	$3.9 \cdot 10^{-2}$	$1.4 \cdot 10^{-1}$
		TETP	$7.4 \cdot 10^{-2}$	$1.4 \cdot 10^{-6}$	$3.0 \cdot 10^{-8}$	$1.7 \cdot 10^{-1}$	$1.5 \cdot 10^{-1}$
		HTP	6.8	1.7	$2.4 \cdot 10^{-3}$	$4.9 \cdot 10^1$	$1.6 \cdot 10^{-1}$
157. Methabenzthiazuron	18691-97-9	AETP _{fresh}	$7.0 \cdot 10^1$	$1.1 \cdot 10^3$	$9.2 \cdot 10^{-5}$	$4.4 \cdot 10^1$	$1.4 \cdot 10^2$
		AETP _{marine}	$2.5 \cdot 10^1$	$2.5 \cdot 10^1$	$4.8 \cdot 10^1$	1.0	3.2
		SETP _{fresh}	$7.6 \cdot 10^1$	$1.2 \cdot 10^3$	$1.0 \cdot 10^{-4}$	$4.8 \cdot 10^1$	$1.5 \cdot 10^2$
		SETP _{marine}	$3.7 \cdot 10^1$	$3.7 \cdot 10^1$	$7.0 \cdot 10^1$	1.5	4.7
		TETP	$4.5 \cdot 10^{-1}$	$2.0 \cdot 10^{-5}$	$6.0 \cdot 10^{-7}$	1.1	$8.8 \cdot 10^{-1}$
		HTP	7.1	2.6	$8.2 \cdot 10^{-3}$	$5.1 \cdot 10^1$	$3.6 \cdot 10^{-1}$
158. Methomyl	16752-77-5	AETP _{fresh}	$1.4 \cdot 10^4$	$1.4 \cdot 10^5$	$8.5 \cdot 10^{-3}$	$1.4 \cdot 10^4$	$2.8 \cdot 10^4$
		AETP _{marine}	$3.9 \cdot 10^3$	$4.2 \cdot 10^3$	$6.9 \cdot 10^3$	$4.4 \cdot 10^2$	$8.9 \cdot 10^2$
		SETP _{fresh}	$1.0 \cdot 10^4$	$1.0 \cdot 10^5$	$6.3 \cdot 10^{-3}$	$1.1 \cdot 10^4$	$2.1 \cdot 10^4$
		SETP _{marine}	$5.0 \cdot 10^3$	$5.4 \cdot 10^3$	$8.9 \cdot 10^3$	$5.7 \cdot 10^2$	$1.1 \cdot 10^3$
		TETP	$1.2 \cdot 10^2$	$2.2 \cdot 10^{-3}$	$7.5 \cdot 10^{-5}$	$3.0 \cdot 10^2$	$2.2 \cdot 10^2$
		HTP	6.2	3.3	$1.4 \cdot 10^{-3}$	$4.3 \cdot 10^1$	$6.9 \cdot 10^{-1}$
159. Methylbromide	74-83-9	AETP _{fresh}	$3.3 \cdot 10^{-2}$	$1.9 \cdot 10^1$	$2.3 \cdot 10^{-3}$	$1.4 \cdot 10^{-1}$	$1.4 \cdot 10^{-1}$
		AETP _{marine}	4.1	3.5	2.4	3.1	3.1
		SETP _{fresh}	$1.7 \cdot 10^{-2}$	$1.0 \cdot 10^1$	$1.2 \cdot 10^{-3}$	$7.2 \cdot 10^{-2}$	$7.3 \cdot 10^{-2}$
		SETP _{marine}	1.1	$9.6 \cdot 10^{-1}$	2.0	$8.3 \cdot 10^{-1}$	$8.3 \cdot 10^{-1}$
		TETP	$1.3 \cdot 10^{-2}$	$1.1 \cdot 10^{-2}$	$9.1 \cdot 10^{-4}$	$3.6 \cdot 10^{-1}$	$3.7 \cdot 10^{-1}$
		HTP	$3.5 \cdot 10^2$	$3.0 \cdot 10^2$	$2.5 \cdot 10^1$	$2.6 \cdot 10^2$	$2.6 \cdot 10^2$

Substance No. Name	CAS No.	Type	Initial emission compartment				
			air	fresh water	sea water	agricult. soil	industria l soil
Pesticides							
160. Metobromuron	3060-89-7	AETP _{fresh}	4.9·10 ¹	4.3·10 ²	1.6·10 ⁻³	9.5·10 ¹	9.5·10 ¹
		AETP _{marine}	4.2·10 ¹	6.4·10 ¹	7.3·10 ¹	1.4·10 ¹	1.4·10 ¹
		SETP _{fresh}	4.8·10 ¹	4.2·10 ²	1.6·10 ⁻³	9.2·10 ¹	9.2·10 ¹
		SETP _{marine}	4.7·10 ¹	7.2·10 ¹	8.2·10 ¹	1.6·10 ¹	1.6·10 ¹
		TETP	9.9·10 ⁻¹	4.6·10 ⁻⁴	3.8·10 ⁻⁵	2.2	2.2
		HTP	5.5·10 ¹	8.0	7.6·10 ⁻²	4.1·10 ²	1.9
161. Metolachlor	51218-45-2	AETP _{fresh}	1.5·10 ³	3.8·10 ⁴	7.0·10 ⁻²	1.9·10 ³	5.8·10 ³
		AETP _{marine}	3.8·10 ²	5.8·10 ²	1.3·10 ³	3.0·10 ¹	9.1·10 ¹
		SETP _{fresh}	1.3·10 ³	3.4·10 ⁴	6.2·10 ⁻²	1.7·10 ³	5.2·10 ³
		SETP _{marine}	5.2·10 ²	8.1·10 ²	1.9·10 ³	4.1·10 ¹	1.3·10 ²
		TETP	1.1·10 ⁻¹	2.1·10 ⁻⁴	5.4·10 ⁻⁶	5.4·10 ⁻¹	4.1·10 ⁻¹
		HTP	2.6	5.5·10 ⁻¹	8.5·10 ⁻⁴	1.1·10 ¹	1.1·10 ⁻¹
162. Mevinphos	7786-34-7	AETP _{fresh}	9.3·10 ³	5.9·10 ⁵	6.9·10 ⁻⁵	3.5·10 ²	1.5·10 ³
		AETP _{marine}	5.4·10 ³	5.7·10 ²	1.1·10 ⁴	3.4·10 ⁻¹	1.4
		SETP _{fresh}	1.2·10 ³	7.4·10 ⁴	8.8·10 ⁻⁶	4.4·10 ¹	1.8·10 ²
		SETP _{marine}	6.0·10 ²	6.3·10 ¹	1.2·10 ³	3.8·10 ⁻²	1.6·10 ⁻¹
		TETP	4.3·10 ¹	2.3·10 ⁻⁵	3.2·10 ⁻⁷	8.7·10 ¹	9.0·10 ¹
		HTP	1.0	1.1·10 ¹	1.8·10 ⁻³	5.7	5.5·10 ⁻²
163. Oxamyl	23135-22-0	AETP _{fresh}	5.6·10 ¹	6.5·10 ²	4.5·10 ⁻⁷	3.0·10 ¹	1.2·10 ²
		AETP _{marine}	1.4	1.8·10 ⁻¹	2.8	8.4·10 ⁻³	3.4·10 ⁻²
		SETP _{fresh}	2.5·10 ¹	3.0·10 ²	2.1·10 ⁻⁷	1.3·10 ¹	5.5·10 ¹
		SETP _{marine}	4.0·10 ⁻¹	5.3·10 ⁻²	8.0·10 ⁻¹	2.4·10 ⁻³	9.9·10 ⁻³
		TETP	2.9	7.1·10 ⁻⁶	2.3·10 ⁻⁸	5.9	6.0
		HTP	1.4	3.6·10 ⁻¹	1.4·10 ⁻⁵	1.0·10 ¹	6.8·10 ⁻²
164. Oxydemethon-methyl	301-12-2	AETP _{fresh}	2.4·10 ³	7.0·10 ⁴	3.0·10 ⁻⁴	9.7·10 ²	3.6·10 ³
		AETP _{marine}	5.0·10 ²	1.4·10 ²	1.0·10 ³	2.0	7.3
		SETP _{fresh}	5.3·10 ²	1.6·10 ⁴	6.8·10 ⁻⁵	2.2·10 ²	8.1·10 ²
		SETP _{marine}	2.1·10 ²	5.8·10 ¹	4.2·10 ²	8.2·10 ⁻¹	3.0
		TETP	4.1·10 ¹	4.6·10 ⁻⁴	5.2·10 ⁻⁶	9.2·10 ¹	8.5·10 ¹
		HTP	1.2·10 ²	7.4·10 ¹	1.0·10 ⁻²	6.1·10 ²	3.8
165. Parathion-ethyl	56-38-2	AETP _{fresh}	2.8·10 ³	1.2·10 ⁶	2.0·10 ⁻¹	5.0·10 ²	1.9·10 ³
		AETP _{marine}	3.1·10 ³	5.3·10 ³	4.1·10 ⁴	2.3	9.2
		SETP _{fresh}	1.9·10 ³	8.0·10 ⁵	1.4·10 ⁻¹	3.4·10 ²	1.3·10 ³
		SETP _{marine}	1.3·10 ³	2.2·10 ³	1.7·10 ⁴	9.6·10 ⁻¹	3.8
		TETP	1.1	3.1·10 ⁻³	8.2·10 ⁻⁵	1.7·10 ¹	1.7·10 ¹
		HTP	3.3	3.1·10 ¹	1.8·10 ⁻¹	2.9	1.1·10 ⁻¹
166. Parathion-methyl	298-00-0	AETP _{fresh}	9.9·10 ²	2.9·10 ⁵	1.2·10 ⁻¹	1.1·10 ³	4.4·10 ³
		AETP _{marine}	7.2·10 ²	1.5·10 ³	8.1·10 ³	5.9	2.3·10 ¹
		SETP _{fresh}	6.0·10 ¹	1.8·10 ⁴	7.4·10 ⁻³	6.8·10 ¹	2.6·10 ²
		SETP _{marine}	3.0·10 ¹	6.2·10 ¹	3.4·10 ²	2.5·10 ⁻¹	9.8·10 ⁻¹
		TETP	5.7	3.4·10 ⁻²	7.1·10 ⁻⁴	8.1·10 ¹	7.9·10 ¹
		HTP	5.3·10 ¹	1.0·10 ²	5.4·10 ⁻¹	2.4·10 ¹	1.7
167. Permethrin	52645-53-1	AETP _{fresh}	1.6·10 ⁴	5.0·10 ⁶	1.0·10 ¹	9.2·10 ²	3.7·10 ³
		AETP _{marine}	3.1·10 ⁴	2.7·10 ⁴	2.8·10 ⁵	5.5	2.2·10 ¹
		SETP _{fresh}	2.1·10 ⁴	6.7·10 ⁶	1.3·10 ¹	1.2·10 ³	4.8·10 ³
		SETP _{marine}	2.3·10 ⁴	2.0·10 ⁴	2.2·10 ⁵	4.2	1.7·10 ¹
		TETP	2.6·10 ¹	3.9·10 ⁻¹	1.7·10 ⁻²	2.5·10 ²	2.5·10 ²
		HTP	8.5·10 ⁻¹	2.3·10 ¹	2.6·10 ⁻¹	1.1·10 ¹	2.1·10 ⁻²

Substance No. Name	CAS No.	Type	Initial emission compartment				
			air	fresh water	sea water	agricult. soil	industria l soil
Pesticides							
168. Phoxim	14816-18-3	AETP _{fresh}	4.4·10 ⁻¹	2.6·10 ³	3.3·10 ⁻²	4.4	7.9
		AETP _{marine}	1.6	5.0	3.0·10 ²	3.1·10 ⁻¹	5.5·10 ⁻¹
		SETP _{fresh}	7.1·10 ⁻²	4.3·10 ²	5.4·10 ⁻³	7.2·10 ⁻¹	1.3
		SETP _{marine}	2.1·10 ⁻¹	6.7·10 ⁻¹	4.1·10 ¹	4.1·10 ⁻²	7.2·10 ⁻²
		TETP	1.7·10 ⁻²	1.5·10 ⁻²	1.3·10 ⁻³	4.7	3.8
		HTP	9.7·10 ⁻¹	1.2·10 ¹	2.9·10 ⁻¹	2.5·10 ¹	3.8·10 ⁻¹
169. Pirimicarb	23103-98-2	AETP _{fresh}	2.4·10 ³	3.6·10 ⁴	8.9·10 ⁻⁴	1.7·10 ³	5.2·10 ³
		AETP _{marine}	4.1·10 ²	1.6·10 ²	8.6·10 ²	7.3	2.3·10 ¹
		SETP _{fresh}	2.4·10 ³	3.6·10 ⁴	9.0·10 ⁻⁴	1.7·10 ³	5.3·10 ³
		SETP _{marine}	6.2·10 ²	2.4·10 ²	1.3·10 ³	1.1·10 ¹	3.5·10 ¹
		TETP	4.6·10 ¹	9.3·10 ⁻⁴	1.7·10 ⁻⁵	1.2·10 ²	9.4·10 ¹
		HTP	3.4	1.7	1.3·10 ⁻³	2.6·10 ¹	2.9·10 ⁻¹
170. Propachlor	1918-16-7	AETP _{fresh}	2.0·10 ¹	1.2·10 ³	5.0·10 ⁻⁴	1.7·10 ¹	6.4·10 ¹
		AETP _{marine}	7.1	2.4	2.7·10 ¹	4.2·10 ⁻²	1.6·10 ⁻¹
		SETP _{fresh}	1.1·10 ¹	6.7·10 ²	2.7·10 ⁻⁴	9.4	3.4·10 ¹
		SETP _{marine}	6.5	2.3	2.5·10 ¹	4.0·10 ⁻²	1.5·10 ⁻¹
		TETP	5.4·10 ⁻¹	8.1·10 ⁻⁴	1.3·10 ⁻⁵	2.5	2.3
		HTP	1.2·10 ¹	1.6	2.6·10 ⁻³	1.5·10 ¹	1.4·10 ⁻¹
171. Propoxur	114-26-1	AETP _{fresh}	2.5·10 ⁴	2.6·10 ⁵	1.2·10 ⁻⁴	2.0·10 ⁴	5.4·10 ⁴
		AETP _{marine}	1.8·10 ³	5.0·10 ²	3.4·10 ³	3.9·10 ¹	1.0·10 ²
		SETP _{fresh}	1.8·10 ⁴	1.8·10 ⁵	8.2·10 ⁻⁵	1.4·10 ⁴	3.8·10 ⁴
		SETP _{marine}	1.8·10 ³	5.2·10 ²	3.6·10 ³	4.0·10 ¹	1.1·10 ²
		TETP	7.0·10 ²	3.1·10 ⁻⁴	3.2·10 ⁻⁶	1.8·10 ³	1.3·10 ³
		HTP	3.7·10 ¹	1.3	3.9·10 ⁻⁴	2.7·10 ²	2.7·10 ⁻¹
172. Pyrazophos	13457-18-6	AETP _{fresh}	1.8·10 ²	4.9·10 ⁴	2.3·10 ⁻³	2.5·10 ²	9.9·10 ²
		AETP _{marine}	9.4·10 ¹	1.2·10 ²	1.1·10 ³	6.8·10 ⁻¹	2.6
		SETP _{fresh}	1.7·10 ²	4.5·10 ⁴	2.0·10 ⁻³	2.3·10 ²	9.0·10 ²
		SETP _{marine}	8.9·10 ¹	1.2·10 ²	1.1·10 ³	6.5·10 ⁻¹	2.5
		TETP	2.3	1.7·10 ⁻³	2.9·10 ⁻⁵	3.0·10 ¹	2.9·10 ¹
		HTP	2.5·10 ¹	5.3·10 ¹	2.3·10 ⁻¹	5.1·10 ¹	1.2
93. Quintozene	82-68-8	AETP _{fresh} AETP _{marine} SETP _{fresh} SETP _{marine} TETP HTP	see pentachloronitrobenzene (halogenated aromatics)				
173. Simazine	122-34-9	AETP _{fresh}	2.1·10 ³	2.7·10 ⁴	4.5·10 ⁻³	2.3·10 ³	5.6·10 ³
		AETP _{marine}	2.8·10 ²	1.4·10 ²	6.7·10 ²	1.3·10 ¹	3.1·10 ¹
		SETP _{fresh}	1.8·10 ³	2.3·10 ⁴	3.8·10 ⁻³	2.0·10 ³	4.8·10 ³
		SETP _{marine}	4.1·10 ²	2.1·10 ²	1.0·10 ³	1.9·10 ¹	4.6·10 ¹
		TETP	8.8	1.0·10 ⁻³	1.9·10 ⁻⁵	2.9·10 ¹	2.1·10 ¹
		HTP	3.3·10 ¹	9.7	1.6·10 ⁻²	2.1·10 ²	2.2
174. 2,4,5-T	93-76-5	AETP _{fresh}	8.5·10 ⁻¹	1.7·10 ¹	1.7·10 ⁻¹⁰	4.4·10 ⁻¹	1.5
		AETP _{marine}	2.0·10 ⁻¹	6.1·10 ⁻²	4.0·10 ⁻¹	1.6·10 ⁻³	5.5·10 ⁻³
		SETP _{fresh}	6.1·10 ⁻¹	1.2·10 ¹	1.2·10 ⁻¹⁰	3.2·10 ⁻¹	1.1
		SETP _{marine}	2.5·10 ⁻¹	7.6·10 ⁻²	4.9·10 ⁻¹	2.0·10 ⁻³	6.8·10 ⁻³
		TETP	3.2·10 ⁻¹	3.6·10 ⁻⁸	6.4·10 ⁻¹¹	7.4·10 ⁻¹	6.4·10 ⁻¹
		HTP	8.9·10 ⁻¹	1.9	5.4·10 ⁻³	5.8	1.8·10 ⁻¹

Substance No. Name	CAS No.	Type	Initial emission compartment				
			air	fresh water	sea water	agricult. soil	industria l soil
Pesticides							
175. Thiram	137-26-8	AETP _{fresh}	2.7·10 ³	9.8·10 ⁴	2.6·10 ⁻²	6.9·10 ²	4.4·10 ³
		AETP _{marine}	3.1·10 ²	7.5·10 ¹	4.2·10 ²	7.0·10 ⁻¹	4.5
		SETP _{fresh}	9.8·10 ²	3.5·10 ⁴	9.5·10 ⁻³	2.5·10 ²	1.6·10 ³
		SETP _{marine}	1.9·10 ¹	6.6	3.7·10 ¹	5.7·10 ⁻²	3.7·10 ⁻¹
		TETP	3.2·10 ¹	9.3·10 ⁻²	3.1·10 ⁻⁴	5.1·10 ¹	8.1·10 ¹
		HTP	1.9·10 ¹	3.3	6.6·10 ⁻⁴	7.9	2.5·10 ⁻¹
176. Tolclophos-methyl	57018-4-9	AETP _{fresh}	1.5·10 ⁻¹	5.0·10 ²	2.9·10 ⁻²	3.1	9.2
		AETP _{marine}	1.4	4.4	1.4·10 ²	1.3·10 ⁻¹	3.9·10 ⁻¹
		SETP _{fresh}	1.6·10 ⁻¹	5.3·10 ²	3.1·10 ⁻²	3.3	9.9
		SETP _{marine}	1.6	5.1	1.6·10 ²	1.5·10 ⁻¹	4.4·10 ⁻¹
		TETP	3.4·10 ⁻⁴	3.2·10 ⁻⁴	6.7·10 ⁻⁵	1.8	1.5
		HTP	6.0·10 ⁻²	1.0	6.5·10 ⁻²	1.1·10 ¹	4.0·10 ⁻²
177. Tri-allaat	2303-17-5	AETP _{fresh}	6.1·10 ¹	4.9·10 ⁴	1.1	5.0·10 ¹	2.0·10 ²
		AETP _{marine}	1.5·10 ²	7.8·10 ²	3.3·10 ³	8.4·10 ⁻¹	3.4
		SETP _{fresh}	2.2·10 ¹	1.7·10 ⁴	4.1·10 ⁻¹	1.8·10 ¹	7.0·10 ¹
		SETP _{marine}	3.9·10 ¹	2.2·10 ²	9.2·10 ²	2.3·10 ⁻¹	9.3·10 ⁻¹
		TETP	6.9·10 ⁻³	2.7·10 ⁻³	1.3·10 ⁻⁴	1.3	1.3
		HTP	9.7	8.3·10 ¹	1.2	5.8	3.6·10 ⁻¹
178. Triazophos	24017-47-8	AETP _{fresh}	3.3·10 ³	1.7·10 ⁵	7.9·10 ⁻²	5.8·10 ³	1.9·10 ⁴
		AETP _{marine}	8.5·10 ²	1.5·10 ³	4.9·10 ³	5.3·10 ¹	1.7·10 ²
		SETP _{fresh}	3.0·10 ³	1.6·10 ⁵	7.4·10 ⁻²	5.4·10 ³	1.8·10 ⁴
		SETP _{marine}	1.2·10 ³	2.1·10 ³	6.8·10 ³	7.3·10 ¹	2.4·10 ²
		TETP	3.4·10 ¹	3.9·10 ⁻²	8.4·10 ⁻⁴	2.5·10 ²	2.0·10 ²
		HTP	2.1·10 ²	3.2·10 ²	1.6	1.2·10 ³	3.7·10 ¹
179. Tributyltin-oxide	56-35-9	AETP _{fresh}	7.7·10 ³	4.5·10 ⁵	3.0	1.1·10 ³	4.2·10 ³
		AETP _{marine}	3.1·10 ⁵	2.1·10 ⁵	5.7·10 ⁵	5.6·10 ²	2.2·10 ³
		SETP _{fresh}	1.0·10 ⁴	6.1·10 ⁵	4.1	1.5·10 ³	5.7·10 ³
		SETP _{marine}	3.9·10 ⁵	2.9·10 ⁵	7.9·10 ⁵	7.7·10 ²	3.0·10 ³
		TETP	1.7·10 ¹	1.1·10 ⁻¹	6.9·10 ⁻³	3.7·10 ¹	3.7·10 ¹
		HTP	7.5·10 ³	3.4·10 ³	5.5·10 ¹	2.9·10 ²	4.3·10 ¹
180. Trichlorfon	52-68-6	AETP _{fresh}	1.3·10 ⁴	4.1·10 ⁵	5.3·10 ⁻⁶	3.3·10 ³	1.8·10 ⁴
		AETP _{marine}	1.8·10 ³	8.3·10 ¹	3.6·10 ³	6.7·10 ⁻¹	3.7
		SETP _{fresh}	2.4·10 ³	7.6·10 ⁴	9.9·10 ⁻⁷	6.1·10 ²	3.4·10 ³
		SETP _{marine}	2.7·10 ²	1.3·10 ¹	5.4·10 ²	1.0·10 ⁻¹	5.6·10 ⁻¹
		TETP	1.2·10 ³	7.0·10 ⁻⁵	4.8·10 ⁻⁷	1.9·10 ³	2.6·10 ³
		HTP	4.4	3.7·10 ⁻¹	3.1·10 ⁻⁵	3.3·10 ¹	2.0·10 ⁻²
181. Trifluarin	1582-9-8	AETP _{fresh}	9.9	2.7·10 ⁴	1.8	4.0·10 ¹	1.6·10 ²
		AETP _{marine}	1.0·10 ²	4.2·10 ²	8.3·10 ³	1.2	4.5
		SETP _{fresh}	8.1	2.2·10 ⁴	1.4	3.3·10 ¹	1.3·10 ²
		SETP _{marine}	4.4·10 ¹	1.8·10 ²	3.6·10 ³	4.9·10 ⁻¹	1.9
		TETP	1.7·10 ⁻²	1.3·10 ⁻²	3.0·10 ⁻³	3.5·10 ¹	3.4·10 ¹
		HTP	1.7	9.7·10 ¹	6.0	1.2·10 ²	6.8·10 ⁻¹
182. Zineb	12122-67-7	AETP _{fresh}	9.4·10 ²	2.8·10 ⁴	3.6·10 ⁻³	3.7·10 ²	1.4·10 ³
		AETP _{marine}	4.1·10 ²	2.5·10 ²	8.1·10 ²	3.5	1.3·10 ¹
		SETP _{fresh}	7.4·10 ²	2.2·10 ⁴	2.9·10 ⁻³	3.0·10 ²	1.1·10 ³
		SETP _{marine}	4.5·10 ²	2.7·10 ²	8.9·10 ²	3.8	1.4·10 ¹
		TETP	7.2	1.3·10 ⁻³	2.8·10 ⁻⁵	1.6·10 ¹	1.5·10 ¹
		HTP	4.8	1.7	8.2·10 ⁻⁴	2.0·10 ¹	1.0·10 ⁻¹

4.2 Relative contribution of the geographical scales

The contribution of the four geographical scales to the toxicity potentials calculated with USES-LCA is analysed for the initial emission compartments air, fresh water and industrial soil. This is done for 12 substances, including the reference substance (→ Table 8).

Table 8: Relative contribution of the four geographical scales to toxicity potentials, after initial emission to the continental compartments air, fresh water and industrial soil, respectively

Emission compartment		Air				Fresh water				Industrial soil			
Substance	Unit	C	M	T	A	C	M	T	A	C	M	T	A
		%	%	%	%	%	%	%	%	%	%	%	%
1,4-Dichlorobenzene	AETP _{salt}	7	21	6	66	8	21	6	65	7	21	6	66
	SETP _{salt}	23	15	4	58	26	15	3	56	23	15	4	58
	TETP	18	34	8	39	18	35	8	39	100	0	0	0
	HTP	39	38	23	1	44	34	21	1	39	37	23	1
Hexachlorobenzene	AETP _{salt}	2	29	22	47	2	29	22	47	2	29	22	47
	SETP _{salt}	9	27	18	46	10	27	18	45	9	27	18	46
	TETP	8	24	7	61	8	24	6	62	97	1	0	2
	HTP	25	43	29	3	59	24	16	1	29	41	27	3
Pentachlorophenol	AETP _{salt}	87	12	0	1	93	7	0	0	92	8	0	0
	SETP _{salt}	97	3	0	0	99	1	0	0	98	2	0	0
	TETP	94	6	0	0	94	6	0	0	100	0	0	0
	HTP	96	3	1	0	100	0	0	0	100	0	0	0
2,3,7,8-TCDD	AETP _{salt}	41	38	5	16	57	30	3	10	52	32	4	12
	SETP _{salt}	77	14	2	7	87	9	1	3	84	10	1	5
	TETP	75	20	1	4	75	20	0	5	100	0	0	0
	HTP	85	14	1	0	98	2	0	0	99	1	0	0
Dichloromethane	AETP _{salt}	6	16	6	72	7	16	6	71	6	17	5	72
	SETP _{salt}	23	12	3	62	26	12	3	59	23	12	4	61
	TETP	15	34	10	41	15	34	10	41	99	0	0	1
	HTP	32	39	28	1	33	38	28	1	32	39	28	1
Endosulfan	AETP _{salt}	91	8	0	1	99	1	0	0	97	3	0	0
	SETP _{salt}	97	2	0	1	100	0	0	0	99	1	0	0
	TETP	91	8	0	1	91	8	0	1	100	0	0	0
	HTP	96	4	0	0	100	0	0	0	100	0	0	0
Lindane	AETP _{salt}	72	20	2	6	93	6	0	1	92	7	0	1
	SETP _{salt}	90	5	0	5	98	1	0	1	98	2	0	0
	TETP	78	17	1	4	78	18	0	4	100	0	0	0
	HTP	89	11	0	0	98	2	0	0	96	4	0	0
Lead	AETP _{salt}	1	26	57	16	1	26	57	16	1	26	57	16
	SETP _{salt}	4	25	55	16	6	24	54	16	6	24	54	16
	TETP	69	26	1	4	9	34	44	13	100	0	0	0
	HTP	71	21	7	1	47	25	27	1	98	1	1	0
Benzo[a]pyrene	AETP _{salt}	82	15	1	2	83	14	1	2	83	14	1	2
	SETP _{salt}	96	3	0	1	96	3	0	1	96	3	0	1
	TETP	99	1	0	0	99	1	0	0	100	0	0	0
	HTP	x	x	x	x	x	x	x	x	x	x	x	x
Benzene	AETP _{salt}	16	18	3	63	21	17	3	59	16	18	3	63
	SETP _{salt}	46	11	1	42	55	9	1	35	46	11	1	42
	TETP	34	36	5	25	34	36	5	25	100	0	0	0
	HTP	58	31	11	0	61	28	10	1	58	31	11	0
Formaldehyde	AETP _{salt}	85	13	0	2	100	0	0	0	99	1	0	0
	SETP _{salt}	96	3	0	1	100	0	0	0	100	0	0	0
	TETP	88	11	0	1	87	11	0	1	100	0	0	0
	HTP	90	10	0	0	100	0	0	0	93	7	0	0
Nitrogen dioxide	HTP	89	10	1	0	x	x	x	x	x	x	x	x

C = continental scale; M = moderate scale; T = tropical scale; A = arctic scale; x = toxicity potential not calculated.

As can be seen in Table 8, the tropical scale contribute less to the TETPs and salt water AETPs and SETPs of all substances than the arctic scale with the salt water AETPs and SETPs for lead as an exception. This difference in contribution can be explained by the fact that the environmental temperature and the corresponding degradation and volatilisation rates for the soil and water compartment are much higher in the tropics in comparison with the arctic. Furthermore, it can be seen that the arctic scale is in general relatively more important for salt water AETPs and SETPs of relatively volatile and persistent substances than for relatively non- volatile and non-persistent substances. This holds also true for TETPs of substances emitted to continental air or fresh water compartment, while for direct emissions to industrial soils TETPs are completely explained by continental concentrations in the soil. This means that after emission to continental soils transport of pollutants to other soils hardly occurs. Moreover, for relatively immobile or rapidly degradable substances, such as benzo[a]pyrene and formaldehyde, the continental and moderate scale are contributing dominantly to the TETPs and salt water AETPs and SETPs of these substances, because in de model calculations initial emissions take place at the continental scale. Finally, the continental scale and in most cases in combination with the moderate scale are important for all HTPs listed in Table 8. The tropical scale is also important for relatively volatile and air persistent substances emitted to the air or fresh water. The arctic scale does not significantly contribute to any HTP, because the population density at this scale is very low.

4.3 Comparison with previous toxicity potentials

This section is devoted to the analysis of the differences between toxicity potentials calculated with either USES 1.0 (Guinée et al., 1996a) or USES-LCA for a selection of substances. The three calculation procedures for toxicity potentials which are compared are:

- USES 1.0 OLD, containing the toxicity potentials calculated by Guinée et al. (1996a);
- USES 1.0 NEW, containing the toxicity potentials calculated by USES 1.0, but now using up-to-date substance-specific input data. In addition, system parameters and human characteristics are set equal to the continental scale in USES-LCA, although air speed and water flow are still minimised to prevent substance flow across the system boundaries;
- USES-LCA, containing the toxicity potentials calculated by the adapted USES 2.0 model, using up-to-date substance-specific input data.

Table 9 shows the results of the comparison of the three calculation procedures mentioned above. In the four columns called 'USES 1.0 NEW / USES 1.0 OLD' the toxicity potentials as calculated by USES 1.0 are compared by dividing the USES 1.0 NEW by the USES 1.0 OLD factors. If the quotient related to a substance and an initial emission compartment is smaller than 1, the toxicity potential calculated with USES 1.0 NEW is lower than the toxicity potential calculated with USES 1.0 OLD. If

the quotient is larger than 1, the reverse is true.²⁰ About 60% of the quotients are smaller than 1, while 40% of the quotients are larger than or equal to 1. Differences, listed in Table 8, may be up to several orders of magnitude, indicating that it is worthwhile to use up-to-date input data and to have a closer look at the system settings of the modelled system. A combination of the following alternations is responsible for the differences found:

- HLVs and PNECs are altered, because (1) more recent or relevant literature sources are consulted, (2) PNECs are derived with the TGD method (EC, 1996), while Guinée et al. (1996a) used the modified EPA-method (Van de Meent et al., 1990), and (3) for substances which are genotoxic or (possibly) carcinogenic by a genotoxic mechanism of action an HLV corresponding with an extra life-time risk of 1.10^{-6} is used instead of 1.10^{-4} . (1) And (2) will both lead to either an increase or decrease of the toxicity potential, and (3) result in a factor 100 increase of human toxicity potentials for genotoxic substances;
- Based on McKone et al. (1995) and Howard et al. (1991), degradation rates for 1,4-dichlorobenzene are estimated much more conservatively for the compartments air, water and soil than Guinée et al. (1996a) did. In contrast, for most other substances worst-case default degradation rates are replaced by more realistic degradation rates. Furthermore, although for other substances too optimistic degradation rates are replaced by more conservative estimates, the new estimates are relatively less conservative than the change in conservativeness of degradation rates for 1,4-dichlorobenzene. The result of this change is that for most substances the toxicity potentials decrease to a large extent in comparison with the toxicity potentials calculated by Guinée et al. (1996a). Using other substance-specific input data in the new calculations, such as experimental partitioning coefficients, bioconcentration factors and bio-accumulation factors may also change the toxicity potentials to some extent.

In the four columns called 'USES-LCA / USES 1.0 NEW' the toxicity potentials as calculated by USES-LCA are compared with the up-to-date USES 1.0 toxicity potentials by dividing the USES-LCA by the USES 1.0 NEW factors. If the quotient is less than 1, the toxicity potential calculated by USES-LCA is lower than the toxicity potential calculated by USES 1.0 NEW. If the quotient is larger than 1, the reverse is true. About 60% of the quotients is smaller than 1, while 40% of the quotients is larger or equal to 1. Differences in toxicity potentials between USES-LCA and USES 1.0 NEW, which are up to several orders of magnitude, may be explained by one or more of the the following alterations:

- USES-LCA is a closed nested multi media model, including a sea compartment and three global scales in contrast to USES 1.0 which does not contain these compartments and must be artificially closed by setting the water flow and wind speed to extreme low levels.
- To prevent "leaking" of substances out of the water compartment in USES 1.0, the hydraulic residence time is maximized by setting the fraction of rain water that runs off the soil to a very low level (Guinée et al., 1996a). This results in a very low mass flow of the chemical from the soil to the water compartment. In USES-LCA this

²⁰ Do not confuse the quotient with the toxicity potential itself. The toxicity potential say something about the toxic potential of substance emitted to a certain compartment for a specific impact category compared to the toxic potential of a reference substance emitted to a reference compartment for the same impact category.

artificial model change is not needed which results in larger fresh water AETPs after initial emissions to industrial soil and agricultural soil and larger HTPs after emission to agricultural soil compared to USES 1.0.

- On the tropical and arctic scale in USES-LCA an environmental temperature of 25 °C and -10 °C are used as typical values, respectively. Therefore, solubility, biodegradation and hydrolysis rates, vapour pressure, and Henry's law constant will be respectively higher and lower on the tropical and arctic scale in comparison with values for parameters on the continental scale in USES 1.0.
- In USES-LCA bioconcentration factors for fish are estimated with a different QSAR than in USES 1.0 and the model for biotransfer from soil and air to plants in USES-LCA is an adapted version of that in USES 1.0. For instance, in USES-LCA photodegradation and metabolism in plants can be taken explicitly taken into account in the human exposure assessment, resulting in lower Human Toxicity Potentials (HTPs) for pentachlorophenol, endosulfan and 2,3,7,8-TCDD in USES-LCA compared to USES 1.0 NEW (up to a factor 5).
- Weighting factors are used in the calculation of toxicity potentials by USES-LCA. In USES 1.0 weighting factors are not necessary for aquatic ecotoxicity and human toxicity and are not applied for terrestrial ecotoxicity.
- TETP-values are calculated very differently in USES-LCA compared to USES 1.0. In USES 1.0 TETPs are calculated by only taking the predicted environmental concentration in the agricultural soil compartment into account and neglecting concentrations in natural soils and industrial soils. In the calculations with USES-LCA TETPs are calculated taking environmental concentrations in all soil compartments into account (→ Equation 8). As can be seen in Table 8, initial emission to the agricultural soil generally result in lower TETPs in USES-LCA compared to USES 1.0, while for emission to industrial soil the opposite is true.
- Introduction of a chemical-specific soil depth at all geographical scales changes toxicity potentials within a factor 3 for all 12 substances listed in Table 8. However, the TETPs for lead increase up to a factor of 6 in comparison with the use of a standard soil depth, indicating that predicted steady state soil concentrations of lead are not strongly influenced by an increase of the soil depth in comparison to the reference substance 1,4-dichlorobenzene.
- Human ingestion of soil does affect the HTP of persistent substances after direct emission to industrial/urban soil (up to a factor 25 for lead).
- In USES-LCA it is assumed that 90% of the total fish intake on the continental scale are salt water species and 10% fresh water species, instead of assuming that all fish intake are fresh water species. This results in differences up to a factor 40 for HTPs after release to fresh water or sea water.
- In USES 1.0 it is not possible to implement specific inhalatory HLVs in the calculation of the human RCR. The inhalatory HLV is always estimated using route-to-route extrapolation on the basis of absorption rates. In USES-LCA experimental inhalatory HLVs can be implemented. This results in differences up to a factor 30 for the HTPs of the 12 selected substances.
- Taking into account pH-dependency of hydrolysis rates for endosulfan and lindane result in differences up to a factor 2 compared with the use of hydrolysis rates at an environmental pH of 7 in USES 1.0 NEW.
- Toxicity potentials of pentachlorophenol are changed up to a factor 800, using a compartment-specific apparent solubility in the fate analysis.

Table 9: Comparison of old and new toxicity potentials.

Substance	Type	USES1.0 NEW/ USES1.0 OLD				USES-LCA / USES1.0 NEW			
		air	fresh water	agricult. soil	industrial soil	air	fresh water	agricult. soil	industrial soil
1,4-dichlorobenzene	AETP _{fresh}	3.3	1.0	9.3·10 ¹	2.7·10 ¹	6.6·10 ⁻²	1.0	3.3·10 ⁻²	4.0·10 ⁻¹
	TETP	1.2·10 ⁻¹	2.0·10 ⁻¹	4.0·10 ⁻²	1.0	1.2·10 ⁻²	1.2·10 ⁻²	5.4·10 ⁻⁵	1.0
	HTP	1.0	1.7	2.2·10 ¹	8.0	1.0	8.7·10 ⁻¹	2.4·10 ⁻¹	3.0
hexachlorobenzene	AETP _{fresh}	4.5	9.9·10 ⁻¹	2.2	3.4	6.9·10 ⁻²	9.7·10 ⁻¹	1.6·10 ⁻¹	2.4·10 ⁻¹
	TETP	1.1·10 ⁻³	1.4·10 ⁻³	2.7·10 ⁻⁴	8.3·10 ⁻⁴	5.8·10 ⁻⁴	6.2·10 ⁻⁴	2.8·10 ⁻⁴	1.1·10 ⁻²
	HTP	1.9·10 ³	2.2·10 ³	8.7·10 ²	1.4·10 ³	3.8·10 ⁻¹	3.5·10 ⁻¹	2.8·10 ⁻¹	5.7
pentachlorophenol	AETP _{fresh}	3.0·10 ⁻¹	1.2	5.3·10 ⁻⁵	1.4·10 ⁻⁴	3.5·10 ⁻¹	1.4	4.6·10 ⁻³	3.2·10 ¹
	TETP	1.5·10 ⁻⁴	5.9·10 ⁻⁶	1.3·10 ⁻⁴	6.8·10 ⁻⁸	6.5·10 ⁻³	2.5·10 ⁻⁵	1.5·10 ⁻⁹	3.9·10 ¹
	HTP	2.7·10 ¹	1.1	2.9·10 ⁻³	1.3·10 ⁻²	9.4·10 ⁻⁴	3.3·10 ⁻²	1.9·10 ⁻¹	8.0·10 ⁻²
2,3,7,8-TCDD	AETP _{fresh}	5.9·10 ⁻¹	8.8·10 ¹	1.5·10 ⁻⁴	4.5·10 ⁻⁴	5.0·10 ⁻¹	1.2	5.7·10 ²	1.3·10 ²
	TETP	6.3·10 ⁻³	8.0·10 ⁻⁵	9.3·10 ⁻³	7.1·10 ⁻⁷	7.4·10 ⁻³	1.1·10 ⁻²	1.4·10 ⁻⁴	7.5·10 ¹
	HTP	2.5	1.3	9.1·10 ⁻³	1.2·10 ⁻³	2.9·10 ⁻²	2.0·10 ⁻¹	7.7·10 ⁻¹	9.0·10 ¹
dichloromethane	AETP _{fresh}	2.7·10 ¹	6.2	2.4·10 ¹	2.6·10 ¹	2.8·10 ⁻³	9.5·10 ⁻²	5.2·10 ⁻⁴	1.4·10 ⁻²
	TETP	1.6·10 ⁻¹	1.5·10 ⁻¹	6.8·10 ⁻²	1.5·10 ⁻¹	3.4·10 ⁻⁴	3.4·10 ⁻⁴	1.3·10 ⁻⁶	2.1·10 ⁻²
	HTP	7.8·10 ⁻¹	6.6·10 ⁻¹	6.5·10 ⁻¹	7.2·10 ⁻¹	2.3·10 ⁻¹	2.3·10 ⁻¹	3.8·10 ⁻²	3.0·10 ⁻¹
endosulfan	AETP _{fresh}	1.8·10 ⁻²	3.2·10 ⁻¹	6.6·10 ⁻⁶	1.0·10 ⁻⁵	2.9·10 ⁻³	9.5·10 ⁻³	3.7·10 ⁻²	9.9·10 ⁻¹
	TETP	9.9·10 ⁻⁶	6.0·10 ⁻⁷	1.4·10 ⁻⁴	5.5·10 ⁻⁹	1.6·10 ⁻³	1.4·10 ⁻³	1.6·10 ⁻⁸	8.3·10 ²
	HTP	5.0·10 ⁻²	1.2·10 ⁻¹	7.1·10 ⁻⁴	2.9·10 ⁻⁵	2.7·10 ⁻¹	2.6·10 ⁻¹	1.2·10 ⁻¹	7.4·10 ¹
lindane	AETP _{fresh}	7.3·10 ⁻²	2.4·10 ⁻¹	2.9·10 ⁻²	3.5·10 ⁻²	3.3·10 ⁻¹	6.6·10 ⁻¹	1.7·10 ⁻¹	4.1·10 ¹
	TETP	5.3·10 ⁻⁵	4.2·10 ⁻⁵	2.2·10 ⁻⁴	2.6·10 ⁻⁵	2.1·10 ⁻³	1.4·10 ⁻³	3.1·10 ⁻⁷	1.8
	HTP	8.5·10 ⁻³	1.7·10 ⁻²	1.6·10 ⁻²	4.1·10 ⁻³	7.3	2.2·10 ⁻¹	2.9·10 ⁻²	8.0·10 ¹
lead	AETP _{fresh}	4.3·10 ⁻¹	4.3·10 ⁻¹	5.5·10 ⁻²	5.5·10 ⁻²	4.6	5.6·10 ⁻¹	1.0·10 ⁻¹²	3.0·10 ¹⁰
	TETP	9.5·10 ⁻⁴	1.9·10 ⁻⁹	9.7·10 ⁻⁴	1.4·10 ⁻⁹	1.5	1.3·10 ⁻⁶	1.2·10 ⁻²²	9.7·10 ¹⁴
	HTP	1.2·10 ⁻⁴	1.1·10 ⁻¹	5.4·10 ⁻²	2.1·10 ⁻⁶	6.0·10 ¹	4.3·10 ⁻¹	3.1	9.6·10 ¹²
benzo[a]pyrene	AETP _{fresh}	9.4·10 ⁻¹	1.1	3.9·10 ⁻³	5.1·10 ⁻³	2.9·10 ⁻¹	2.3·10 ¹	2.5·10 ¹	2.9·10 ³
	TETP	3.1·10 ⁻⁵	1.2·10 ⁻⁵	3.6·10 ⁻⁵	1.7·10 ⁻⁷	1.2·10 ⁻⁴	2.6·10 ⁻³	9.7·10 ⁻⁸	7.6·10 ¹
	HTP	x	x	x	x	x	x	x	x
benzene	AETP _{fresh}	3.7·10 ⁻¹	8.9·10 ⁻²	3.3	1.1	1.7·10 ⁻¹	1.0	2.0·10 ⁻²	1.5
	TETP	9.8·10 ⁻³	1.4·10 ⁻²	4.4·10 ⁻³	2.9·10 ⁻²	2.6·10 ⁻²	2.6·10 ⁻²	7.3·10 ⁻⁶	5.6
	HTP	6.1·10 ¹	8.4·10 ¹	1.0·10 ³	1.8·10 ²	1.1	9.7·10 ⁻¹	3.9·10 ⁻²	8.7
formaldehyde	AETP _{fresh}	9.0·10 ⁻¹	1.9	7.3·10 ¹	6.3·10 ¹	1.5	9.4·10 ⁻¹	1.0·10 ⁻²	2.0·10 ²
	TETP	5.9·10 ⁻²	1.1·10 ⁻¹	1.3·10 ⁻¹	4.2	6.1·10 ⁻³	5.7·10 ⁻³	1.9·10 ⁻⁸	2.7
	HTP	6.7·10 ⁻¹	5.8·10 ⁻¹	3.1·10 ¹	4.7·10 ¹	2.9	1.8·10 ⁻¹	2.9·10 ⁻⁵	5.9·10 ²
nitrogen dioxide	AETP _{fresh}	x	x	x	x	x	x	x	x
	TETP	x	x	x	x	x	x	x	x
	HTP	3.8	x	x	x	1.3	x	x	x

x = toxicity potential is not calculated

4.4 Terrestrial vegetation compartment

Although a terrestrial vegetation compartment is not included in USES-LCA, terrestrial vegetation may have a large influence on the fate of chemicals (Bennett et al., 1998; Calamari et al., 1991; Simonich & Hites, 1994). The effect on the toxicity potentials of adding a vegetation compartment on the continental scale²¹, described in Brandes et al. (1996) and Severinsen & Jager (1998), is analysed in this section. This terrestrial vegetation compartment is not suited for anorganic substances, such as metals. Therefore, no comparison is made for these substances. As can be seen in Table 10, including a terrestrial vegetation compartment on the continental scale does not significantly change toxicity potentials of the selected substances.

Table 10: Comparison of toxicity potentials calculated with USES-LCA either excluding or including a terrestrial vegetation compartment on the continental scale

Substance ^a	Type	USES-LCA DEFAULT / USES-LCA VEGETATION				
		air	fresh water	sea water	agricultural soil	industrial soil
1,4-dichlorobenzene	AETP _{fresh}	1	1	1	1	1
	SETP _{fresh}	1	1	1	1	1
	TETP	1	1	1	1	1
	HTP	1	1	1	1	1
hexachlorobenzene	AETP _{fresh}	1	1	1	1.1	1
	SETP _{fresh}	1	1	1	1	1
	TETP	1	1	1	1.1	1
	HTP	1	1	1	1.1	1
pentachlorophenol	AETP _{fresh}	1.1	1	1	1	1
	SETP _{fresh}	1.1	1	1	1	1
	SETP	1.1	1.1	1.1	1	1
	HTP	1.1	1	1	1	1
2,3,7,8-TCDD	AETP _{fresh}	1.1	1	1	1	1
	SETP _{fresh}	1.1	1	1	1.1	1
	TETP	1.1	1.1	1.1	1	1
	HTP	1.1	1	1	1	1
dichloromethane	AETP _{fresh}	1	1	1	1	1
	SETP _{fresh}	1	1	1	1	1
	TETP	1	1	1	1	1
	HTP	1	1	1	1	1
endosulfan	AETP _{fresh}	1	1	1	1	1
	SETP _{fresh}	1	1	1	1	1
	TETP	1	1.1	1.1	1	1
	HTP	1	1	1	1	1
lindane	AETP _{fresh}	1	1	1	0.9	1
	SETP _{fresh}	1	1	1	1	1
	TETP	1	1	1	1	1
	HTP	1	1	1	1	1
benzo[a]pyrene	AETP _{fresh}	1	1	1	1	1
	SETP _{fresh}	1	1	1	1	1
	TETP	1	1	1	1	1
	HTP	x	x	x	x	x
benzene	AETP _{fresh}	1	1	1	1	1
	SETP _{fresh}	1	1	1	1	1
	TETP	1	1	1	1	1
	HTP	1	1	1	1	1
formaldehyde	AETP _{fresh}	1	1	1	0.7	1
	SETP _{fresh}	1	1	1	1.1	1
	TETP	1	1	1	1	1
	HTP	1	1	1	1	1

²¹ On the global scales, no terrestrial vegetation compartment is implemented.

^a effect of terrestrial vegetation compartment is unknown for lead and NO₂ ; x = toxicity potential is not calculated

5. Validity of toxicity potentials

The significance of the toxicity potentials calculated with USES-LCA is dependent on the validity of the assumptions concerning the model structure, input data, and use in LCA case studies. The validity of the toxicity potentials is assessed by a critical discussion of these assumptions, because experimental validation is not feasible within the context of this study.

Model structure

One implicit assumption in the calculation of toxicity potentials is that the model sufficiently covers all relevant compartments and environmental processes. However, this may not be the case. Several simplifications in USES-LCA may have an effect on the outcome of the priority assessment. First, the groundwater compartment is not implemented in the model as a full compartment. Because predicted porewater concentrations of chemicals are used as a first approximation for concentrations in drinking water produced by groundwater, intake of chemicals via drinking water will be overestimated. Secondly, a terrestrial vegetation compartment is not included in the current model calculations. A preliminary assessment including a terrestrial vegetation compartment on the continental scale, however, indicate that terrestrial vegetation do not have a large effect on the toxicity potentials. Furthermore, all compartments in USES-LCA are assumed to be 'well-mixed' and chemicals are assumed to be homogeneously distributed in the compartments which is a simplification of reality. In addition, on the global scale no differentiation between types of soil and water compartments is implemented. Dividing the world in more compartments, as is the case in the global distribution model developed by Wania & Mackay (1995), may improve the validity of the toxicity potentials to some extent. In the human exposure assessment the use of the octanol-water partition coefficient to predict chemical biotransfer of organic chemicals from cattle diet into beef and milk, and from soil into the above-ground vegetation may also cause unreliable model results (Dowdy et al., 1996; Dowdy & McKone, 1997; Garten & Trabalka, 1983; Lowenbach et al., 1995; Polder et al., 1998). Dowdy et al. (1996) and Dowdy & McKone (1997) showed that using a QSAR method based on the Molecular Connectivity Index instead of the octanol-water partition coefficient improved these model predictions to a large extent. It is likely that metabolism variations of chemicals are an important contribution to the observed variation in biotransfer factors and bioconcentration factors. This type of variation is not captured by the variation in octanol-water partition coefficients, while it is by the Molecular Connectivity Index (Dowdy et al., 1996; Dowdy & McKone, 1997). Another simplification in USES-LCA is the implicit assumption that all humans consume food only from their own geographical region. However, a large proportion of the food intake may be imported from other geographical scales. Finally, human characteristics, such as food intake rates, are considered to be identical for all geographical scales which is obviously not the case. The influence of above mentioned simplifications on the calculated toxicity potentials is difficult to assess, because only the relative difference between the reference substance, 1,4-dichlorobenzene, and all other substances caused by above mentioned simplifications is of importance. This should be the subject of further research.

LCA-specific alternations in the model structure may also have an effect on the validity

of the model results. An important choice in the calculation of toxicity potentials is that it is assumed that all life cycle emissions take place in Western Europe. Of course, this is a simplification of reality because emissions in many product life cycles also take partly place outside Western Europe. Another problem of using Western Europe as the initial emission compartment is that in this way all emissions are assumed to be homogeneously distributed over Western Europe, not allowing computation of specific toxicity potentials per West European country. Both problems may be reduced by dividing the world in a standard set of regions. For each region then specific toxicity potentials should be calculated and life cycle inventory outcomes should list their emissions per geographical region instead of a fully accumulated list of emissions. Another arbitrary choice in the calculation of toxicity potentials is that aggregation of salt water aquatic RCRs take place on the basis of volumes of the compartments involved, and aggregation of terrestrial and salt water sediment RCRs on the basis of compartment weights. Other weighting methods, for instance, on the basis of species density per compartment may result in other AETPs, TETPs and SETPs. A third LCA choice in this assessment is to consider warm-blooded predators (mammals and birds) as a separate impact category, although impact factors have not been calculated, yet. Another option may be to consider fish-eating predators and worm-eating predators as an integral part of the aquatic and terrestrial environment, respectively. Following this line of reasoning three ecotoxicological impact categories have to be assessed instead of five. However, integration of these impact impact categories is only valid if in the derivation of aquatic and terrestrial PNECs potential toxic effects of higher predators are accounted for. Methods to account for secondary poisoning may be used for this purpose (see Van de Plassche, 1994). Finally, in the calculation of human toxicity potentials oral and inhalatory effects are added. Because every type of impact that firstly occurs is used in the derivation of oral and inhalatory HLVs, different severity and effect are added, implicitly giving the same weight to all effects.

Substance-specific data

Although much effort is spent in obtaining relevant input data for the model calculations, still a number of shortcomings can be found. First the use of USES-LCA for metals is debatable. No attempt is made to take metal speciation into account in the assessment. Both the PNECs and predicted environmental concentrations are expressed as total metal concentrations and not as bioavailable additions and concentrations. This introduces uncertainty into the assessment since bioavailability may not be the same for exposure levels and PNECs. Furthermore, dependency of metal K_p -values to soil characteristics (in particular pH) is not taken into account in the assessment. Moreover, the use of bioconcentration and bioaccumulation factors for metals in the human exposure assessment may not be valid. As has been pointed out by Chapman (1996), bioconcentrations factors for metals, especially essential metals, may not be valid, because uptake is only partially related to the concentration in the environment. Referring to the topic of essential metals, a more general question is whether essential metals should be treated differently than non-essential substances. Essential elements are indispensable for life and may be deficient in some situations with associated problems for plants, animals and humans. This may be considered as a negative effect, although naturally occurring deficiencies may play an important role in maintaining biodiversity. A discussion on how to deal with the possible positive and negative effects of essential elements in the derivation of PNECs for these elements has been ongoing for some years. These discussions have not resulted yet in new derivation

procedures. In the derivation procedures of PNECs for humans, terrestrial and aquatic ecosystems used in this study this ongoing discussion on the essential aspects of some elements has not been taken into account yet (if possible at all). For the time being it is assumed that the current background concentrations will supply a sufficient level of essential elements for many existing species (Crommentuijn et al., 1997). It is therefore advised to treat the antropogenic addition of essential metals to the environment in the same way as releases of non-essential chemicals.

Chemicals which are transformed into stable or more toxic metabolites in the environment also form a problem in the computation of toxicity potentials. For instance, aldicarb will be transformed to the stable metabolites aldicarb-sulfon and aldicarb-sulfoxide which may have different toxicity characteristics as aldicarb, and 2-chloro-4-methyl-phenol is more toxic than its parent compound MCPA (Crommentuijn et al., 1997b). Another example is that NO_x , NH_3 , and SO_2 form secondary aerosols in the atmosphere which are also important for human toxicity. The fate and toxicity of these transformation products should also be taken into account in the computation of toxicity potentials. However, in the current USES-LCA model it is not possible to simultaneously model the fate of the parent compound and its metabolites.

A third group of substances which is difficult to assess in USES-LCA, are ionising substances, such as chlorophenols. As pointed out by Shiu et al. (1994) and Mackay et al. (1995), the solubility and K_{oc} of ionising chemicals are dependent on the pH of the environment. This is also the case for uptake of dissociating substances in plants (Briggs et al., 1987). As a consequence the fate and human intake of these substances may be highly dependent on the expected pH of the environment. As a first approximation, the apparent solubility and K_{oc} is estimated using simple formulas given by Shiu et al. (1994), and uptake of dissociating pesticides by plants is estimated on the basis of results of Briggs et al. (1987). This approximation causes substantial uncertainty in the toxicity potentials of this type of substances.

Carcinogenic PAHs are also difficult to assess. Toxicity potentials for this group of substances are calculated, assuming a default composition of carcinogenic PAHs occurring in the environment. Substantial uncertainty is, however, attached to this default composition. Other default composition estimates may result in other toxicity potentials.

Finally, substantial error in the toxicity potentials may be introduced by the estimation of air degradation rates with the atmospheric oxidation program of Syracuse Research Corporation (1993), based on QSAR-methods developed by Atkinson (1985, 1987, 1988). As has been pointed by Kwok & Atkinson (1995), these QSAR methods may produce too optimistic rate constants for polycyclic and heteroatom-containing aromatic compounds, such as pesticides.

There are also problems concerned with input data in the calculation of toxicity potentials in general. First of all, the effects assessment is seriously hampered by the lack of relevant data. The inhalatory HLV is in most cases derived by applying route-to-route extrapolation, although this extrapolation procedure is not very reliable (Vermeire et al., 1998) and due to a lack of ecotoxicity data about 60% of the terrestrial PNECs and 100% of the sediment PNECs are based on aquatic PNECs.

Furthermore, for almost all substances a considerable amount of uncertainty is attached to input data, such as environmental degradation rates, partitioning coefficients, bioconcentration factors and no effect levels. The combined effect of these input uncertainties on the uncertainty of toxicity potentials can be assessed with help of Monte Carlo simulation. Thissen (1999) performed such an uncertainty analysis for a small number of substances for which toxicity potentials are derived here.

Application of toxicity potentials

The current calculation of impact scores has some serious limitations. First, it implies that there is a single overall endpoint per impact category. This may be true for terrestrial ecotoxicity and aquatic ecotoxicity, because only effect parameters which exclusively affect the species on the population level, such as mortality, growth, reproduction and photosynthesis, are taken into account in the derivation of PNECs (Slooff, 1992). For human toxicity, however, this is not the case, because every type of impact that firstly occurs, is used in the derivation of HLVs. This means that in the calculation of the impact score for human toxicity, impacts of different severity and effect are added, implicitly giving the same weight to all effects (Olsen & Hauschild, 1998). Furthermore, the toxicity potentials calculated with USES-LCA can not be used for the impact assessment of airborne emissions low above ground, such as airborne emissions of pesticides during application. The fate of this type of airborne emissions is very different from the way USES-LCA treats airborne emissions. Moreover, the calculation procedure assumes linearity between emissions and responses (Owens, 1997). An assumption that deviates from real life. Finally, interactions between substances, such as antagonistic or synergistic effects related to the exposure to multiple substances, are disregarded in the aggregation procedure.

The first limitation may be overcome by distinguishing human toxicity in several subcategories. For instance, Burke et al. (1995) proposed to distinguish substances causing human toxicity in three categories which are (1) irreversible effects, (2) reversible but life-threatening effects, and (3) reversible and no life-threatening effects. Expert-based weighting factors of these three impact categories for human toxicity are set to 100, 10 and 1, respectively. Although such a proposal needs additional information about the type of impact on which the HLV is based, for most substances this information can be obtained (see Lu, 1995; USEPA, 1998b). Aggregation may also be established with the concept of Disability Adjusted Life Years (DALYs), as described in detail by Hofstetter (1999). Furthermore, the limitation that current toxicity potentials are not valid for airborne emissions low above ground can be overcome by using other models for the calculation of toxicity potentials for these type of emissions.²² The other limitations are far more difficult to deal with, because solving these limitations requires much more detailed data than currently available. For instance, to take the non-linearity in emissions and responses into account, the complete dose-response curve of the chemical for each impact category must be known and spatially differentiated information about background concentrations of all chemicals and inventory data must be available.

However, the implementation of the toxicity potentials, calculated with USES-LCA, in LCAs already requires more spatial information than is currently available in most

²² The local part of USES 2.0 provides the option to assess the fate of airborne pesticide emissions

cases. Emissions to the aquatic environment, used in the calculations of life cycle inventories and normalisation data, must be reported separately for sea water and fresh water, because toxicity potentials are calculated for both emissions to sea water and fresh water. The same is true for emissions to soil which should be distinguished in emissions to industrial and agricultural soil.

6. Conclusions

The use of the nested global multi-media fate model USES-LCA has improved the calculation of toxicity potentials in comparison with previous research. First, the artificial change to a closed system and the lack of relevant compartments in the currently used multi media fate models is overcome by modelling a larger part of the world. Furthermore, temperature dependency of solubility, vapour pressure, Henry's law constant, and degradation rates is taken into account. Additional improvements in USES-LCA are the implementation of (1) a chemical specific soil depth on all scales, (2) specific hydrolysis rates per individual compartment, (3) soil ingestion in the human exposure assessment, and (4) chemical transport from the troposphere to stratosphere. Apart from the improved model structure, much effort is expended to prevent the use of estimation procedures or worst-case default estimates for input data in the model calculations.

Although method and input data are both improved, still a number of issues needs to be addressed. Model improvements in USES-LCA, such as the implementation of scale-specific human characteristics and a ground water compartment, are needed. The fate and toxicity of metabolites should also be taken into account in the computation of toxicity potentials. Furthermore, the simple compartment aggregation procedure on the basis of volumes or mass for the ecotoxicological impact categories, respectively, may be replaced by a more complex aggregation procedure perhaps based on other compartment characteristics, such as species density. Moreover, a discussion is needed about which toxic impact categories should be distinguished. Questions to be solved are (1) "Should higher predators be considered as separate impact categories or can they become integrated in the ecotoxicological impact categories considered in this report?" and (2) "Which types of human impact categories should be distinguished and which method should be used to weight these impact categories?". In addition, safety factors in both the derivation of human and ecotoxicological no-effect values should be based on typical estimates. It is also necessary to calculate toxicity potentials for additional substances and additional regions other than Western Europe. Finally, an uncertainty (importance) analysis should be applied to operationalise data uncertainty in the computation of toxicity potentials and to be able to focus further research on parameters which contributes dominantly to the uncertainty in toxicity potentials.

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