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Uncertainty and variability in environmental life-cycle assessment

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Aan Fanny en Renske

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Chapter 1

General introduction

Increased rates of resource depletion, land use, solid waste generation and emissions of pollutants became issues of broad public concern in the beginning of the seventies (Meadows *et al.*, 1972). Unfortunately, most of these problems are still with us today, and some of them have increased substantially (World Resources Institute, 1996). One way to decrease the environmental pressure of human activities is the environmental improvement of production processes (Reijnders, 1996). In this respect, an important question to be answered is 'how exactly can we measure the environmental improvement of production processes?' Environmental life-cycle assessment (LCA) aims to answer that question. The first section of this chapter provides an overview of the LCA framework. Although the framework itself is well-established, the application of the framework is in many aspects problematic. A brief overview of the problems associated with the actual implementation of the framework is described in second paragraph. Finally, the aim and the structure of the present thesis is outlined in the third paragraph.

§ 1.1 Environmental life cycle assessment

Environmental life cycle assessment (LCA) is a tool for the assessment of the environmental impact of product systems (Heijungs *et al.* 1992). It considers the full life cycle of a product from resource extraction to waste disposal. LCA is generally divided into four phases: goal and scope definition, inventory analysis, impact assessment, and interpretation (Figure 1.1; ISO, 1997a).

Figure 1.1 Phases taken in environmental life-cycle assessment (from ISO, 1997a).

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 'the consumption of 100 kg apples' with, for instance, the aim to compare the environmental impacts of different agricultural production processes of apples. In the inventory analysis, for each of the product systems considered data are gathered for all the relevant processes involved in the life cycle. A product system can be considered as a combination of processes needed for the functioning of a product or service. The outcome of the inventory analysis is a list of all extractions of resources and emissions of substances caused by the functional unit for every product system considered, generally disregarding place and time of the extractions and releases. The matrix method can be used to perform the inventory analysis (Heijungs, 1996, 1997):

$$i = H \cdot G^{-1} \cdot u$$

where i is the vector of environmental interventions, H is the environmental intervention matrix, representing the extractions of resources and emissions of substances per unit process, G is the technology matrix representing the inter-process flows needed for the functioning of the product system, and u is the external supply vector, related to the functional unit.

Life cycle impact assessment (LCIA) aims to improve the understanding of the inventory result. Firstly, it is determined which extractions and emissions contribute to which impact categories. An impact category can be defined as ‘a class representing environmental issues of concern into which results from the inventory analysis may be assigned’ (ISO, 1998a). Table 1.1 shows a comprehensive list of commonly applied impact categories in LCA (Udo de Haes, 1996; Guinée, 2000).

<i>Input related categories ("resource depletion or competition")</i>
1. Abiotic resources
2. Biotic resources
3. Effect of land use
4. Dessication
<i>Output related categories ("pollution")</i>
5. Global warming
6. Depletion of stratospheric ozone
7. Human toxicological impacts
8. Ecotoxicological impacts
9. Photo-oxidant formation
10. Acidification
11. Eutrophication
12. Odour
13. Noise
14. Radiation
15. Casualties
16. Waste heat

Table 1.1
Default list of generally recognised impact categories for LCIA (from Udo de Haes 1996; Guinée, 2000)

The next step in the impact assessment is the characterisation. The aim of the characterisation is to aggregate the releases of pollutants and the extractions of resources of a product system for a number of predefined environmental impact categories (see Table 1.1). As many LCA applications tend to be change-oriented (“what is the additional environmental impact if one extra product is produced?”), the approach of ‘marginal change’ is advocated in life cycle impact assessment (Udo de Haes *et al.*, 1999). It assumes that an additional amount of a certain stressor introduces very small changes on top of a *ceteris paribus* background situation. The change in impact per unit amount of additional ‘release’ represents the relative importance of the stressor to an impact category (Heijungs *et al.*, 1992). This conversion factor is referred to as the

characterisation factor q for the pollutant and impact category considered. Other names for characterisation factor are 'potential', 'equivalency factor' or 'impact factor'. Fate and effects of a substance are preferably taken into account in the calculation of the characterisation factor (Heijungs, 1997; Joliet, 1996; Nichols *et al.*, 1996):

$$\mathbf{Q} = \mathbf{E} \cdot \mathbf{F}^{-1}$$

where $\mathbf{Q}$ is the matrix of characterisation factors, $\mathbf{E}$ is the effect matrix and $\mathbf{F}$ is the fate matrix. Various models may be used to include fate and effects in the calculation of characterisation factors (Hertwich *et al.*, 2001; Potting *et al.*, 2001; Hauschild and Pennington, 2001; Krewitt *et al.*, 2001). Fate factors may be calculated with multi-media fate box models, such as Simplebox (Brandes *et al.*, 1996), or spatially explicit models, such as EcoSense (Krewitt *et al.*, 1998). The effect factor ($\mathbf{E}$) may be a simple measure of impact, such as the inverse of a predicted no effect concentration (1/PNEC) for toxic effects towards ecosystems (Guinée and Heijungs, 1993). It may also be derived from a detailed description of the dose-response curve (Krewitt *et al.*, 1998; Goedkoop and Spriensma, 1999). Commonly applied sets of characterisation factors are global warming potentials (Albritton *et al.*, 1996), ozone depletion potentials (Solomon *et al.*, 1995) and photochemical ozone creation potentials (Derwent *et al.*, 1998). Multiplication of the characterisation factor matrix $\mathbf{Q}$ with the environmental intervention vector $\mathbf{i}$ gives a vector $\mathbf{r}$ of environmental impact scores:

$$\mathbf{r} = \mathbf{Q} \cdot \mathbf{i}$$

The last (optional) step of the impact assessment is the calculation of an environmental index by aggregation of the impact categories (Heijungs, 1997; Finnveden *et al.*, 2001):

$$x = \mathbf{w} \cdot \mathbf{r}$$

in which x is the environmental index and $\mathbf{w}$ is the vector of weighting factors representing the relative importance of the impact categories involved. For example, an authorised weighting set may be based on political reduction targets, environmental control and damage costs or panel preferences in reducing environmental impacts (Powell *et al.*, 1997; Finnveden *et al.*, 2001). The final phase in an LCA study is the interpretation of the results from the previous three steps, to draw conclusions and to formulate recommendations for decision makers.

§ 1.2 Problem setting

Although the LCA framework, as presented in Section 1.1, is conceptually straightforward, the actual implementation of the framework is not without problems. When it comes to scientific merit, there are major uncertainties about the extent to which outcomes of LCAs reflect (changes in) real-life environmental impacts. A major source of uncertainty in LCA is that fate modelling of toxic, acidifying and eutrophying substances is in its early development or not implemented at all (Guinée, 1995; Heijungs, 1997). Another important issue is the general lack of site and time dependency in the LCA methodology (Udo de Haes, 1996). This lack is caused by the fact that both the inventory analysis and the impact assessment generally disregards place and time. Environmental impacts, may, however, be strongly affected by the site-dependent nature of environmental interventions, because geographically different targets may differ in their sensitivity an/or background exposure (Potting *et al.*, 1999). Another major problem affecting the application of LCA-based tools concerns the input data needed. The availability of reliable data is a general concern in life cycle inventories (Weidema and Wesnæs 1996). Many producers do not provide full data, and the monitoring of the adequacy of data provided by producers is usually poor. Furthermore, in the calculation of characterisation factors various estimates of environmental and substance specific input parameters may be used which in turn may strongly affect the model outcomes (Hertwich *et al.*, 1999). Normative choices may also give rise to uncertainty. An example of choices leading to uncertainty in the inventory analysis is the choice of an allocation procedure for multi-output processes, multi-waste processes and open-loop recycling. According to Kortman *et al.* (1996), different allocation procedures may have a significant effect on the outcome of an LCA. The choice of a particular characterisation factor may also give rise to uncertainty. For instance, in dealing with contributions to climate forcing, different time horizons may be used (Albritton *et al.* 1996), which may have a significant effect on the outcome of LCA case studies. An overview of all the value choices to be considered in LCA and the actual possibility to assess the importance of these value choices, is, however, lacking. All in all, it appears that there are a large range of possibilities available to improve the LCA methodology. This also concerns the availability of reliable data and the handling of uncertainty. Although such improvements may not make LCA-based tools perfect, it may be worthwhile to find out if substantial improvements are a realistic possibility.

§ 1.3 Aim and outline of the thesis

As argued in the previous section, uncertainty and variability are not systematically addressed in LCA research. However, decreasing uncertainties in the application of the LCA framework and a quantitative insight into the level of the (remaining) uncertainty and variability may improve the quality of the decision making process. The aim of this thesis is to contribute to a quantitative evaluation of uncertainty and variability in

environmental life-cycle assessment. It also intends to improve the characterisation factors used for the evaluation of toxic, acidifying and eutrophying emissions.

In Chapter 2 a framework to classify types of uncertainty and variability in LCAs is developed and tools how to deal with these types of uncertainty and variability are discussed in detail. Furthermore, for parameter uncertainty and uncertainty due to choices it is shown in a simplified example how they can be evaluated in the inventory analysis and the impact assessment.

Chapter 3 outlines the global nested multi-media fate, exposure and effects model USES-LCA. This model is used to improve the calculation of characterisation factors for toxic emissions. USES-LCA was used to calculate for 181 substances toxicity potentials for the six impact categories fresh water aquatic ecotoxicity, marine aquatic ecotoxicity, fresh water sediment ecotoxicity, marine sediment ecotoxicity, terrestrial ecotoxicity and human toxicity, after initial emission to the compartments air, fresh water, seawater, industrial soil and agricultural soil, respectively. For Atrazine, 2,3,7,8-TCDD and Lead the variance in toxicity potentials resulting from input parameter uncertainties and human variability was quantified. In addition, the variance in toxicity potentials resulting from choices in the modelling procedure was assessed. A first scenario analysis showed to what extent potential impacts in the relatively short term are obscured by the inclusion of impacts on the very long term. The second scenario analysis addressed to what extent potential impacts on the continental scale are obscured by the inclusion of impacts on the global scale.

Chapter 4 outlines the spatially explicit model RAINS-LCA which was developed for the calculation of acidification and terrestrial eutrophication potentials of ammonia (NH_3) and nitrogen oxide (NO_x) air emissions and acidification potentials for sulfur dioxide (SO_2) air emissions for Europe and a number of European regions, taking fate, background depositions and effects into account. Two impact definitions are explored in the calculations: the marginal change in the hazard index of all ecosystems in Europe, and the marginal change in the hazard index of ecosystems in Europe where the critical load is actually exceeded. Chapter 4 also shows the results of including fate in the calculation of aquatic eutrophication potentials of NH_3 and NO_x emitted to the air, N and P emitted to water, and N and P emitted to soil. These characterisation factors were calculated for the Netherlands, West-Europe and the world, respectively.

In Chapter 5, the environmental comparison of insulation thickness in buildings serves as a case study for the evaluation of uncertainty in LCA. This case study addressed (1) parameter uncertainties in defining the functional unit, the inventory analysis, and the impact assessment; (2) the influence of choices concerning the allocation of environmental burdens in recycling processes, future waste scenarios, and the timing, geographical scale and definition of environmental impacts; and (3) model uncertainty due to the lack of spatial and temporal differentiation and due to the lack of suitable characterisation factors for sum emissions.

Finally, Chapter 6 contains the general conclusions and recommendations for future research.

Chapter 2

Application of uncertainty and variability in LCA

§ 2.1 Framework

As yet, the application of an uncertainty and variability analysis is not common practice in LCAs. A proper analysis will be facilitated when it is clear which types of uncertainties and variabilities exist in LCAs and which tools are available to deal with them. Therefore, a framework is developed to classify types of uncertainty and variability in LCAs. Uncertainty is divided in (1) parameter uncertainty, (2) model uncertainty, and (3) uncertainty due to choices, while variability covers (4) spatial variability, (5) temporal variability, and (6) variability between objects and sources. A tool to deal with parameter uncertainty and variability between objects and sources in both the inventory and the impact assessment is probabilistic simulation. Uncertainty due to choices can be dealt with in a scenario analysis or reduced by standardisation and peer review. The feasibility of dealing with temporal and spatial variability is limited, implying model uncertainty in LCAs. Other model uncertainties can be reduced partly by more sophisticated modelling, such as the use of non-linear inventory models in the inventory and multi media models in the characterisation phase.

Introduction

Uncertainty and variability are often mentioned as factors complicating the interpretation of outcomes of LCAs. Variability is understood here as stemming from inherent variations in the real world, while uncertainty comes from inaccurate measurements, lack of data, model assumptions, etc. that are used to 'convert' the real world into LCA outcomes. The implementation of an uncertainty and variability analysis in LCAs may be helpful for decision makers in judging the significance of the differences in product comparisons, options for product improvements or the assignment of ecolabels.

Although the importance of dealing with uncertainty and variability is broadly accepted, a proper framework to distinguish types of uncertainty and variability in LCAs is lacking. Therefore, a classification of uncertainty and variability in LCAs seems useful. This is all the more so because different types of uncertainty and variability need to be made operational or reduced in different ways. Several authors have proposed classifications for uncertainty and variability (e.g. Morgan and Henoion, 1990; Funtowitz and Ravetz, 1990; US-EPA, 1997). This paper presents a general framework to address uncertainty and variability in LCA and builds on these classifications. The following types of uncertainty and variability are distinguished and elaborated in the sections below: (1) parameter uncertainty; (2) model uncertainty; (3) uncertainty due to choices; (4) spatial variability; (5) temporal variability and (6) variability between objects/sources (Figure 2.1). Moreover, techniques and methods to deal with these types of uncertainty and variability are discussed.

Figure 2.1 Transferring the real world in LCA outcomes

Parameter uncertainty

A large amount of data is usually needed in the inventory analysis and in the models which calculate characterisation and weighting factors in the impact assessment. Uncertainty of these parameters also causes uncertainty in the outcome of an LCA. Empirical inaccuracy (imprecise measurements), unorepresentativity (incomplete or outdated measurements) and lack of data (no measurements) are common sources of parameter uncertainty. Weidema and Wesnæs (1996) describe a comprehensive procedure for estimating the combined inaccuracy and unorepresentativity of inventory data both qualitatively and quantitatively. Although this procedure may substantially improve the credibility of the outcomes of LCAs, uncertainty analysis is generally complicated by a lack of knowledge of uncertainty distributions and correlations between parameters. A substitute for lack of knowledge is the use of expert judgement to estimate uncertainty ranges of inputs in and outputs of industrial processes. In addition, a description in databases of uncertainty ranges of environmental interventions per unit process will substantially improve the feasibility of performing a standard uncertainty analysis in LCAs. A first step in this respect is the development of a common database format, in which uncertainty ranges for average life cycle inventory data should be listed (Singhofen *et al.*, 1996). However, lack of knowledge about specific processes, material use and emissions related to a product system is not compensated by assessing inaccuracy and unoreliability. Additional data research and standard estimation techniques may provide useful information for filling in these data gaps (Bretz and Frankhouser, 1996). Various methods have been proposed to make uncertainty operational in LCA outcomes due to parameter uncertainty: Hoffman *et al.* (1995) and Heijungs (1996) promoted the use of analytical uncertainty propagation methods; Chevalier and Le Têno (1996) performed calculations with intervals; Beccali *et al.* (1997) applied fuzzy logic computations, which is an extension of the interval concept; Petersen (1997) developed a method, based on Bayesian statistics, which makes it possible to treat subjective uncertainty estimates with the usual statistical calculation rules; and Kennedy *et al.* (1996) used stochastic modelling, describing parameters as uncertainty distributions. Stochastic modelling, which can be performed by Monte Carlo or Latin Hypercube simulation, seems to be an especially promising technique for making uncertainty in model output operational. An advantage in relation to the other methods mentioning is that, dependent on the available information, various parameter distributions, such as uniform, triangular, normal, or lognormal distributions, can be used in the model. Furthermore, if correlations between parameters can be estimated, it is technically easy to deal with these correlations in the simulations.

To perform Monte Carlo simulation, parameters have to be specified as uncertainty distributions. The method varies all the parameters at random, but the variation is restricted by the given uncertainty distribution for each parameter. The randomly selected values from all the parameter uncertainty distributions are inserted in the output-equation. Repeated calculations produce a distribution of the predicted output

values, reflecting the combined parameter uncertainties. Latin Hypercube simulation works in the same way with one exception. This method segments the uncertainty distribution of a parameter into a number of non-overlapping intervals, each having equal probability. In addition, from each interval, a value is selected at random according to the probability distribution within the interval, leading to generally more precise random samples than Monte Carlo simulation

Probabilistic uncertainty analysis is useful in making the influence of parameter uncertainty on the uncertainty of the model outcomes operational. For the reduction of parameter uncertainty, however, more reliable data must be provided by additional literature research, expert judgement or measurements. Parameters which cause the largest spread in the model outcome should have been given priority. The contribution of the separate parameters to the total uncertainty may be estimated through the use of statistical correlation and regression techniques (Janssen *et al.*, 1990). Besides the possibility to perform probabilistic simulation in spreadsheets, probabilistic simulation programs, such as Crystal Ball[®] (Decisioneering, 1996), provide correlation techniques to perform an uncertainty importance analysis.

Model uncertainty

Some aspects cannot be modelled within the present LCA structure. For instance, spatial and temporal characteristics are lost by the aggregation of emissions in the inventory analysis. Furthermore, in the impact assessment it is assumed that ecological processes respond in a linear manner to environmental interventions and that thresholds of interventions are disregarded (Owens, 1996). In addition, the derivation of characterisation factors causes model uncertainty. Characterisation factors are computed with the help of simplified environmental models which also suffer from model uncertainties. For instance, the fate of substances and the sensitivity of the receiving environment are not taken into account in the computation of acidification and eutrophication factors (Nichols *et al.*, 1996). With the help of multi media modelling, fate of substances and the sensitivity of the environment could be taken into account in the computation of acidification and eutrophication factors (Wegener Sleeswijk and Heijungs, 1996; Potting *et al.*, 1997), reducing model uncertainty in the impact assessment.

When a model suffers from large model uncertainties, the results of a parameter uncertainty analysis may be misleading. For instance, currently only information of the molecular weight and the amount of potentially produced acid of emitted substances and a reference substance are needed to compute acidification factors (Heijungs *et al.*, 1992). Parameter uncertainty in this case is negligible, but model uncertainty is certainly not, because fate of the substances and site-specific critical loads are not taken into account. The result of decreasing model uncertainty will in most cases be the implementation of more parameters in the computation of acidification factors, thereby increasing the importance of operationalising parameter uncertainty in the model.

Uncertainty due to choices

When performing LCAs, choices are unavoidable. Examples of choices leading to uncertainty in the inventory analysis are the choice of the functional unit and the choice of the allocation procedure for multi-output processes, multi-waste processes and open-loop recycling. Furthermore, in some cases different characterisation methods can be used for the same impact category. Moreover, the weighting phase in LCAs is an area in which choices play a crucial role. Although many weighting methods have been suggested by LCA experts, only a few are operational and no general agreement exists as to which one should be preferred. For example, an authorised weighting set could potentially be based on political reduction targets, environmental control and damage costs and panel preferences in reducing environmental impacts (Powell *et al.*, 1997). The problem is even more complicated, because reduction targets are formulated at many policy levels and the panel preference may reflect the opinion of a societal group, of scientific experts, of governments or international bodies. Moreover, there is still some discussion about whether to use generic weighting sets or to perform weighting case-by-case for different product systems in LCAs (Lindeijer, 1996).

The standardisation of procedures, such as the guidelines given by Lindfors *et al.* (1995b) and ISO (1997a, b, 1998a, b), is useful for reducing uncertainty due to choices to a broadly accepted level and stimulate unity in LCA practice. In addition, peer review can be used to judge choices on their merits. When standard procedures are not fully applicable, uncertainty due to choices may be made operational with the help of a scenario analysis, which can show the effect on LCA outcomes of several combinations of choices (Lindfors *et al.*, 1995a; Kortman *et al.*, 1996). For instance, a scenario analysis can show differences in LCA outcomes due to the application of different allocation procedures, characterisation methods and weighting methods.

Spatial variability

In LCA variability across locations, such as physico-chemical and ecological properties of the environment, background concentrations of chemicals and human population density, is generally not taken into account in LCA (Heijungs *et al.*, 1992; Guinée *et al.*, 1996a). In most LCAs all environmental interventions are summed up regardless of the spatial context of the intervention, introducing model uncertainty in LCAs. A distinction between outdoor versus indoor emissions and emissions to land versus emissions to sea, for instance, could make the results of LCAs more appropriate (Potting and Blok, 1994). A way to address real world spatial variability is to distinguish compartments by choosing appropriate subregions for LCA purposes. Both inventory analysis and impact assessment have to be modified to incorporate the appropriate spatial variability for the interpretation of environmental interventions.

In LCAs the feasibility of dealing with spatial variability is limited. The first reason is that

a detailed regional context of emissions is in some cases not known or irretrievable. For instance, only accumulated average environmental interventions associated with plastics, produced by European plants, are published (e.g. Boustead, 1993). Data of all the individual plants are not available and environmental interventions due to transport and the production of energy carriers, such as electricity, oil and gas have already been summed up with the process-specific interventions. As a consequence, in these cases it is not possible to use spatially differentiated classification factors. Furthermore, detailed environmental information, such as physico-chemical properties, ecological properties and background concentrations is needed to compute site-dependent classification factors. Although this kind of information is available to compute country-specific acidification, eutrophication and photochemical ozone creation factors in Europe (Potting *et al.*, 1997), such detailed information may be lacking for other continents. In addition, detailed information relevant for other impact categories, such as human toxicity and ecotoxicity, may not be available.

Temporal variability

Temporal variation is present in both the inventory and the impact assessment of LCAs. However, variations of environmental interventions over a relatively short time period, such as differences in industrial emissions on week days versus weekends or even short calamitous emissions, are not taken into account, because LCA emission data are commonly obtained by dividing yearly emission by yearly production. Temporal variability over the years may be made operational when inventory data of several years are collected (Hanssen and Asbjørnsen, 1996). However, it will be very difficult to obtain yearly variations of environmental interventions for the entire life cycle. Furthermore, caution is needed in the interpretation of the yearly variations, because the variation could also be caused by unreliable or inaccurate measurements. In practice, it seems very hard to operationalise temporal variability in inventory data for the whole life cycle of a product system.

Not incorporating temporal variation in the inventory analysis also has consequences for the operationalisation of temporal variability in the impact assessment. Substance-independent variables, such as wind speed and temperature, are used for the computation of characterisation factors, such as toxicity potentials (Guinée *et al.*, 1996a). Although these variables obviously vary temporally, it is not possible to match the temporal variation of these variables with the inventory data, because temporal variation over short time periods is not made operational in the inventory analysis. Moreover, emissions of a certain substance, which often take place in different years for the several unit processes, have been summed up in the inventory. Instead of operationalising the temporal variability of these variables in the impact assessment, the mean (and uncertainty of the mean) for these parameters has to be estimated for the representative geographic region and time period.

A second type of temporal variability in the impact assessment, however, is operational.

Global warming potentials (GWPs), ozone depletion potentials (ODPs) and photochemical ozone creation potentials (POCPs) differ, depending on the chosen time horizon to integrate potential effects (Albritton *et al.*, 1996; Solomon *et al.*, 1995; Andersson-Sköld *et al.*, 1992). The temporal variability in these characterisation factors is caused by the difference in life times between the reference substance, chosen per impact category, and the remaining substances. This kind of temporal variability can be made operational by comparing model outcomes for several chosen time horizons, changing temporal variability in uncertainty due to choices. Characterisation factors computed for a short time horizon may serve as indicators for short-term effects, while longer time horizons may serve as indicators for longer-term effects.

Variability between sources and objects

In both the inventory and the impact assessment, variability between sources and objects may influence LCA outcomes. Inherent differences in inputs and emissions of comparable processes in a product system, for example due to the use of different technologies in factories which produce the same material, cause variability in life cycle inventories (e.g. Boustead, 1993; Hanssen and Asbjørnsen, 1996). Furthermore, variability between objects exist in the characterisation phase. For example, variability in human characteristics, such as body weight, consumption of food products and sensitivity for toxic substances, may cause variation in human toxicity potentials. Moreover, the weighting of environmental problems in the impact assessment could introduce variability between human preferences. When, for instance, the panel method is used to weight environmental problems, differences between individual preferences cause inherent variation in the final environmental indicator.

The effect on LCA outcomes of variability between sources and objects can be made operational by probabilistic simulation, analogous to the procedure for operationalising parameter uncertainty. Variability between objects should preferably always be taken into account in the impact assessment. The operationalisation in the inventory analysis, however, is dependent on the goal of the study. For example, if the goal is to improve the environmental profile of a product system, it could be informative to know the actual range of the environmental interventions in the inventory. Factories which produce the same product or material within one product system may have considerably different environmental interventions. When the output distribution of the environmental profile is analysed with a correlation analysis, it may become clear which data variability in the inventory mainly contributes to the range of environmental profiles. Consequently, a reduction of the sources which contribute to the upper tail of the data variability could be the main focus for product system optimisation. If, however, the goal of the study is to perform a product comparison, the average environmental profiles of the product systems is of particular interest. Consequently, variability between sources in the inventory should be transformed into the uncertainty of the mean. However, the

representation of both variability between sources and uncertainty of the mean in probabilistic simulations is still interfered by measurement inaccuracies. A quantitative example of how to deal with this complication is given in the Appendix.

Integration in LCA research

Ideally, LCAs cover all the types of uncertainty and variability mentioned in the previous sections (Table 2.1), although for the inventory phase this may depend on the goal and scope of the analysis. In the near future, however, it will neither be possible nor feasible in product assessments to perform such a large-scale analysis. It seems at least feasible to deal with the following types of uncertainty and variability (Table 2.2): (1) parameter uncertainty and/or variability between objects and sources in the inventory analysis through the use of stochastic modelling, uncertainty/variability importance analysis or other techniques; (2) uncertainty due to choices in the inventory analysis, the choice of impact categories and the characterisation phase by means of standardisation, peer review and scenario analysis.

Table 2.1 Examples of types of uncertainty and variability related to the phase of LCA.

Phase	Goal and scope	Inventory	Choice of impact categories	Classification	Characterisation	Weighting
Source						
Parameter uncertainty		Inaccurate emission measurements	Impact categories are not known		Uncertainty in life times of substances	Inaccurate normalisation data
Model uncertainty		Linear instead of non-linear modelling	Leaving out known impact categories	Contribution to impact category is not known	Characterisation factors are not known	Weighting criteria are not operational
Uncertainty due to choices	Functional unit	Use of several allocation methods			Using several characterisation methods within one category	Using several weighting methods
Temporal variability		Differences in yearly emission inventories			Change of temperature over time	Change of social preferences over time
Spatial variability		Regional differences in emission inventories			Regional differences in environmental sensitivity	Regional differences in distance to (political) targets
Variability between objects/sources		Differences in emissions between factories which produce same product			Differences in human characteristics	Differences in individual preferences, when using panel method

Table 2.2 Overview of tools available to address types of uncertainty and variability in LCAs.

Tools	Types	Parameter uncertainty	Model uncertainty	Uncertainty due to choices	Spatial variability	Temporal variability	Variability in objects/sources
Probabilistic simulation		+					+
Correlation and regression analysis		+					+
Additional measurements		+					+
Scenario modelling				+		+	
Standardisation				+			
Expert judgement/peer review		+		+			+
Non-linear modelling			+				
Multi media modelling			+		+		

Operationalisation of parameter uncertainty and variability between objects and sources in the inventory phase, however, is most probably limited to the process data which are specific for the given product system under study, such as material use, energy use and process emissions. For widely used inventory data, such as the environmental interventions related to the production of electricity, heat and widely used bulk materials, like plastics, steel, aluminium, wood, etc., it is favourable to provide uncertainty estimates in general databases. However, in contrast to other environmental models, thousands of parameters are involved in the inventory analysis of product assessments, which make the feasibility of estimating underpinned uncertainty ranges for all these parameters in LCAs doubtful. Therefore, finding ways to simplify the uncertainty analysis in a systematic and transparent way is an important LCA research issue. Some possibilities to simplify the parameter uncertainty analysis are discussed in Huijbregts (1998b).

In addition to the above-mentioned analysis of uncertainty and variability in product assessments, other structural developments are necessary. The following developments focus on more general aspects in LCAs, such as (1) the reduction of model uncertainties in the inventory analysis through use of non-linear, suggested by Wrisberg *et al.* (1997); (2) the reduction of model uncertainty in the characterisation phase, through use of multi-media modelling (Guinée *et al.*, 1996a; Wegener Sleeswijk and Heijungs, 1996); (3) the operationalisation of parameter uncertainty and, if applicable, variability between objects in the environmental models which are used to compute characterisation factors; (4) the standardisation of the weighting procedure to guide uncertainty due to choices (Lindeijer, 1996); and (5) the operationalisation of spatial variability in inventories and

characterisation factors (Potting *et al.*, 1997). Co-operation with specialists of other scientific disciplines will facilitate the implementation of these improvement options. If widely accepted results of model improvements and uncertainty c.q. variability estimates in characterisation factors are available, incorporation of these developments in product assessments will be possible.

Although dealing with uncertainty and variability is possible in product assessments, it remains unclear what the exact implications are for decision makers. Clear guidance needs to be developed how to take uncertainty and variability into account in decision-making processes. In this respect, special care is needed in the interpretation of model uncertainty. To some extent, it is not possible to reduce or operationalise model uncertainties, such as the lack of a detailed spatial and temporal differentiation in LCAs. Other environmental information, such as risk assessment results, may provide complementary information for decision makers. How to combine the results of the different methods also remains to be explored.

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Appendix: Combining measurement inaccuracies with either 'variability between sources' or 'uncertainty of the mean'.

To calculate the distribution characteristics of the inventory data, the effects of measurement inaccuracies with either 'variability between sources' or 'uncertainty of the mean' should be combined. The implications are shown in a simplified example. It is assumed that the SO₂ process emissions of five factories, which produce the product P, are known (Table 2.3). Furthermore, it is assumed that the five factories are a representative sample of all product P producing factories, and that the emissions caused by these factories are described by a normal distribution. If inaccuracies in the measurement of SO₂ emissions are neglected, the variation in SO₂ emissions is represented by the standard deviation of the sample (SDs), while the standard error of the mean (SEMs) represents the uncertainty of the average SO₂ emission. Basic statistical rules can be applied to compute the SDs and the SEMs.

Of course, the exact SO₂ emissions of the five factories are not known precisely. The measurement inaccuracies are represented by the standard deviations per SO₂ emission

(Table 2.3). If these inaccuracies are taken into account, the computation of the SD and the SEM changes. The $SD_{combined}$, which reflects both the variation between factories and the inaccuracy in measurements, is computed with the following equation:

$$SD_{combined} = \sqrt{\frac{1}{N} \times \left(\sum_{x=1}^{x=N} SD_s^2 + \sum_{x=1}^{x=N} SD_x^2 \right)}$$

where $SD_{combined}$ is the combined standard deviation of SO_2 emissions due to variation between factories and inaccuracy in measurements; SD_s is the standard deviation of SO_2 emissions due to variation between the five factories; SD_x is the standard deviation of SO_2 emissions due to inaccurate measurements in factory x ; x is the factory identification number; and N is the number of factories.

The $SEM_{combined}$ is computed by means of the following equation:

$$SEM_{combined} = \frac{SD_{combined}}{\sqrt{N}}$$

in which all variables equal those mentioned above, and the $SEM_{combined}$ represents the error introduced by both the generalisation of the sample emission average to the emission average of all product P producing factories and inaccurate measurements. As can be seen in Table 2.3, the characteristics of the emission profile will change, depending on whether inaccuracy in combination with either variability ($SD_{combined}$) or uncertainty of the mean ($SEM_{combined}$) is taken into account.

Table 2.3 Characteristics of g SO_2 process emissions per kg product P

Emission	Factory A mean (sd)	Factory B mean (sd)	Factory C mean (sd)	Factory D mean (sd)	Factory E mean (sd)	Mean	SD_s	SEM_s	$SD_{combined}$	$SEM_{combined}$
g SO_2	16 (5)	20 (4)	18 (3)	25 (5)	30 (6)	21.8	5.7	2.5	7.4	3.3

§ 2.2 Parameter uncertainty and uncertainty due to choices

Results of product assessments are often criticised as to their handling of uncertainty. Therefore, it is necessary to develop a comprehensive methodology reflecting parameter uncertainty in combination with uncertainty due to choices in the outcome of LCAs. This paper operationalises the effect of combined parameter uncertainties in the inventory and in the characterisation factors for global warming and acidification for the comparison of two exemplary types of roof gutters. For this purpose, Latin Hypercube sampling is used in the matrix (inventory) method. To illustrate the influence of choices, the effect on LCA outcomes is shown of two different allocation procedures in open-loop recycling and three time horizons for global warming potentials. Furthermore, an uncertainty importance analysis is performed to show which parameter uncertainties mainly contribute to uncertainties in the comparison and the separate environmental profiles of the product systems. These results can be used to prioritise further data research.

Introduction

The ultimate goal of environmental life cycle assessments (LCAs) is to provide information for decisions which will lead to environmental improvement of economies. However, LCAs may give rise to incorrect decisions when uncertainty and variability are not properly taken into account. Although at present model uncertainties due to the lack of spatial variability and temporal variability in the assessment generally cannot be made operational in LCA case studies, other types of uncertainty, such as parameter uncertainty and uncertainty due to choices, potentially can (Huijbregts, 1998a).

To illustrate parameter uncertainty and uncertainty due to choices, this paper compares two types of roof gutters with respect to their potential contribution to the environmental categories global warming (time horizon 20, 100 and 500 years) and acidification, using simplified inventory data. Using probabilistic modelling and scenario analysis, it shows the influence on LCA model outcomes of parameter uncertainties, of the choice of different allocation rules applied to open-loop recycling processes, and of different time horizons for global warming potentials. Furthermore, it couples the uncertainty analysis with an uncertainty importance analysis, which verifies the parameters that introduce the largest uncertainty in model outcomes. Finally, it discusses the feasibility of the application of this methodology in 'real-life' LCAs and possibilities for simplifying the analysis. These studies may help in developing a comprehensive methodology for the inclusion of parameter uncertainty and uncertainty due to choices in LCA studies.

Data input

Inventory

The matrix method, developed by Heijungs (1994, 1996), is used to perform the inventory analysis. The inventory table I is computed with the following formula (Heijungs, 1996):

$$I = H \cdot G^{-1} \cdot u$$

where I is the inventory table, H is the environmental intervention matrix, G is the technology matrix, and u is the external supply vector, related to the functional unit. An important advantage of the matrix method over other inventory methods is that the method easily deals with self-referring groups of processes (Heijungs, 1994). The matrix method has already been used for extensive life cycle inventories, such as the inventories for energy systems (Frischknecht *et al.*, 1996).

The functional unit used in the comparison of roof gutters A1 and A2 is 'the discharge of rain water falling on the roof of a one-family building during fifty years'. The

application of 10m of roof gutter fulfils this function for about 25 years. It is expected that part of both types of roof gutters will be recycled in the product system 'Sewage pipes'. The cut-off method and the avoided-impacts method are used to allocate the environmental burdens associated with the recycling of the products. These methods reflect two extreme visions on how to allocate environmental burdens in open-loop recycling processes and both were judged defensible by experts (Kortman *et al.*, 1996). The cut-off method allocates the environmental interventions caused by the waste recycling process to the receiving product system S, while the avoided-impacts method allocates the environmental interventions caused by the waste recycling process to the product system A_x , but also credits system A_x by subtracting the avoided environmental interventions from the original inventory table of A_x . The inventory data of the two roof gutter systems are given in Tables 2.4 through 2.6.

Table 2.4 Inventory data of product system 'Roof gutter A1'.

Commodity	Process	Electricity production	Oil production	Plastic P1 production	Gutter A1 production	Gutter A1 use and demolition	Incineration of P1/A1	Recycling process ^c	Material B production ^{c,e}	Product system
MJ electricity	1	-1.10 ⁻²	-50	-1	0	-1	-25	40	0	
kg oil	-6.10 ⁻³	1	-0.8	0	0	-0.5	-0.1	0.3	0	
kg plastic P1	0	0	1	-325	0	0	0	0	0	
100m produced A1	0	0	0	1	-1	0	0	0	0	
100m installed A1	0	0	0	0	1	0	0	0	0.2 ^f	
kg incinerated P1/A1	0	0	-0.01 ^a	-0.05 ^a	-65 ^{a,b}	1	-0.1 ^a	0	0	
kg A1 in recycling	0	0	0	0	-260 ^{a,b}	0	1	0	0	
kg avoided material B	0	0	0	0	0	0	-1.8 ^{a,d}	1	0	
kg CO ₂	1.10 ⁻²	0.5	2	0	0	3	2	-1.5		
kg CH ₄	3.10 ⁻⁴	4.10 ⁻³	0	0	0	5.10 ⁻⁵	4.10 ⁻³	0		
kg N ₂ O	1.10 ⁻⁶	1.10 ⁻⁴	1.10 ⁻⁵	0	0	5.10 ⁻⁵	3.10 ⁻⁴	-2.10 ⁻⁴		
kg NO _x	3.10 ⁻⁴	2.10 ⁻³	5.10 ⁻²	0	0	8.10 ⁻⁴	2.10 ⁻²	-4.10 ⁻³		
kg SO ₂	6.10 ⁻⁴	3.10 ⁻³	0.1	0	0	2.10 ⁻⁴	1.10 ⁻²	-5.10 ⁻³		

^a in addition to economic inflows economic outflows have a negative sign in the technology matrix; ^b the amount of 'kg A1 to the recycling process' is computed by multiplying 'kg plastic P1' used in the production of 100m of roof gutter A1 with the 'recycling fraction of roof gutter A1'. The computation of the amount of waste to the incineration process is done in the same way, but '1 - recycling fraction' is used in the multiplication; ^c the process data of the recycling process and Material B production are only used if the avoided-impacts allocation method is applied; ^d the amount of avoided material B per kg A1 going into the recycling process is computed by multiplying 'the amount of A1 going to product system S' with the ratio of the mass of material B1 and the mass of product A1 related to the functional unit of the receiving product system S; ^e the signs of the economic process data and the environmental interventions per kg material B are reversed, because the avoided-impacts allocation method subtracts the environmental interventions related to the amount of avoided material B from original product system A1; ^f The fraction of 100m roof gutter needed to fulfil the functional unit is computed by multiplying 'the fraction of 100m of roof gutter, initially applied to a one-family house' with 50 years, divided by the expected lifetime of the roof gutter.

Table 2.5 Inventory data of product system 'Roof gutter A2'.

Process Commodity	Electricity production	Oil production	Plastic P2 production	Gutter A2 production	Gutter A2 use and demolition	Incineration of P2/A2	Recycling process ^c	Material B production ^{c,e}	Product system
MJ electricity	1	-1.10 ⁻²	-40	-2	0	-1	-40	40	0
kg oil	-6.10 ⁻³	1	-0.6	0	0	-0.5	-0.5	0.3	0
kg plastic P2	0	0	1	-200	0	0	0	0	0
100m produced A2	0	0	0	1	-1	0	0	0	0
100m installed A2	0	0	0	0	1	0	0	0	0.2 ^f
kg incinerated P2/A2	0	0	-0.02 ^a	-0.05 ^a	-20 ^{a,b}	1	-0.2 ^a	0	0
kg A2 in recycling	0	0	0	0	-180 ^{a,b}	0	1	0	0
kg avoided material B	0	0	0	0	0	0	-2 ^{a,d}	1	0
kg CO ₂	1.10 ⁻²	0.5	1.5	0	0	2	2.5	-1.5	
kg CH ₄	3.10 ⁻⁴	4.10 ⁻³	0	0	0	3.10 ⁻⁵	2.10 ⁻³	0	
kg N ₂ O	1.10 ⁻⁶	1.10 ⁻⁴	3.10 ⁻⁴	0	0	6.10 ⁻⁶	4.10 ⁻⁴	-2.10 ⁻⁴	
kg NO _x	3.10 ⁻⁴	2.10 ⁻³	0.5	0	0	6.10 ⁻⁴	3.10 ⁻²	-4.10 ⁻³	
kg SO ₂	6.10 ⁻⁴	3.10 ⁻³	1.10 ⁻²	0	0	4.10 ⁻⁴	2.10 ⁻²	-5.10 ⁻³	

a,b,c,d,e,f same comments as in Table 2.4

Table 2.6 Additional input data and uncertainty factors applied to the product systems A1 and A2.

Parameters	Product sytem A1	Product system A2	UF ^b
Recycling fraction Ax	0.80	0.90	1.1
Mass of product Ax related to the functional unit of the receiving product system S	250	200	1.1
Mass of material B related to functional unit of the receiving product system S ^a	500	500	1.1
Fraction of 100m roof gutter, initially applied to a one-family house ^a	0.1	0.1	1.05
Lifetime of roofgutter A1 and A2 (years) ^a	25	25	1.25

^a it is assumed that these parameters are not product system specific; ^b UF = uncertainty factor

Parameter uncertainty in the inventory analysis of the two product systems is characterised with the help of ‘Uncertainty factors (UFs)’ which are given in the Tables 2.6 and 2.7. UFs are used to represent inventory data uncertainties as a triangular uncertainty distribution. The minimum and maximum values¹ of parameter P_x are assumed to be:

$$P_{x, \min} = \frac{P_{x, \text{modus}}}{UF_x} \quad \text{and} \quad P_{x, \max} = P_{x, \text{modus}} \times UF_x$$

where $P_{x, \min}$ is the minimum value of parameter x , $P_{x, \text{modus}}$ is the most likely value of parameter x , $P_{x, \max}$ is the maximum value of parameter x , and UF_x is the uncertainty factor applied to parameter x . By way of simplification, estimates of the UFs and the applied distribution form are entirely arbitrary. Furthermore, the UFs for the product-specific process data in the two product systems are assumed to be the same, which would not be necessarily true in ‘real life’ cases.

Table 2.7 Uncertainty factors applied to the inventory data of the product systems A1 and A2.

Process Commodity	Electricity production	Oil production	Plastic P2 production	Gutter A2 production	Gutter A2 use and demolition	Incineration of P2/A2	Recycling process ^c	Material B production ^{c,e}	Product system
MJ electricity	1.01	1.1	1.05	1.05	1	1.1	1.05	1.1	1
kg oil	1.05	1.01	1.05	1	1	1.1	1.05	1.1	1
kg plastic	1	1	1.01	1.05	1	1	1	1	1
100m produced gutter	1	1	1	1.01	1	1	1	1	1
100m installed gutter	1	1	1	1	1	1	1	1	n.a. ^a
kg incinerated waste	1	1	1.2	1.1	n.a. ^a	1.01	1.05	1	1
kg gutter in recycling	1	1	1	1	n.a. ^a	1	1.01	1	1
kg avoided material B	1	1	1	1	1	1	n.a. ^a	1.01	1
kg CO ₂	1.1	1.1	1.05	1	1	1.05	1.05	1.05	
kg CH ₄	2	2	1	1	1	2	1.1	1	
kg N ₂ O	5	5	3	1	1	5	3	4	
kg NO _x	1.5	1.5	1.1	1	1	1.5	1.1	1.2	
kg SO ₂	1.5	1.5	1.1	1	1	1.5	1.1	1.2	

^a n.a. = not applicable: uncertainty factors are only applied to input data and not applied to computation outcomes

1. When $P_{x, \text{modus}} < 0$, $P_{x, \max}$ and $P_{x, \min}$ change places in the formulas

Global warming

The Global Warming Potential (GWP) of a gas is ‘the cumulative radiative forcing between the present and some chosen later time “horizon” caused by a unit mass of gas emitted now, expressed relative to some reference gas’ (Albritton *et al.*, 1996). Generally, CO₂ is taken as the reference gas. As a consequence, the uncertainty of the GWP of any trace gas other than CO₂ depends upon the substance-specific uncertainties in the integrated radiative forcing (IF) of the gas itself and on the IF of CO₂ (Albritton *et al.*, 1995, 1996).

A typical uncertainty in the direct IF of various gases, such as N₂O, is estimated to be $\pm 35\%$, caused by uncertainties in the parameters ‘radiative forcing per molecule’ and ‘lifetimes in the atmosphere of the trace gases’ (Albritton *et al.*, 1995, 1996). Because a further explanation of the uncertainty distribution is lacking in the IPCC reports, it is assumed in this assessment that the $\pm 35\%$ uncertainty represents the 95% confidence range of a normal uncertainty distribution (Table 2.8). In addition to the direct radiative forcing capacity, the IF of CH₄ depends on indirect contributions to the radiative forcing of CH₄ due to stratospheric ozone and water vapour production. Uncertainty ranges for the IF of CH₄ for the time horizons 20, 100 and 500 years, given by Albritton *et al.* (1995), are in the same order as the above-mentioned $\pm 35\%$ uncertainty range. Uncertainties in the IF for CO₂ depend on uncertainties in the carbon cycle. The effect of these uncertainties is not known, because of the large model uncertainties involved (Albritton *et al.*, 1995). As a result, it is impossible to quantify the uncertainties in probabilistic simulation.

Variation in future scenarios of CO₂ and other trace gas emissions also have an effect on GWP-values, although the IF of CO₂ is relatively insensitive to these emission scenarios (Caldeira and Kasting, 1993; Albritton *et al.*, 1995). When two very different extreme scenarios are compared with the reference scenario, a maximum difference of $\pm 15\%$ in GWP-values is found (Albritton *et al.*, 1995). The choice of a reference future atmosphere for a GWP is not a parameter uncertainty, but rather an agreement upon a selection of a future scenario for atmospheric composition, and therefore it causes uncertainty due to choices. This uncertainty is not taken into account in the further assessment here. Nor are other uncertainties and limitations of GWPs quantified. For instance, the GWP concept is not applicable to gases and aerosols that are very unevenly distributed. For this reason, GWPs for sulphur oxides, which probably contribute to negative radiative forcing through aerosol, and NO_x are not estimated by Albritton *et al.* (1995, 1996).

Acidification

Heijungs *et al.* (1992) proposed an “acid equivalents approach” in the computation of the acidification factor (AF) of a substance, in which the proton release per kg emission of the substance in the environment is divided by the proton release per kg emission of

a reference substance, assuming that emitted substances are fully transformed into protons. Realization of the maximum proton release depends on whether or not the anions which accompany the released protons are completely leached out of the system. The contribution to acidification is reduced when the anions are bound in the soil or removed in biomass (Hauschild and Wenzel, 1998). When SO_2 is taken as the reference substance, the AF of an acidifying substance is caused by the uncertainty in the proton release of SO_2 and the proton release of the substance itself.

For SO_2 emissions the average release of approximately two protons is thought to be representative for terrestrial conditions, because the soil retention of SO_3^{2-} and SO_4^{2-} ions, formed by deposition of SO_2 , is considered to be small (Finnveden *et al.*, 1992; Hauschild and Wenzel, 1998). In this assessment a relatively small uncertainty range for average proton release due to SO_2 emissions is considered (Table 2.8). For NO_x emissions, the actual proton release is more complicated to derive. The first problem may be that NO and NO_2 emissions are taken together as NO_x which may cause uncertainty in the value of 'x'. NO, however, is measured and represented as NO_2 in NO_x inventories. Thus, 'x' has a value of 2 which is in line with Hauschild and Wenzel (1998) and Heijungs *et al.* (1992). Furthermore, it is unclear what average fraction of NO_3^- ions, following from the deposition of nitrogen oxides, is taken up by plants and removed from the system. As a first approximation, the minimum and maximum values for average removal of NO_3^- ions due to harvesting are chosen to be respectively 10% and 50%, resulting in a net release of protons of 50% to 90% of the theoretical maximum (Table 2.8).

Table 2.8 Characteristics of the Global Warming Potentials (20, 100 and 500 years time horizon) and Acidification Factors for the emissions considered in this example

	Units	CO_2	CH_4 mean (sd)	N_2O mean (sd)	NO_x [min - max]	SO_2 [min - max]	UD ^a
GWP20	CO_2 -eq. (kg)	1	56 (9.8)	280 (49.0)	?	?	normal
GWP100	CO_2 -eq. (kg)	1	21 (3.7)	310 (54.3)	?	?	normal
GWP500	CO_2 -eq. (kg)	1	6.5 (1.1)	170 (29.8)	?	?	normal
Proton release	-	?	0	0	[0.5 - 0.9]	[1.9 - 2.0]	uniform

^a UD = uncertainty distribution

Environmental profiles

To show the effect on LCA outcomes of uncertainty in the input data, Latin Hypercube simulation is performed with Crystal Ball[®] (Decisioneering, 1996) in the spreadsheet program Microsoft Excel 7.0[®] (Microsoft, 1995). This method segments the uncertainty

distribution of a parameter into a number of non-overlapping intervals, each having equal probability. In addition, a value from each interval is randomly selected according to the probability distribution within the interval. The randomly selected values from all the parameter uncertainty distributions are inserted in the output equation. Repeated calculations produce a distribution of the predicted output values, reflecting the combined parameter uncertainties. Each model run consisted of 10,000 iterations, which is considered sufficient to obtain a representative frequency chart of the output variables (Morgan and Henrion, 1990).

The quotients of product system A1 and product system A2 for their potential contribution to global warming and acidification are computed and used to indicate the significance of differences between the two product systems.

$$CI_e = \frac{\sum_{x=1}^{x=n} CF_{e,x} \times E_{A1,x}}{\sum_{x=1}^{x=n} CF_{e,x} \times E_{A2,x}}$$

where CI_e is the comparison indicator for environmental category e (dimensionless), $CF_{e,x}$ is the characterisation factor of substance x in the environmental category e (dimensionless), $E_{A1,x}$ is the amount of emitted substance x related to product system A1 (kg), $E_{A2,x}$ is the amount of emitted substance x related to product system A2 (kg), x is the emission identification number (dimensionless), and n is the number of emission types (dimensionless). When a quotient is significantly lower than 1, product system A1 contributes less to an environmental category than product system A2. When a quotient is significantly higher than 1, the reverse is true. A certain result is considered to be significant if 95% of the iterations lies above or below 1.

Figures 2.2 and 2.3 respectively show the frequency charts of the Global Warming Comparison Indicator with a chosen time horizon of 100 years ($GWCI_{100}$) and the Acidification Comparison Indicator (ACI), when using either the cut-off method or the avoided-impacts method to allocate environmental burdens associated with the open-loop recycling process. Table 2.9 shows some statistical characteristics of the respective comparison indicators. This table also lists the statistics of the potential contribution to global warming and acidification of the two product systems A1 and A2. The results show that the $GWCI_{100}$ lies 100% above 1 regardless of the allocation method used. The same is true for $GWCI_{20}$ and $GWCI_{500}$. The ACI lies 28.6% and 6.9% above 1, when the cut-off and avoided-impacts allocation method are used, respectively. Thus, product system A2 contributes significantly less to global warming than product system A1; however, when considering the contribution to acidification using the above-mentioned criterion for significance, no significant differences are found between the two product systems.

Table 2.9 Statistical characteristics of the potential contribution of product systems A1 and A2 respectively to Global Warming (time horizons 20, 100 and 500 years) and Acidification, and the Comparison Indicators for Global Warming (time horizons 20, 100 and 500 years) and Acidification.

	Units	Global warming (20y)		Global warming (100y)		Global warming (500y)		Acidification	
		C ^a	A ^b	C ^a	A ^b	C ^a	A ^b	C ^a	A ^b
Product system A1	CO ₂ /SO ₂ -eq								
Mean		304.7	212.6	258.4	189.7	236.6	180.1	11.0	9.4
Standard deviation		38.1	30.3	27.9	25.8	24.6	23.5	1.2	1.1
Distribution ^c		LN	LN	LN	LN	LN	LN LN	LN	
Product system A2	CO ₂ /SO ₂ -eq								
Mean		137.8	99.8	115.9	91.6	103.1	85.4	11.9	11.5
Standard deviation		17.9	17.6	12.9	15.3	11.0	13.4	2.1	2.2
Distribution ^c		LN	LN	LN	LN	LN	LN LN	LN	
Comparison Indicator	-								
Mean		2.22	2.13	2.23	2.10	2.30	2.16		
Standard deviation		0.11	0.28	0.12	0.30	0.13	0.32		
Modus							0.85	0.75	
Range							[0.7 - 1.25]	[0.6 - 1.15]	
Distribution ^c		LN	LN	LN	LN	LN	LN T	T	
Percentage A1 > A2	-	100%	100%	100%	100%	100%	100%	31.9%	7.8%

^a C = Cut-off allocation method, ^b A = Avoided-impacts allocation method; ^c LN = Lognormal, T= Triangular

Uncertainty importance analysis

Crystal Ball[®] is also equipped with a tool which calculates the uncertainty importance of each parameter. This tool calculates the uncertainty importance by computing rank correlation coefficients between every parameter uncertainty and every model outcome, such as the ACI, during the simulation. If a parameter and a model outcome have a high correlation coefficient, this means that the uncertainty in the parameter has a relatively large impact on the uncertainty in the model outcome. In the current assessment, the relative contribution of each parameter uncertainty to the uncertainty of the Comparison Indicators is approximated by the square values of the rank correlation coefficients r normalized to 100%. Table 2.10 lists the parameters which make a relatively large contribution (>5%) to the uncertainty of the GWCI₁₀₀ and ACI. In this respect, parameters which dominantly cause uncertainty in the ACI are of most interest, because statistically significant results are not obtained for the ACI as opposed to the GWCI. Uncertainty in the ACI is almost entirely caused by uncertainty in the proton release due to NO_x emissions, regardless of the allocation method used (Table 2.10). Research priority should in this case be given to reducing the uncertainty in the average removal of NO₃⁻ ions due to harvesting.

Figure 2.2 Frequency charts of the Global Warming Comparison Indicator (time horizon 100 years) after 10,000 model iterations, when using either the cut-off method or the avoided-impacts method to allocate environmental burdens associated with the open-loop recycling process.

Figure 2.3 Frequency charts of the Acidification Comparison Indicator after 10,000 model iterations, when using either the cut-off method or the avoided-impacts method to allocate environmental burdens associated with the open-loop recycling process.

Table 2.10 Uncertainty importance of input parameters, expressed in percentage contribution to the output uncertainty, relevant (> 5%) in the determination of the significance of differences between the product systems A1 and A2 for the GWCI₁₀₀ and the ACI

Parameter	Global Warming (100y)		Acidification	
	C ^a	A ^b	C ^a	A ^b
Recycling fraction roofgutter A1 (-)	23.4%	14.7%		
Recycling fraction roofgutter A2 (-)	26.6%	12.6%		
Plastic P1 input in production roofgutter A1 (kg)	14.0%			
Plastic P2 input in production roofgutter A2 (kg)	12.5%			
Mass of product A1 related to the functional unit of the receiving product system S (kg)		13.2%		
Mass of product A2 related to the functional unit of the receiving product system S (kg)		31.3%		
N ₂ O emission in roofgutter A2 recycling process (kg)	10.8%			
Proton release due to 1 mol NO _x emission (mol)			82.9%	81.0%
NO _x emission in plastic P2 production (kg)			6.7%	6.6%
Total uncertainty importance, explained by above factors	87.3%	71.8%	89.6%	87.6%

^a C = Cut-off allocation method; ^b A = Avoided-impacts allocation method

If the main goal of the assessment is not to compare products but, for example, to find product improvement options, an uncertainty importance analysis, performed for each product system separately, will be relevant. Tables 2.11 and 2.12 show that other parameter uncertainties, such as uncertainty of the lifetime of roof gutters, become important in the separate analyses. The partly changed relevance of parameter uncertainty is explained by the fact that some parameters are not specified per separate product system but are implemented only once in the simulation model. As a consequence, these parameters are mainly 'divided out' in the product comparison, while in a separate analysis of the product systems they are not.

Table 2.11 Uncertainty importance of input parameters, expressed in percentage contribution to the output uncertainty, relevant (> 5%) in the determination of the contribution to global warming (time horizon 100 years) and acidification of *product system A1*

Parameter	Global Warming (100y)		Acidification	
	C ^a	A ^b	C ^a	A ^b
Lifetime of roof gutter A1 (years)	73.9%	45.1%	68.2%	66.2%
Recycling fraction roofgutter A1 (-)	5.4%	12.9%		
Mass of product A1 related to the functional unit of the receiving product system S (kg)		11.9%		
Mass of product B related to the functional unit of the receiving product system S (kg)		12.1%		
Fraction of 100m roof gutter, initially applied to a one-family house (-)	7.7%	5.0%	6.8%	6.7%
Proton release due to 1 mol NOx emission (mol)			9.1%	11.5%
SO ₂ emission per MJ produced electricity (kg)			7.3%	
Total uncertainty importance, explained by above factors	87.0%	87.0%	91.4%	84.4%

^a C = Cut-off allocation method; ^b A = Avoided-impacts allocation method

Table 2.12 Uncertainty importance of input parameters, expressed in percentage contribution to the output uncertainty, relevant (> 5%) in the determination of the contribution to global warming (time horizon 100 years) and acidification of *product system A2*

Parameter	Global Warming (100y)		Acidification	
	C ^a	A ^b	C ^a	A ^b
Lifetime of roof gutter A2 (years)	69.1%	30.4%	23.0%	21.3%
Recycling fraction roofgutter A2 (-)	6.5%	7.2%		
Mass of product A2 related to the functional unit of the receiving product system S (kg)		19.2%		
Mass of product B related to the functional unit of the receiving product system S (kg)		18.9%		
Fraction of 100m roof gutter, initially applied to a one-family house (-)	7.1%			
NO ₂ emission per kg material B production (kg)		5.5%		
Proton release due to 1 mol NOx emission (mol)			68.3%	70.3%
Total uncertainty importance, explained by above factors	82.7%	81.2%	91.3%	91.6%

^a C = Cut-off allocation method; ^b A = Avoided-impacts allocation method

Discussion

As shown in this simplified example, the procedure to operationalise uncertainty due to choices and parameter uncertainty in LCAs is relatively straightforward. However, when 'real-life' LCAs are analysed, feasibility problems will occur. It will probably not be feasible in LCA case studies to analyse the effect of all possible combinations of choices, to underpin the uncertainty ranges of all the input data used in the inventory, and to perform an extensive parameter uncertainty analysis in the characterisation phase. Options to deal with these problems are discussed below.

When performing LCAs, choices are unavoidable. Aside from the choice how to allocate environmental burdens in open-loop recycling processes, several other choices will lead to uncertainty in LCA outcomes, such as the choice how to allocate environmental burdens in multi-output and multi-waste processes, and the choice of a functional unit. The following procedure, partly based on recommendations in Kortman *et al.* (1996), may help to decrease the number of choice combinations in LCA case studies: (1) formulate several options for every LCA choice; (2) find the two 'extreme' options for every choice; (3) construct two 'extreme' combinations of options and compute the effect of the two combinations on the LCA outcomes.

Furthermore, in practice it will be very difficult to underpin the uncertainty ranges for the huge number of parameters involved in the inventory analysis. Focusing on key parameter uncertainties will increase the feasibility of the uncertainty analysis and will decrease the validity of the uncertainty analysis only in a limited extent. Heijungs (1996) proposes to first perform a broad sensitivity analysis, using standard uncertainty estimates, to find out what parameters may contribute substantially to the uncertainty in environmental profiles. In a probabilistic simulation program it is possible to perform a sensitivity analysis in the same way as in the uncertainty importance analysis described in the previous section. Each parameter is then characterised with the same percentile sensitivity range and distribution, for example $\pm 10\%$ of most likely numbers as a uniform distribution. The parameters which together cover 90% of the sensitivity range, for instance, should then get priority to find accurate measurements or better uncertainty estimates. However, a disadvantage of using one standard sensitivity range is that parameters which are initially thought to present a minor contribution to LCA outcomes, but has an expected large unknown uncertainty range, are thrown out of the analysis beforehand. A very rough solution is perhaps found in the use of a number of standard sensitivity ranges for types of environmental interventions, such as the application of several 'uncertainty factors' in the roof gutter example used in this article. A complementary strategy to simplify the uncertainty analysis is to implement uncertainty ranges for accumulated environmental interventions rather than individual parameters in LCA inventories (see Kennedy *et al.*, 1996). This simplification could be particularly useful in the analysis of the potential importance of background data in the uncertainty analysis. For example, ranges for accumulated emissions per MJ electricity use could be implemented in the sensitivity analysis. If it appears that some of the

accumulated emissions may contribute substantially to the uncertainty in model outcomes, a reconstruction of parts of the inventory for electricity production will be necessary. Moreover, a second sensitivity analysis could be performed to find the dominant parameter uncertainties in the computation of the most important accumulated emissions. If potentially dominant parameter uncertainties are found, more sophisticated methods, such as the method described by Weidema and Wesnæs (1996) combined with expert judgement, and measurement of inaccuracies may be used to estimate uncertainty ranges in detail.

In addition to the lack of uncertainty estimates for process data in the inventory analysis, uncertainty pertinent to characterisation factors is generally unknown or very poorly known. An important difference between process data of the inventory and characterisation factors, however, is that process data are directly measured, while characterisation factors are computed with (simplified) environmental models. Therefore, uncertainty ranges for characterisation factors can only be found by a parameter uncertainty analysis within these models. Developers of characterisation factors should pay attention to this aspect, if necessary in co-operation with environmental model experts.

Finally, although operationalising the effect of parameter uncertainties and uncertainty due to choices is important, model uncertainties should not be disregarded. As pointed out in the introduction, model uncertainties, such as the lack of temporal and spatial variability in the assessment, have not been quantified in LCAs (Huijbregts, 1998a). Because of these inherent model uncertainties, it is important to avoid the appearance that uncertainty in LCAs is totally quantified with the techniques used in this paper. Other analytical instruments are needed to deal with these model uncertainties.

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Chapter 3

Life-cycle impact assessment of toxic substances

§ 3.1 Model development and application

Toxicity potentials are standard values used in life cycle assessment (LCA) to enable a comparison of toxic impacts between substances. In most cases, toxicity potentials are calculated with multi-media fate models. Up till now, unoealistic system settings were used for these calculations. The present paper outlines an improved model to calculate toxicity potentials: the global nested multi-media fate, exposure and effects model USES-LCA. It is based on the Uniform System for the Evaluation of Substances 2.0 (USES 2.0). USES-LCA was used to calculate for 181 substances toxicity potentials for the six impact categories fresh water aquatic ecotoxicity, marine aquatic ecotoxicity, fresh water sediment ecotoxicity, marine sediment ecotoxicity, terrestrial ecotoxicity and human toxicity, after initial emission to the compartments air, fresh water, seawater, industrial soil and agricultural soil, respectively. Differences of several orders of magnitude were found between the new toxicity potentials and previously calculated ones.

Published in *Chemosphere* 41: 541-573 (2000) under the title `Priority assessment of toxic substances in life cycle assessment. Part I: Calculation of toxicity potentials for 181 substances with the nested multi-media fate, exposure and effects model USES-LCA'. Co-authors are U. Thissen, J.B. Guinée, T. Jager, D. Kalf, D. van de Meent, A.M.J. Ragas, A. Wegener Sleeswijk and L. Reijnders.

Introduction

Life Cycle Assessment (LCA) is a tool for the assessment of the potential environmental impact of a product system (Heijungs *et al.*, 1992). It considers the entire life cycle of a product from resource extraction to waste disposal. According to ISO standardisation guidelines (ISO, 1997a, b, 1998a, b), an LCA study can be divided into four steps: goal and scope definition, inventory analysis, impact assessment, and interpretation. 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 types of television sets. In the inventory analysis, all extractions of resources and emissions of substances attributable to the studied functional unit are listed. In the impact assessment, it is first determined which impact categories have to be considered and which extractions and emissions contribute to these impact categories. Impact categories correspond with environmental problems, such as 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 the aggregated emission for each individual substance with an characterisation factor (Heijungs *et al.*, 1992).

$$IS_p = \sum_e \sum_x CF_{p,x,e} \times E_{x,e}$$

where IS_p is the impact score for impact category p per functional unit (kg), $CF_{p,x,e}$ is the characterisation Factor for impact category p of substance x emitted to compartment e (dimensionless), and $E_{x,e}$ is the emission of substance x to compartment e per functional unit (kg).

Characterisation factors, also called 'potentials', are substance-specific, quantitative representations of potential impacts per unit emission of a substance. They are calculated for each impact category to which a substance may potentially contribute. Examples are the Human Toxicity Potential and the Ozone Depletion Potential. Thus, within one impact category, characterisation factors are used as assessment factors to determine the relative contribution of a substance to an impact category. This should not be confused with the determination of environmental risks. The last (optional) step of the impact assessment is the calculation of an environmental index by aggregation of the impact categories. This can be done by attributing weighting factors to the different 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.

Guinée *et al.* (1996a, b) 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 model, developed by McKone (1993). Although multi-media fate and exposure modelling is in

itself a powerful tool to compute toxicity potentials, application of USES 1.0 and CalTOX for LCA purposes involves some drawbacks:

- 1 The models were originally developed for regional risk assessment purposes. They allow import and export of pollutants across their system boundaries, which effectively results in loss of substance from the system. This is inappropriate for LCA studies because the fate of a substance should be fully accounted for. Therefore, the open systems of USES 1.0 and CalTOX were closed by setting wind speed and water flow to an extremely low level in the calculations (Guinée *et al.*, 1996a; Hertwich *et al.*, 1998). These settings are unoealistic, which reduces the credibility of the model predictions.
- 1 Not all relevant compartments are included in these models. For instance, the sea is omitted.
- 2 Guinée *et al.* (1996a, b) used a considerable amount of questionable substance-specific default values as inputs in the computation of toxicity potentials.

The present article outlines the global multi-media fate and exposure model USES-LCA that eliminated most of the above mentioned drawbacks. It is based upon the *Uniform System for the Evaluation of Substances 2.0* (USES 2.0; RIVM *et al.*, 1998). USES-LCA is used to calculate toxicity potentials for 181 substances with a minimum use of default values or QSAR estimates. Below, first both USES 2.0 and USES-LCA will be discussed. Then, the calculated toxicity potentials will be presented and compared with those calculated by Guinée *et al.* (1996a, b).

Methods

USES 2.0

USES 2.0 has been developed for quantitative assessment of the risks on the local and regional scale posed by new and existing substances to man and the environment (RIVM *et al.*, 1998). USES 2.0 consists of six modules: (1) the input module for substance-specific data; (2) the emission module; (3) the distribution module; (4) the exposure module; (5) the effects module; and (6) the risk characterisation module.

The distribution module of USES 2.0 consists of local fate models and the nested multi-media fate model Simplebox 2.0, which are used to calculate steady-state concentrations, based on the data from the emission and input module. "Nested" means that chemicals can be transported from one scale to a higher scale and vice versa. Simplebox 2.0 has three spatial scales (regional, continental and global) and three climate zones, reflecting arctic, moderate and tropic climatic zones of the Northern hemisphere (Figure 3.1; Brandes *et al.*, 1996).

The regional and continental scales are defined within the moderate climate zone and each consists of six compartments: air, fresh water, seawater, natural soil, agricultural soil, and industrial soil. The global scale comprises the arctic, moderate and tropical climate

Figure 3.1 Schematic representation of SimpleBox 2.0 (Brandes *et al.*, 1996).

zones, each of which consists of three compartments: air, seawater, and soil. Because the global scale is modelled as a closed system without transport across the system boundaries, emitted substances cannot escape. For this reason, USES 2.0 can be used to calculate toxicity potentials without unoealistic system settings like an extremely low wind speed and water flow.

USES 2.0 distinguishes seven protection targets: aquatic ecosystems, terrestrial ecosystems, sediment ecosystems, fish-eating predators, worm-eating predators, micro-organisms in sewage treatment plants, and humans. The exposure module is used to calculate an exposure concentration for humans and fish-eating and worm-eating predators. For the other targets of protection, the exposure concentration is set equal to the environmental concentration predicted by the distribution module. In the effects assessment module, a Predicted No-Effect Concentration (PNEC) or a 'No-(Low)-Observed-Adverse-Effect' Level (N(L)OAEL) is calculated, corresponding with each of the targets of protection. Finally, risks are characterised by the ratio of the outcomes of the exposure assessment and the effects assessment modules. These ratios are called Risk Characterisation Ratios (RCR), also known as the PEC/PNEC ratio, and are calculated on the local and/or the regional scale.

USES-LCA

USES 2.0 has been adapted to meet LCA-specific demands. Furthermore, some general modifications have been made. These changes are discussed briefly below. A detailed discussion can be found in the technical report underlying this paper (Huijbregts, 1999a).

- 1 *Replacement of worst-case estimates.* In USES 2.0 some system parameters, such as purification factors for drinking water, are worst-case estimates. Worst-case values may be appropriate for initial risk assessment purposes, but their use in LCA is questionable. Because LCA is concerned with relative comparisons between product systems, worst-case values are replaced by realistic estimates.
- 2 *Discarding the local and regional scales.* In almost all current life cycle inventories, emissions are summed up per pollutant regardless of their geographical place of occurrence. This results in an inventory outcome that lacks any retrievable relation with a particular region. Consequently, the local and regional scales of USES 2.0 are not used in the calculation of toxicity potentials.
- 3 *Switch off 'economic' processes.* In line with the ISO standardisation guidelines (ISO, 1997a), 'economic' processes, such as sewage treatment, are 'switched off' in USES-LCA. These processes should be taken into account in the inventory analysis. An exception was made for drinking water purification, because this process is generally not taken into account in the inventory analysis (Guinée *et al.* (1996a, b).
- 4 *The use of standard emissions at the continental scale.* The built-in substance-specific emission estimation procedures of USES 2.0 were not used. Instead, standard emissions were implemented at the continental scale ($1 \cdot 10^6$ kg-day⁻¹) into one of the following continental compartments: air, fresh water, seawater, agricultural soil, industrial soil.
- 5 *Implementing exposure and effects assessment at all available scales.* The effects assessment for humans and ecosystems and the human exposure assessment were newly implemented at the continental scale and the three climate zones of the global scale of USES-LCA. In theory, characteristic human input values, such as daily meat intake, must be derived and implemented separately for the continental, moderate, arctic and tropic scales. However, here the practical choice is made to use the human characteristics of the continental scale for the global scale as well.
- 6 *Human effects assessment.* Extrapolation of NOAELs or LOAELs for mammals to oral and inhalatory Human Limit Values (HLVs) is not 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 a fair comparison between substances in LCA. Therefore, chronic HLVs as published by the Health Council of the Netherlands (1996), JECFA (1982, 1986, 1989) FAO/WHO (1993, 1998, 1999), WHO (1987, 1996, 1997), RIVM (Annema *et al.*, 1996; Janssen *et al.*, 1995, 1998; Janus, *et al.*, 1994; Rademaker, *et al.*, 1993; Rademaker and Van de Plassche, 1993; Slooff *et al.*, 1989; Vermeire *et al.*, 1991; Vermeire, 1993), USEPA (1999) and others (Environmental Defense Fund, 1999; Guinée *et al.*, 1996a; Tomlin, 1994) were implemented in USES-LCA. For genotoxic and carcinogenic substances the human intake value corresponding with an extra life-time risk of $1 \cdot 10^{-6}$ was used. This dose is sometimes referred to as the virtually safe dose (VSD; Food Safety Council, 1980) or as the risk-specific dose (RSD; Krewski *et al.*, 1990).

- 7 *Chemical-specific penetration depth.* In USES-LCA, the implementation of a chemical-specific penetration depth in the soil was extended from the regional and continental scales to the global scale.
- 8 *Transport to the stratosphere.* Because transport to the stratosphere may influence tropospheric air concentrations of very air-persistent substances, it was included in USES-LCA. It was assumed that every year 1/60th of the volume of the air in the troposphere advects to the stratosphere (Huijbregts, 1999a).
- 9 *Soil ingestion.* Chemical uptake via direct ingestion of soil particles was incorporated in USES-LCA (Table 1), because this route may be an important human exposure route for metals and persistent organic substances (Van de Meent *et al.*, 1995).
- 10 *Temperature dependency.* Temperature-dependent OH-radical reaction rates in air of 14 substances were implemented, based on information in Atkinson (1985) and Brubaker and Hites (1997).
- 11 *pH-dependency.* pH-dependency of some substance-specific characteristics was taken into account in the model calculations for (1) solubility, K_{oc} and plant uptake of dissociating substances, such as chlorophenols, and (2) rates of hydrolysis in water, soil and sediments.
- 12 *Metals.* USES-LCA was made suitable for the assessment of metals and other inorganic substances by using experimentally derived parameters. An example thereof is the usage of the experimentally determined metal solids-water partition coefficient (K_p) instead of the K_p estimated on the basis of the organic carbon extend.

Toxicity potentials

A toxicity potential is an indicator of the relative impact of a substance on a specific impact category after emission to a specific environmental compartment. In this study, toxicity potentials were calculated for six different toxic impact categories: the fresh water aquatic environment, the marine aquatic environment, the fresh water sediment environment, the marine sediment environment, the terrestrial environment and humans. Furthermore, five compartments were considered to which emission can take place: air, fresh water, seawater, agricultural soil and industrial soil. Each is referred to as an emission scenario. Thus, ultimately, 30 toxicity potentials were calculated for each substance; one for each combination of six impact categories and five emission compartments.

Risk Characterisation Ratios (RCRs) form the basis of the calculation of toxicity potentials. For each emission scenario and impact category, RCRs are calculated for the continental scale and the three climate zones of the global scale. For the impact categories aquatic, terrestrial and sediment ecotoxicity the RCRs are calculated by

$$RCR_{x,c,e} = \frac{PEC_{x,c,e}}{PNEC_{x,c}}$$

where $RCR_{x,c,e}$ is the Risk Characterisation Ratio of substance x in aquatic, terrestrial or sediment compartment c after emission to compartment e (dimensionless), $PEC_{x,c,e}$ is the Predicted Environmental Concentration of substance x in aquatic, terrestrial or sediment compartment c due to an emission to compartment e ($\text{kg}\cdot\text{m}^{-3}$ or $\text{kg}\cdot\text{kg}_{\text{wwt}}^{-1}$), and $PNEC_{x,c}$ is the Predicted No-Effect Concentration of substance x in aquatic, terrestrial or sediment compartment c ($\text{kg}\cdot\text{m}^{-3}$ or $\text{kg}\cdot\text{kg}_{\text{wwt}}^{-1}$). The RCRs for the impact category human toxicity are calculated by

$$RCR_{human,x,s,e} = \sum_r \frac{PDI_{r,x,s,e}}{HLV_{r,x}}$$

where $RCR_{human,x,s,e}$ is the Human Risk Characterisation Ratio of substance x at geographical scale s due to an emission to compartment e (dimensionless), $PDI_{r,x,s,e}$ is the Predicted Daily Intake via exposure route r (oral and inhalatory) of substance x for humans at geographical scale s after emission to compartment e ($\text{kg}\cdot\text{kg}_{\text{bw}}^{-1}\cdot\text{day}^{-1}$), and $HLV_{r,x}$ is the Human Limit Value for exposure route r (oral and inhalatory) of substance x ($\text{kg}\cdot\text{kg}_{\text{bw}}^{-1}\cdot\text{day}^{-1}$). An exception is made for the inorganic substances nitrogen dioxide (NO_2), sulphur dioxide (SO_2), ammonia (NH_3), hydrogen sulphide (H_2S), hydrogen chloride (HCl) and primary fine particulate matter (PM_{10}). For these substances only inhalatory exposure is taken into account in the calculation of human RCRs, instead of both inhalatory and oral exposure.

Computation of one toxicity potential per initial emission compartment for four of the six impact categories can only take place after aggregating the RCRs of the different environmental scales. This aggregation was performed with weighting factors resulting in a weighted RCR for each toxicity category. The RCRs of the marine aquatic compartments were aggregated on the basis of the compartment's volume, and the RCRs of the marine sediment and terrestrial compartments were both aggregated on the basis of the compartment's mass. For humans, the human population present at a certain scale has been used as a weighting factor. Per toxicity category, the weighted RCR of a substance after emission to a certain continental compartment was calculated by:

$$\text{Weighted } RCR_{i,x,e} = \sum_{c/s} RCR_{i,x,e,c/s} \times W_{i,c/s}$$

where $\text{Weighted } RCR_{i,x,e}$ is the weighted Risk Characterisation Ratio of impact category i for substance x emitted to compartment e (-, m^3 or kg_{wwt}), $RCR_{i,x,e,c/s}$ is the Risk Characterisation Ratio of impact category i for substance x at compartment c or geographical scale s after an emission to compartment e (-), and $W_{i,c/s}$ is the impact-specific weighting factor of compartment c or scale s (-, m^3 or kg_{wwt}).

As suggested by Guinée and Heijungs (1993), a reference substance was used in the

calculation of toxicity potentials which follows the established use of carbon dioxide (CO₂), ethylene (C₂H₄), and chlorofluorocarbon (CFC11) for evaluating global warming, photochemical ozone formation, and stratospheric ozone depletion, respectively (Albritton *et al.*, 1996; Derwent *et al.*, 1998; Solomon *et al.*, 1995). For the calculation of toxicity potentials, 1,4-dichlorobenzene was taken as a reference substance (cf. Guinée *et al.*, 1996a, b). Furthermore, one (continental) reference emission compartment per toxic impact category is chosen: the air compartment for human toxicity, the fresh water compartment for fresh water aquatic ecotoxicity and fresh water sediment ecotoxicity, the seawater compartment for marine aquatic ecotoxicity and marine sediment ecotoxicity, and the industrial soil compartment for terrestrial ecotoxicity. 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:

$$TP_{i,x,e} = \frac{\text{Weighted } RCR_{i,x,e}}{\text{Weighted } RCR_{ref}}$$

where $TP_{i,x,e}$ is the toxicity Potential of impact category i for substance x emitted to compartment e (1,4-DCB equivalents), $\text{Weighted } RCR_{i,x,e}$ is the weighted Risk Characterisation Ratio of impact category i for substance x emitted to compartment e (-, m³ or kg_{wwt}), and $\text{Weighted } RCR_{ref}$ is the weighted Risk Characterisation Ratio of impact category i for 1,4-DCB emitted to the defined reference compartment e (-, m³ or kg_{wwt}).

Input data

Distinction is made between environmental and substance-specific input parameters. For environmental parameters, default values in USES 2.0 were used. However, default values for the system areas of the three climate zones at the global scale and some plant properties were changed into more realistic estimates (Huijbregts, 1999a). Because the human characteristics of the exposure assessment of USES 2.0, such as food intake values, reflect worst-case assumptions, these were replaced by typical values (Table 3.1). 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 ultimately be protected, may also be defensible.

Table 3.1 Human characteristics in USES-LCA.

Parameter	Unit	USES-LCA	Source
Daily intake of drinking water	l.d ⁻¹	1.4	a
Daily intake of fishd	kg _{wwt} .d ⁻¹	0.03	b
Daily intake of leaf crops (incl. fruit and cereals)	kg _{wwt} .d ⁻¹	0.77	b
Daily intake of root crops	kg _{wwt} .d ⁻¹	0.18	b
Daily intake of meat	kg _{wwt} .d ⁻¹	0.26	b
Daily intake of dairy products	kg _{wwt} .d ⁻¹	0.28	b
Daily inhalation rate	m ³ .d ⁻¹	13.3	a
Body weight	kg	70	c
Daily soil ingestione	mg _{wwt} .d ⁻¹	50	a

^a USEPA (1997b); ^b ECETOC (1994); ^c RIVM *et al.* (1998); ^d 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; ^e it is assumed that on the continental scale all ingested soil comes from industrial/urban soils.

An extensive literature research was performed to find representative experimental substance-specific input parameters for 181 substances and thereby avoid as much as possible estimation routines or worst-case default values. All experimental substance-specific values used can be found in Huijbregts (1999a, b) and Van de Zande-Guinée *et al.* (1999). Avoiding estimation routines is especially important for dissociating substances, heavy metals and other inorganic chemicals, because these USES-LCA routines are valid only for non-ionic organic chemicals (RIVM *et al.*, 1998). When several reported values for one parameter seemed equally reasonable, the geometric mean of these values was calculated as this is the best representation of the usually skewed distributions (Seiler and Alvarez, 1996; Slob, 1994). If no experimental values for organic chemicals were found, USES 2.0 estimation routines were applied. Where necessary, air degradation rates were estimated with the atmospheric oxidation program of the Syracuse Research Corporation (1993), based on QSAR-methods developed by Atkinson (1985, 1988).

It was impossible to calculate HTPs for individual carcinogenic PAHs, because the inhalatory HLV for carcinogenic PAHs is representative for the over-all group of carcinogenic PAHs and not for the individual substances (Slooff *et al.*, 1989). Therefore, only the HTP for the total group of carcinogenic PAHs was calculated. Vermeire (1993) calculated the oral HLV for the carcinogenic PAHs from the individual oral HLVs of carcinogenic PAHs by assuming typical concentration ratios for carcinogenic PAH occurrence, derived from the occurrence of individual carcinogenic PAHs in industrial soils. These typical concentration ratios of carcinogenic PAHs were also used here to calculate the weighted averaged substance-specific input data for the fate analysis.

Results

Toxicity potentials

Table 3.2 lists the toxicity potentials for the 181 evaluated substances calculated by USES-LCA.

Table 3.2 Toxicity potentials of 181 substances related to the initial emission compartments and impact categories. FAETP = fresh water Aquatic Ecotoxicity Potential; MAETP = marine Aquatic Ecotoxicity Potential; FSETP = fresh water Sediment Ecotoxicity Potential; MSETP = marine Sediment Ecotoxicity Potential; TETP = Terrestrial Ecotoxicity Potential; HTP = Human Toxicity Potential; x = toxicity potential was not calculated.

Substance Name	CAS No.	Type	Initial emission compartment				
			air	fresh water	sea water	agricult. soil	indust. soil
Metals							
Antimony	7440-36-0	FAETP	3.7	2.0·10 ¹	7.6·10 ⁻²¹	1.0·10 ¹	1.0·10 ¹
		MAETP	3.3·10 ⁴	2.7·10 ⁴	4.9·10 ⁴	1.4·10 ⁴	1.4·10 ⁴
		FSETP	9.1	4.8·10 ¹	1.8·10 ⁻²⁰	2.4·10 ¹	2.4·10 ¹
		MSETP	3.1·10 ⁴	2.5·10 ⁴	4.6·10 ⁴	1.3·10 ⁴	1.3·10 ⁴
		TETP	6.1·10 ⁻¹	1.7·10 ⁻²⁰	3.0·10 ⁻²⁰	1.3	1.3
		HTP	6.7·10 ³	5.1·10 ³	8.6·10 ³	8.9·10 ³	2.6·10 ³
Arsenic	7440-38-2	FAETP	5.0·10 ¹	2.1·10 ²	3.8·10 ⁻²⁰	1.3·10 ²	1.3·10 ²
		MAETP	2.3·10 ⁵	1.2·10 ⁵	3.4·10 ⁵	7.7·10 ⁴	7.7·10 ⁴
		FSETP	1.3·10 ²	5.3·10 ²	9.8·10 ⁻²⁰	3.4·10 ²	3.4·10 ²
		MSETP	2.3·10 ⁵	1.2·10 ⁵	3.4·10 ⁵	7.7·10 ⁴	7.7·10 ⁴
		TETP	1.6·10 ³	1.0·10 ⁻¹⁷	3.0·10 ⁻¹⁷	3.3·10 ³	3.3·10 ³
		HTP	3.5·10 ⁵	9.5·10 ²	2.4·10 ³	3.2·10 ⁴	1.0·10 ³
Barium	7440-39-3	FAETP	4.3·10 ¹	2.3·10 ²	2.4·10 ⁻¹⁹	1.1·10 ²	1.1·10 ²
		MAETP	7.8·10 ⁵	8.3·10 ⁵	1.1·10 ⁶	4.2·10 ⁵	4.2·10 ⁵
		FSETP	9.7·10 ¹	5.1·10 ²	5.4·10 ⁻¹⁹	2.6·10 ²	2.6·10 ²
		MSETP	6.7·10 ⁵	7.1·10 ⁵	9.3·10 ⁵	3.6·10 ⁵	3.6·10 ⁵
		TETP	4.9	5.1·10 ⁻¹⁹	6.6·10 ⁻¹⁹	1.0·10 ¹	1.0·10 ¹
		HTP	7.6·10 ²	6.3·10 ²	8.0·10 ²	3.6·10 ²	3.2·10 ²
Beryllium	7440-41-7	FAETP	1.7·10 ⁴	9.1·10 ⁴	1.6·10 ⁻¹⁶	4.6·10 ⁴	4.6·10 ⁴
		MAETP	4.7·10 ⁸	5.4·10 ⁸	6.4·10 ⁸	2.7·10 ⁸	2.7·10 ⁸
		FSETP	2.0·10 ⁴	1.1·10 ⁵	1.8·10 ⁻¹⁶	5.4·10 ⁴	5.4·10 ⁴
		MSETP	2.0·10 ⁸	2.3·10 ⁸	2.8·10 ⁸	1.2·10 ⁸	1.2·10 ⁸
		TETP	1.8·10 ³	3.3·10 ⁻¹⁶	3.9·10 ⁻¹⁶	3.6·10 ³	3.6·10 ³
		HTP	2.3·10 ⁵	1.4·10 ⁴	1.6·10 ⁴	1.3·10 ⁴	7.0·10 ³
Cadmium	7440-43-9	FAETP	2.9·10 ²	1.5·10 ³	2.5·10 ⁻²⁰	7.8·10 ²	7.8·10 ²
		MAETP	1.1·10 ⁶	2.2·10 ⁵	1.8·10 ⁶	1.1·10 ⁵	1.1·10 ⁵
		FSETP	7.4·10 ²	3.9·10 ³	6.5·10 ⁻²⁰	2.0·10 ³	2.0·10 ³
		MSETP	1.1·10 ⁶	2.2·10 ⁵	1.9·10 ⁶	1.1·10 ⁵	1.1·10 ⁵
		TETP	8.1·10 ¹	1.4·10 ⁻²⁰	1.1·10 ⁻¹⁹	1.7·10 ²	1.7·10 ²
		HTP	1.5·10 ⁵	2.3·10 ¹	1.0·10 ²	2.0·10 ⁴	6.7·10 ¹

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

Substance Name	CAS No.	Type	Initial emission compartment				
			air	fresh water	sea water	agricult. soil	indust. soil
Metals							
Nickel	7440-2-0	FAETP	6.3·10 ²	3.2·10 ³	6.1·10 ⁻¹⁹	1.7·10 ³	1.7·10 ³
		MAETP	3.8·10 ⁶	2.2·10 ⁶	5.8·10 ⁶	1.2·10 ⁶	1.2·10 ⁶
		FSETP	1.6·10 ³	8.3·10 ³	1.6·10 ⁻¹⁸	4.3·10 ³	4.3·10 ³
		MSETP	3.7·10 ⁶	2.2·10 ⁶	5.7·10 ⁶	1.2·10 ⁶	1.2·10 ⁶
		TETP	1.2·10 ²	1.0·10 ⁻¹⁸	2.6·10 ⁻¹⁸	2.4·10 ²	2.4·10 ²
		HTP	3.5·10 ⁴	3.3·10 ²	7.5·10 ²	2.7·10 ³	2.0·10 ²
Selenium	7782-49-2	FAETP	5.5·10 ²	2.9·10 ³	7.4·10 ⁻¹⁸	1.5·10 ³	1.5·10 ³
		MAETP	2.1·10 ⁷	2.5·10 ⁷	2.9·10 ⁷	1.3·10 ⁷	1.3·10 ⁷
		FSETP	6.4·10 ²	3.4·10 ³	8.6·10 ⁻¹⁸	1.7·10 ³	1.7·10 ³
		MSETP	9.0·10 ⁶	1.1·10 ⁷	1.2·10 ⁷	5.4·10 ⁶	5.4·10 ⁶
		TETP	5.3·10 ¹	1.6·10 ⁻¹⁷	1.8·10 ⁻¹⁷	1.1·10 ²	1.1·10 ²
		HTP	4.8·10 ⁴	5.6·10 ⁴	6.3·10 ⁴	2.9·10 ⁴	2.8·10 ⁴
Thallium	7440-28-0	FAETP	1.6·10 ³	8.0·10 ³	7.9·10 ⁻¹⁸	4.2·10 ³	4.2·10 ³
		MAETP	2.6·10 ⁷	2.7·10 ⁷	3.6·10 ⁷	1.4·10 ⁷	1.4·10 ⁷
		FSETP	3.9·10 ³	2.0·10 ⁴	2.0·10 ⁻¹⁷	1.1·10 ⁴	1.1·10 ⁴
		MSETP	2.4·10 ⁷	2.5·10 ⁷	3.4·10 ⁷	1.3·10 ⁷	1.3·10 ⁷
		TETP	3.4·10 ²	3.1·10 ⁻¹⁷	4.2·10 ⁻¹⁷	7.0·10 ²	7.0·10 ²
		HTP	4.3·10 ⁵	2.3·10 ⁵	2.9·10 ⁵	2.0·10 ⁶	1.2·10 ⁵
Tin	7440-31-5	FAETP	2.5	1.0·10 ¹	9.5·10 ⁻²³	6.9	6.9
		MAETP	7.5·10 ³	1.2·10 ³	1.2·10 ⁴	8.3·10 ²	8.3·10 ²
		FSETP	1.3	5.2	4.8·10 ⁻²³	3.5	3.5
		MSETP	1.5·10 ³	2.5·10 ²	2.5·10 ³	1.7·10 ²	1.7·10 ²
		TETP	1.4·10 ¹	7.9·10 ⁻²²	7.2·10 ⁻²¹	3.0·10 ¹	3.0·10 ¹
		HTP	1.7	1.7·10 ⁻²	1.1·10 ⁻¹	1.3·10 ¹	5.2·10 ⁻¹
Vanadium	7440-62-2	FAETP	1.7·10 ³	9.0·10 ³	2.4·10 ⁻¹⁸	4.7·10 ³	4.7·10 ³
		MAETP	1.2·10 ⁷	8.6·10 ⁶	1.8·10 ⁷	4.5·10 ⁶	4.5·10 ⁶
		FSETP	4.1·10 ³	2.1·10 ⁴	5.7·10 ⁻¹⁸	1.1·10 ⁴	1.1·10 ⁴
		MSETP	1.1·10 ⁷	7.9·10 ⁶	1.7·10 ⁷	4.1·10 ⁶	4.1·10 ⁶
		TETP	6.7·10 ²	1.0·10 ⁻¹⁷	2.2·10 ⁻¹⁷	1.4·10 ³	1.4·10 ³
		HTP	6.2·10 ³	3.2·10 ³	6.2·10 ³	1.9·10 ⁴	1.7·10 ³
Zinc	7440-66-6	FAETP	1.8·10 ¹	9.2·10 ¹	1.8·10 ⁻²¹	4.8·10 ¹	4.8·10 ¹
		MAETP	6.7·10 ⁴	1.4·10 ⁴	1.1·10 ⁵	7.2·10 ³	7.2·10 ³
		FSETP	4.6·10 ¹	2.4·10 ²	4.5·10 ⁻²¹	1.2·10 ²	1.2·10 ²
		MSETP	6.8·10 ⁴	1.4·10 ⁴	1.1·10 ⁵	7.3·10 ³	7.3·10 ³
		TETP	1.2·10 ¹	2.5·10 ⁻²¹	1.9·10 ⁻²⁰	2.5·10 ¹	2.5·10 ¹
		HTP	1.0·10 ²	5.8·10 ⁻¹	3.2	6.4·10 ¹	4.2·10 ⁻¹

Substance Name	CAS No.	Type	Initial emission compartment				
			air	fresh water	sea water	agricult. soil	indust. soil
Inorganics							
Ammonia	7664-41-7	FAETP	x	x	x	x	x
		MAETP	x	x	x	x	x
		FSETP	x	x	x	x	x
		MSETP	x	x	x	x	x
		TETP	x	x	x	x	x
		HTP	1.0·10 ⁻¹	x	x	x	x
Hydrogen sulphide	10102-44-0	FAETP	x	x	x	x	x
		MAETP	x	x	x	x	x
		FSETP	x	x	x	x	x
		MSETP	x	x	x	x	x
		TETP	x	x	x	x	x
		HTP	2.2·10 ⁻¹	x	x	x	x
Hydrogen chloride	7446-9-5	FAETP	x	x	x	x	x
		MAETP	x	x	x	x	x
		FSETP	x	x	x	x	x
		MSETP	x	x	x	x	x
		TETP	x	x	x	x	x
		HTP	5.0·10 ⁻¹	x	x	x	x
Nitrogen dioxide	7783-6-4	FAETP	x	x	x	x	x
		MAETP	x	x	x	x	x
		FSETP	x	x	x	x	x
		MSETP	x	x	x	x	x
		TETP	x	x	x	x	x
		HTP	1.2	x	x	x	x
Sulphur dioxide	7647-1-0	FAETP	x	x	x	x	x
		MAETP	x	x	x	x	x
		FSETP	x	x	x	x	x
		MSETP	x	x	x	x	x
		TETP	x	x	x	x	x
		HTP	3.1·10 ⁻¹	x	x	x	x
PM10		FAETP	x	x	x	x	x
		MAETP	x	x	x	x	x
		FSETP	x	x	x	x	x
		MSETP	x	x	x	x	x
		TETP	x	x	x	x	x
		HTP	9.6·10 ⁻²	x	x	x	x

Substance Name	CAS No.	Type	Initial emission compartment				
			air	fresh water	sea water	agricult. soil	indust. soil
Non-aromatics							
Acrylonitrile	107-13-1	FAETP	4.1·10 ⁻¹	7.9·10 ¹	6.0·10 ⁻³	6.5	8.1
		MAETP	9.1·10 ⁻¹	5.4·10 ⁻¹	3.1	2.1·10 ⁻¹	2.7·10 ⁻¹
		FSETP	2.7·10 ⁻¹	5.2·10 ¹	3.9·10 ⁻³	4.2	5.3
		MSETP	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
Acrolein	107-2-8	FAETP	5.2·10 ²	2.5·10 ⁵	5.0	4.5·10 ⁴	4.5·10 ⁴
		MAETP	5.7·10 ²	1.1·10 ³	8.9·10 ³	2.5·10 ²	2.5·10 ²
		FSETP	3.9·10 ²	1.9·10 ⁵	3.7	3.4·10 ⁴	3.4·10 ⁴
		MSETP	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
1,3-Butadiene	75-15-0	FAETP	3.3·10 ⁻⁷	3.0	5.6·10 ⁻⁸	5.7·10 ⁻⁵	5.7·10 ⁻⁵
		MAETP	2.7·10 ⁻⁶	8.7·10 ⁻³	7.3·10 ⁻¹	2.9·10 ⁻⁶	2.9·10 ⁻⁶
		FSETP	2.2·10 ⁻⁷	2.0	3.8·10 ⁻⁸	3.8·10 ⁻⁵	3.8·10 ⁻⁵
		MSETP	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
Carbon disulfide	106-99-0	FAETP	3.3·10 ⁻²	1.1·10 ²	6.5·10 ⁻³	3.4·10 ⁻¹	3.4·10 ⁻¹
		MAETP	1.5	1.8	3.0·10 ¹	1.4	1.4
		FSETP	2.7·10 ⁻²	8.6·10 ¹	5.4·10 ⁻³	2.8·10 ⁻¹	2.8·10 ⁻¹
		MSETP	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
Ethylene	74-85-1	FAETP	1.4·10 ⁻¹¹	2.2·10 ⁻²	1.0·10 ⁻¹²	1.1·10 ⁻⁹	1.1·10 ⁻⁹
		MAETP	7.9·10 ⁻¹¹	2.8·10 ⁻⁵	2.6·10 ⁻³	7.8·10 ⁻¹¹	7.8·10 ⁻¹¹
		FSETP	9.0·10 ⁻¹²	1.4·10 ⁻²	6.6·10 ⁻¹³	7.1·10 ⁻¹⁰	7.1·10 ⁻¹⁰
		MSETP	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
Formaldehyde	50-00-0	FAETP	8.3	2.8·10 ²	2.1·10 ⁻⁴	1.5·10 ¹	4.4·10 ¹
		MAETP	1.6	1.9·10 ⁻¹	5.6	1.8·10 ⁻²	5.5·10 ⁻²
		FSETP	4.5	1.5·10 ²	1.2·10 ⁻⁴	7.9	2.4·10 ¹
		MSETP	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
Propylene oxide	75-56-9	FAETP	3.7·10 ⁻²	4.0	4.4·10 ⁻⁴	4.2·10 ⁻¹	4.8·10 ⁻¹
		MAETP	1.2·10 ⁻¹	5.8·10 ⁻²	1.4·10 ⁻¹	2.9·10 ⁻²	3.3·10 ⁻²
		FSETP	2.0·10 ⁻²	2.1	2.4·10 ⁻⁴	2.3·10 ⁻¹	2.5·10 ⁻¹
		MSETP	6.4·10 ⁻²	3.3·10 ⁻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

Substance Name	CAS No.	Type	Initial emission compartment				
			air	fresh water	sea water	agricult. soil	indust. soil
Aromatics							
Benzene	71-43-2	FAETP	8.4·10 ⁻⁵	9.1·10 ⁻²	9.2·10 ⁻⁶	7.2·10 ⁻⁴	7.2·10 ⁻⁴
		MAETP	2.8·10 ⁻³	2.7·10 ⁻³	1.5·10 ⁻²	2.4·10 ⁻³	2.4·10 ⁻³
		FSETP	6.4·10 ⁻⁵	7.0·10 ⁻²	7.0·10 ⁻⁶	5.4·10 ⁻⁴	5.4·10 ⁻⁴
		MSETP	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
Toluene	108-88-3	FAETP	7.0·10 ⁻⁵	2.9·10 ⁻¹	8.3·10 ⁻⁶	1.1·10 ⁻³	1.1·0 ⁻³
		MAETP	7.0·10 ⁻⁴	1.2·10 ⁻³	5.1·10 ⁻²	4.5·10 ⁻⁴	4.5·10 ⁻⁴
		FSETP	5.0·10 ⁻⁵	2.1·10 ⁻¹	5.9·10 ⁻⁶	7.5·10 ⁻⁴	7.5·10 ⁻⁴
		MSETP	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
Styrene	100-42-5	FAETP	5.1·10 ⁻⁵	4.4·10 ⁻¹	1.0·10 ⁻⁵	1.5·10 ⁻³	2.6·10 ⁻³
		MAETP	5.1·10 ⁻⁴	2.2·10 ⁻³	1.2·10 ⁻¹	1.1·10 ⁻⁴	1.8·10 ⁻⁴
		FSETP	3.5·10 ⁻⁵	3.0·10 ⁻¹	7.0·10 ⁻⁶	1.1·10 ⁻³	1.8·10 ⁻³
		MSETP	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
Phenol	108-95-2	FAETP	1.5	2.4·10 ²	1.7·10 ⁻⁵	3.5	1.3·10 ¹
		MAETP	5.5·10 ⁻¹	5.6·10 ⁻²	4.7	1.7·10 ⁻³	6.1·10 ⁻³
		FSETP	5.6·10 ⁻¹	8.8·10 ¹	6.4·10 ⁻⁶	1.3	4.7
		MSETP	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
Ethylbenzene	100-41-4	FAETP	1.3·10 ⁻⁴	5.5·10 ⁻¹	9.4·10 ⁻⁶	1.8·10 ⁻³	1.8·10 ⁻³
		MAETP	8.0·10 ⁻⁴	1.4·10 ⁻³	6.2·10 ⁻²	4.1·10 ⁻⁴	4.1·10 ⁻⁴
		FSETP	8.7·10 ⁻⁵	3.6·10 ⁻¹	6.3·10 ⁻⁶	1.2·10 ⁻³	1.2·10 ⁻³
		MSETP	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
m-Xylene	108-38-3	FAETP	4.4·10 ⁻⁵	6.0·10 ⁻¹	7.2·10 ⁻⁶	1.9·10 ⁻³	1.9·10 ⁻³
		MAETP	3.9·10 ⁻⁴	2.1·10 ⁻³	1.4·10 ⁻¹	2.5·10 ⁻⁴	2.5·10 ⁻⁴
		FSETP	2.8·10 ⁻⁵	3.9·10 ⁻¹	4.7·10 ⁻⁶	1.2·10 ⁻³	1.2·10 ⁻³
		MSETP	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
o-Xylene	95-47-6	FAETP	9.3·10 ⁻⁵	5.6·10 ⁻¹	1.5·10 ⁻⁵	2.5·10 ⁻³	2.5·10 ⁻³
		MAETP	9.1·10 ⁻⁴	2.5·10 ⁻³	1.3·10 ⁻¹	5.5·10 ⁻⁴	5.5·10 ⁻⁴
		FSETP	7.4·10 ⁻⁵	4.5·10 ⁻¹	1.2·10 ⁻⁵	2.0·10 ⁻³	2.0·10 ⁻³
		MSETP	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
p-Xylene	106-42-3	FAETP	6.1·10 ⁻⁵	5.5·10 ⁻¹	1.0·10 ⁻⁵	1.4·10 ⁻³	1.4·10 ⁻³
		MAETP	6.1·10 ⁻⁴	2.2·10 ⁻³	1.3·10 ⁻¹	3.2·10 ⁻⁴	3.2·10 ⁻⁴
		FSETP	3.7·10 ⁻⁵	3.3·10 ⁻¹	6.1·10 ⁻⁶	8.6·10 ⁻⁴	8.7·10 ⁻⁴
		MSETP	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

Substance Name	CAS No.	Type	Initial emission compartment				
			air	fresh water	sea water	agricult. soil	indust. soil
Aromatics							
Butyl-benzylphthalate	85-68-7	FAETP	4.0·10 ⁻¹	7.6·10 ¹	3.2·10 ⁻⁵	2.5·10 ⁻²	1.0·10 ⁻¹
		MAETP	3.2·10 ⁻¹	5.3·10 ⁻²	1.6	2.9·10 ⁻⁵	1.2·10 ⁻⁴
		FSETP	1.3·10 ⁻¹	2.5·10 ¹	1.0·10 ⁻⁵	8.2·10 ⁻³	3.3·10 ⁻²
		MSETP	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
Di(2ethylhexyl)-phtalate	117-81-7	FAETP	3.5·10 ⁻¹	7.9·10 ¹	1.6·10 ⁻³	1.5·10 ⁻³	6.0·10 ⁻³
		MAETP	2.4	3.7·10 ⁻¹	1.5·10 ¹	1.6·10 ⁻⁵	6.2·10 ⁻⁵
		FSETP	4.7·10 ⁻¹	1.0·10 ²	2.1·10 ⁻³	2.0·10 ⁻³	7.9·10 ⁻³
		MSETP	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
Dibutylphthalate	84-74-2	FAETP	5.6·10 ⁻¹	7.9·10 ¹	2.9·10 ⁻⁵	7.9·10 ⁻²	3.1·10 ⁻¹
		MAETP	4.4·10 ⁻¹	7.7·10 ⁻²	1.7	1.2·10 ⁻⁴	4.8·10 ⁻⁴
		FSETP	7.3·10 ⁻²	1.0·10 ¹	3.8·10 ⁻⁶	1.0·10 ⁻²	4.1·10 ⁻²
		MSETP	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
Diethylphthalate	84-66-2	FAETP	4.2·10 ⁻¹	3.4·10 ¹	7.9·10 ⁻⁵	1.6·10 ⁻¹	6.3·10 ⁻¹
		MAETP	3.4·10 ⁻¹	1.1·10 ⁻¹	8.0·10 ⁻¹	7.1·10 ⁻⁴	2.8·10 ⁻³
		FSETP	2.8·10 ⁻¹	2.2·10 ¹	5.2·10 ⁻⁵	1.1·10 ⁻¹	4.1·10 ⁻¹
		MSETP	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
Dihexylphthalate	84-75-3	FAETP	5.0·10 ⁻¹	1.1·10 ²	1.1·10 ⁻²	1.8·10 ⁻²	7.4·10 ⁻²
		MAETP	1.7	1.2	9.7	4.3·10 ⁻⁴	1.7·10 ⁻³
		FSETP	1.2	2.6·10 ²	2.6·10 ⁻²	4.4·10 ⁻²	1.8·10 ⁻¹
		MSETP	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
Diisooctylphthalate	27554-26-3	FAETP	1.2·10 ⁻¹	2.1·10 ¹	3.9·10 ⁻³	6.2·10 ⁻⁴	2.5·10 ⁻³
		MAETP	3.6	4.3·10 ⁻¹	1.6·10 ¹	6.5·10 ⁻⁵	2.6·10 ⁻⁴
		FSETP	2.8·10 ⁻¹	4.7·10 ¹	8.7·10 ⁻³	1.4·10 ⁻³	5.5·10 ⁻³
		MSETP	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
Diisodecylphthalate	26761-40-0	FAETP	5.6·10 ⁻¹	8.6·10 ¹	3.8·10 ⁻²	4.6·10 ⁻³	1.8·10 ⁻²
		MAETP	4.7	2.3	1.9·10 ¹	8.6·10 ⁻⁴	3.4·10 ⁻³
		FSETP	1.2	1.9·10 ²	8.5·10 ⁻²	1.0·10 ⁻²	4.1·10 ⁻²
		MSETP	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
Dimethylphthalate	133-11-3	FAETP	5.2·10 ⁻²	3.1	3.8·10 ⁻⁷	7.4·10 ⁻³	2.9·10 ⁻²
		MAETP	2.7·10 ⁻²	1.7·10 ⁻³	5.2·10 ⁻²	9.7·10 ⁻⁶	3.8·10 ⁻⁵
		FSETP	1.3·10 ⁻²	7.9·10 ⁻¹	9.8·10 ⁻⁸	1.9·10 ⁻³	7.5·10 ⁻³
		MSETP	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

Substance Name	CAS No.	Type	Initial emission compartment				
			air	fresh water	sea water	agricult. soil	indust. soil
Aromatics							
Diocetylphthalate	117-84-0	FAETP	1.6·10 ⁻²	2.8	1.4·10 ⁻⁴	4.2·10 ⁻⁵	1.7·10 ⁻⁴
		MAETP	5.4·10 ⁻¹	3.5·10 ⁻²	2.5	1.3·10 ⁻⁶	5.2·10 ⁻⁶
		FSETP	2.7·10 ⁻²	4.7	2.4·10 ⁻⁴	7.1·10 ⁻⁵	2.8·10 ⁻⁴
		MSETP	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
Phthalic anhydride	85-44-9	FAETP	8.2·10 ⁻³	5.5·10 ⁻¹	4.6·10 ⁻¹¹	4.8·10 ⁻⁵	3.1·10 ⁻⁵
		MAETP	8.5·10 ⁻³	4.1·10 ⁻⁶	1.7·10 ⁻²	1.8·10 ⁻⁸	1.2·10 ⁻⁸
		FSETP	1.7·10 ⁻⁵	1.1·10 ⁻³	9.4·10 ⁻¹⁴	9.8·10 ⁻⁸	6.3·10 ⁻⁸
		MSETP	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							
Naphtalene	91-20-3	FAETP	5.0·10 ⁻¹	6.6·10 ²	1.1·10 ⁻²	3.8	1.2·10 ¹
		MAETP	9.1·10 ⁻¹	1.1	3.3·10 ¹	5.7·10 ⁻²	1.9·10 ⁻¹
		FSETP	1.9·10 ⁻¹	2.6·10 ²	4.5·10 ⁻³	1.5	4.9
		MSETP	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
Anthracene	120-12-7	FAETP	1.4·10 ²	5.7·10 ⁴	1.7·10 ¹	8.2·10 ¹	3.2·10 ²
		MAETP	1.7·10 ³	3.0·10 ³	1.8·10 ⁴	6.2	2.5·10 ¹
		FSETP	1.9·10 ²	8.0·10 ⁴	2.3·10 ¹	1.1·10 ²	4.5·10 ²
		MSETP	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
Phenanthrene	85-1-8	FAETP	1.3	5.2·10 ²	5.8·10 ⁻²	2.9·10 ⁻¹	1.2
		MAETP	7.3	1.0·10 ¹	7.4·10 ¹	8.7·10 ⁻³	3.5·10 ⁻²
		FSETP	1.4	5.6·10 ²	6.3·10 ⁻²	3.2·10 ⁻¹	1.3
		MSETP	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
Fluoranthrene	206-44-0	FAETP	1.8·10 ¹	1.3·10 ⁴	8.7·10 ⁻¹	1.9·10 ¹	7.6·10 ¹
		MAETP	2.0·10 ²	8.7·10 ²	4.2·10 ³	1.3	5.3
		FSETP	5.3·10 ¹	3.9·10 ⁴	2.6	5.7·10 ¹	2.3·10 ²
		MSETP	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
Benzo-[a]anthracene	56-55-3	FAETP	4.2·10 ¹	1.1·10 ⁵	1.1	6.2·10 ¹	2.5·10 ²
		MAETP	1.0·10 ³	8.3·10 ³	8.5·10 ⁴	4.5	1.8·10 ¹
		FSETP	1.3·10 ²	3.5·10 ⁵	3.2	1.9·10 ²	7.4·10 ²
		MSETP	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
Chrysene	218-1-9	FAETP	3.9·10 ¹	1.9·10 ⁴	2.6·10 ⁻¹	7.4·10 ¹	2.9·10 ²
		MAETP	4.1·10 ²	3.0·10 ³	7.6·10 ³	1.2·10 ¹	4.7·10 ¹
		FSETP	1.3·10 ²	5.9·10 ⁴	8.3·10 ⁻¹	2.4·10 ²	9.3·10 ²
		MSETP	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

Substance Name	CAS No.	Type	Initial emission compartment				
			air	fresh water	sea water	agricult. soil	indust. soil
Polycyclic aromatics							
Benzo-[k]fluoranthrene	207-8-9	FAETP	3.9·10 ³	1.2·10 ⁶	9.1	5.2·10 ³	2.0·10 ⁴
		MAETP	1.2·10 ⁵	4.4·10 ⁵	1.5·10 ⁶	2.0·10 ³	7.8·10 ³
		FSETP	1.3·10 ⁴	3.9·10 ⁶	3.0·10 ¹	1.7·10 ⁴	6.8·10 ⁴
		MSETP	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
Benzo[a]pyrene	50-32-8	FAETP	8.8·10 ¹	2.5·10 ⁵	2.8·10 ⁻¹	1.3·10 ²	5.3·10 ²
		MAETP	1.4·10 ³	1.2·10 ⁴	1.2·10 ⁵	6.5	2.6·10 ¹
		FSETP	2.5·10 ²	7.2·10 ⁵	8.0·10 ⁻¹	3.8·10 ²	1.5·10 ³
		MSETP	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
Benzo-[ghi]perylene	191-24-2	FAETP	4.4·10 ¹	5.2·10 ⁴	4.9·10 ⁻²	6.1·10 ¹	2.4·10 ²
		MAETP	1.7·10 ³	9.1·10 ³	6.5·10 ⁴	1.1·10 ¹	4.3·10 ¹
		FSETP	1.4·10 ²	1.7·10 ⁵	1.6·10 ⁻¹	2.0·10 ²	7.8·10 ²
		MSETP	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
Indeno [1,2,3-cd]pyrene	193-39-5	FAETP	1.7·10 ²	7.7·10 ⁴	7.4·10 ⁻⁴	9.0·10 ¹	3.6·10 ²
		MAETP	7.3·10 ³	1.5·10 ⁴	1.1·10 ⁵	1.7·10 ¹	6.8·10 ¹
		FSETP	5.3·10 ²	2.5·10 ⁵	2.4·10 ⁻³	2.9·10 ²	1.2·10 ³
		MSETP	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
Carcinogenic PAHs		FAETP	1.7·10 ²	2.8·10 ⁴	1.2·10 ⁻¹	5.8·10 ¹	2.3·10 ²
		MAETP	4.3·10 ³	5.5·10 ³	2.4·10 ⁴	1.2·10 ¹	4.8·10 ¹
		FSETP	5.6·10 ²	8.9·10 ⁴	3.8·10 ⁻¹	1.9·10 ²	7.5·10 ²
		MSETP	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
Halogenated non-aromatics							
Dichloromethane	75-9-2	FAETP	3.3·10 ⁻⁵	1.2·10 ⁻²	5.0·10 ⁻⁶	1.6·10 ⁻⁴	1.6·10 ⁻⁴
		MAETP	3.8·10 ⁻³	3.5·10 ⁻³	3.2·10 ⁻³	2.5·10 ⁻³	2.5·10 ⁻³
		FSETP	2.4·10 ⁻⁵	8.8·10 ⁻³	3.6·10 ⁻⁶	1.1·10 ⁻⁴	1.1·10 ⁻⁴
		MSETP	1.4·10 ⁻³	1.3·10 ⁻³	3.8·10 ⁻³	9.2·10 ⁻⁴	9.2·10 ⁻⁴
		TETP	4.3·10 ⁻⁶	3.9·10 ⁻⁶	6.5·10 ⁻⁷	2.5·10 ⁻⁴	2.5·10 ⁻⁴
		HTP	2.0	1.8	3.0·10 ⁻¹	2.4	1.3
Trichloromethane	67-66-3	FAETP	9.5·10 ⁻⁵	4.2·10 ⁻²	4.5·10 ⁻⁵	4.7·10 ⁻⁴	4.7·10 ⁻⁴
		MAETP	5.9·10 ⁻²	5.8·10 ⁻²	5.6·10 ⁻²	4.7·10 ⁻²	4.7·10 ⁻²
		FSETP	4.9·10 ⁻⁵	2.2·10 ⁻²	2.3·10 ⁻⁵	2.4·10 ⁻⁴	2.4·10 ⁻⁴
		MSETP	1.6·10 ⁻²	1.6·10 ⁻²	3.3·10 ⁻²	1.3·10 ⁻²	1.3·10 ⁻²
		TETP	4.0·10 ⁻⁵	3.9·10 ⁻⁵	1.9·10 ⁻⁵	1.6·10 ⁻³	1.6·10 ⁻³
		HTP	1.3·10 ¹	1.3·10 ¹	6.0	1.4·10 ¹	1.0·10 ¹

Substance Name	CAS No.	Type	Initial emission compartment				
			air	fresh water	sea water	agricult. soil	indust. soil
Halogenated non-aromatics							
Tetrachloro-methane	56-23-5	FAETP	2.5·10 ⁻⁴	2.1·10 ⁻¹	1.9·10 ⁻⁴	5.6·10 ⁻⁴	5.6·10 ⁻⁴
		MAETP	1.2	1.1	1.1	1.1	1.1
		FSETP	1.4·10 ⁻⁴	1.2·10 ⁻¹	1.1·10 ⁻⁴	3.2·10 ⁻⁴	3.2·10 ⁻⁴
		MSETP	3.1·10 ⁻¹	3.1·10 ⁻¹	4.6·10 ⁻¹	3.0·10 ⁻¹	3.0·10 ⁻¹
		TETP	4.7·10 ⁻⁴	4.7·10 ⁻⁴	3.6·10 ⁻⁴	2.1·10 ⁻³	2.1·10 ⁻³
		HTP	2.2·10 ²	2.2·10 ²	1.7·10 ²	2.2·10 ²	2.2·10 ²
1,2-Dichloro-ethane	107-6-2	FAETP	1.2·10 ⁻⁴	2.3·10 ⁻²	8.8·10 ⁻⁵	7.5·10 ⁻⁴	7.5·10 ⁻⁴
		MAETP	8.2·10 ⁻²	8.1·10 ⁻²	9.1·10 ⁻²	5.9·10 ⁻²	5.9·10 ⁻²
		FSETP	1.0·10 ⁻⁴	1.9·10 ⁻²	7.4·10 ⁻⁵	6.3·10 ⁻⁴	6.3·10 ⁻⁴
		MSETP	3.1·10 ⁻²	3.1·10 ⁻²	6.1·10 ⁻²	2.2·10 ⁻²	2.2·10 ⁻²
		TETP	2.6·10 ⁻⁵	2.6·10 ⁻⁵	2.0·10 ⁻⁵	1.7·10 ⁻³	1.7·10 ⁻³
		HTP	6.8	2.8·10 ¹	5.5	1.3·10 ³	5.7
1,1,1-Trichloro-ethane	71-55-6	FAETP	1.2·10 ⁻⁴	1.1·10 ⁻¹	7.1·10 ⁻⁵	3.7·10 ⁻⁴	3.7·10 ⁻⁴
		MAETP	3.0·10 ⁻¹	3.0·10 ⁻¹	2.7·10 ⁻¹	2.9·10 ⁻¹	2.9·10 ⁻¹
		FSETP	1.0·10 ⁻⁴	9.0·10 ⁻²	5.9·10 ⁻⁵	3.1·10 ⁻⁴	3.1·10 ⁻⁴
		MSETP	1.0·10 ⁻¹	1.0·10 ⁻¹	1.9·10 ⁻¹	9.6·10 ⁻²	9.6·10 ⁻²
		TETP	1.8·10 ⁻⁴	1.8·10 ⁻⁴	1.0·10 ⁻⁴	1.5·10 ⁻³	1.5·10 ⁻³
		HTP	1.6·10 ¹	1.6·10 ¹	9.6	1.6·10 ¹	1.6·10 ¹
Trichloroethylene	79-1-6	FAETP	3.8·10 ⁻⁵	9.7·10 ⁻²	1.6·10 ⁻⁵	4.6·10 ⁻⁴	4.6·10 ⁻⁴
		MAETP	2.7·10 ⁻³	3.3·10 ⁻³	5.7·10 ⁻²	2.5·10 ⁻³	2.5·10 ⁻³
		FSETP	3.2·10 ⁻⁵	8.2·10 ⁻²	1.3·10 ⁻⁵	3.9·10 ⁻⁴	3.9·10 ⁻⁴
		MSETP	1.7·10 ⁻³	2.7·10 ⁻³	8.1·10 ⁻²	1.5·10 ⁻³	1.5·10 ⁻³
		TETP	4.7·10 ⁻⁶	4.6·10 ⁻⁶	1.9·10 ⁻⁶	2.1·10 ⁻³	2.1·10 ⁻³
		HTP	3.4·10 ¹	3.3·10 ¹	1.4·10 ¹	3.2·10 ¹	3.2·10 ¹
Tetrachloro-ethylene	127-18-4	FAETP	4.1·10 ⁻⁴	7.0·10 ⁻¹	2.0·10 ⁻⁴	2.2·10 ⁻³	2.2·10 ⁻³
		MAETP	3.4·10 ⁻¹	3.4·10 ⁻¹	6.5·10 ⁻¹	3.1·10 ⁻¹	3.1·10 ⁻¹
		FSETP	3.9·10 ⁻⁴	6.7·10 ⁻¹	1.9·10 ⁻⁴	2.1·10 ⁻³	2.1·10 ⁻³
		MSETP	1.2·10 ⁻¹	1.3·10 ⁻¹	7.8·10 ⁻¹	1.1·10 ⁻¹	1.1·10 ⁻¹
		TETP	8.1·10 ⁻³	7.9·10 ⁻³	4.0·10 ⁻³	3.0·10 ⁻¹	3.0·10 ⁻¹
		HTP	5.5	5.7	2.8	6.4	5.2
Vinylchloride	75-1-4	FAETP	2.9·10 ⁻⁶	2.8·10 ⁻²	1.4·10 ⁻⁶	6.4·10 ⁻⁵	6.4·10 ⁻⁵
		MAETP	1.3·10 ⁻⁴	3.8·10 ⁻⁴	2.0·10 ⁻²	1.3·10 ⁻⁴	1.3·10 ⁻⁴
		FSETP	2.3·10 ⁻⁶	2.3·10 ⁻²	1.1·10 ⁻⁶	5.2·10 ⁻⁵	5.2·10 ⁻⁵
		MSETP	1.2·10 ⁻⁴	4.9·10 ⁻⁴	2.9·10 ⁻²	1.2·10 ⁻⁴	1.2·10 ⁻⁴
		TETP	2.6·10 ⁻⁷	2.6·10 ⁻⁷	1.3·10 ⁻⁷	3.1·10 ⁻⁴	3.1·10 ⁻⁴
		HTP	8.4·10 ¹	1.4·10 ²	4.3·10 ¹	5.2·10 ²	8.3·10 ¹
Hexachloro-1,3-butadiene	87-68-3	FAETP	4.6·10 ¹	4.5·10 ⁴	2.3·10 ¹	7.0·10 ¹	8.4·10 ¹
		MAETP	7.7·10 ⁴	7.5·10 ⁴	7.0·10 ⁴	2.8·10 ⁴	3.4·10 ⁴
		FSETP	5.4·10 ¹	5.2·10 ⁴	2.6·10 ¹	8.0·10 ¹	9.7·10 ¹
		MSETP	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

Substance Name	CAS No.	Type	Initial emission compartment				
			air	fresh water	sea water	agricult. soil	indust. soil
Halogenated aromatics							
Chlorobenzene	108-90-7	FAETP	4.7·10 ⁻⁴	3.6·10 ⁻¹	2.6·10 ⁻⁴	3.2·10 ⁻³	3.2·10 ⁻³
		MAETP	1.1·10 ⁻¹	1.1·10 ⁻¹	3.5·10 ⁻¹	8.3·10 ⁻²	8.3·10 ⁻²
		FSETP	4.4·10 ⁻⁴	3.4·10 ⁻¹	2.4·10 ⁻⁴	3.0·10 ⁻³	3.0·10 ⁻³
		MSETP	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
1,2-Dichloro- benzene	95-50-1	FAETP	2.9·10 ⁻³	1.0	1.3·10 ⁻³	1.9·10 ⁻²	1.9·10 ⁻²
		MAETP	6.7·10 ⁻¹	6.6·10 ⁻¹	9.5·10 ⁻¹	5.1·10 ⁻¹	5.1·10 ⁻¹
		FSETP	2.7·10 ⁻³	9.5·10 ⁻¹	1.2·10 ⁻³	1.8·10 ⁻²	1.8·10 ⁻²
		MSETP	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	
1,3-Dichloro- benzene	541-73-1	FAETP	2.4·10 ⁻³	1.2	1.1·10 ⁻³	1.8·10 ⁻²	1.8·10 ⁻²
		MAETP	4.6·10 ⁻¹	4.6·10 ⁻¹	1.0	3.7·10 ⁻¹	3.7·10 ⁻¹
		FSETP	2.2·10 ⁻³	1.2	1.0·10 ⁻³	1.6·10 ⁻²	1.6·10 ⁻²
		MSETP	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
1,4-Dichloro- benzene	106-46-7	FAETP	2.4·10 ⁻³	1.0	1.1·10 ⁻³	1.4·10 ⁻²	1.4·10 ⁻²
		MAETP	7.4·10 ⁻¹	7.3·10 ⁻¹	1.0	5.5·10 ⁻¹	5.5·10 ⁻¹
		FSETP	2.4·10 ⁻³	1.0	1.1·10 ⁻³	1.4·10 ⁻²	1.4·10 ⁻²
		MSETP	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
1,2,3-Trichloro- benzene	87-61-6	FAETP	8.5·10 ⁻³	4.0	3.9·10 ⁻³	2.3·10 ⁻²	3.0·10 ⁻²
		MAETP	2.1	2.1	3.6	6.5·10 ⁻¹	8.6·10 ⁻¹
		FSETP	9.3·10 ⁻³	4.4	4.3·10 ⁻³	2.5·10 ⁻²	3.3·10 ⁻²
		MSETP	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
1,2,4-Trichloro- benzene	120-82-1	FAETP	9.9·10 ⁻³	3.5	4.4·10 ⁻³	2.0·10 ⁻²	3.2·10 ⁻²
		MAETP	2.0	2.0	3.1	4.3·10 ⁻¹	7.1·10 ⁻¹
		FSETP	1.1·10 ⁻²	3.8	4.8·10 ⁻³	2.2·10 ⁻²	3.6·10 ⁻²
		MSETP	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
1,3,5-Trichloro- benzene	108-70-3	FAETP	1.6·10 ⁻²	5.0	7.0·10 ⁻³	5.4·10 ⁻²	6.6·10 ⁻²
		MAETP	3.0	3.0	4.5	1.1	1.3
		FSETP	1.7·10 ⁻²	5.2	7.2·10 ⁻³	5.6·10 ⁻²	6.9·10 ⁻²
		MSETP	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 Name	CAS No.	Type	Initial emission compartment				
			air	fresh water	sea water	agricult. soil	indust. soil
Halogenated aromatics							
1,2,3,4-Tetra-chlorobenzene	634-66-2	FAETP	1.0·10 ⁻¹	1.6·10 ¹	3.8·10 ⁻²	2.8·10 ⁻²	1.0·10 ⁻¹
		MAETP	1.7·10 ¹	1.6·10 ¹	1.5·10 ¹	3.9·10 ⁻¹	1.5
		FSETP	1.2·10 ⁻¹	1.9·10 ¹	4.5·10 ⁻²	3.2·10 ⁻²	1.2·10 ⁻¹
		MSETP	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
1,2,3,5-Tetra-chlorobenzene	634-90-2	FAETP	7.3·10 ⁻²	1.4·10 ¹	3.0·10 ⁻²	8.3·10 ⁻²	1.9·10 ⁻¹
		MAETP	1.8·10 ¹	1.7·10 ¹	1.6·10 ¹	2.3	5.1
		FSETP	8.1·10 ⁻²	1.6·10 ¹	3.3·10 ⁻²	9.3·10 ⁻²	2.1·10 ⁻¹
		MSETP	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
1,2,4,5-Tetra-chlorobenzene	95-94-3	FAETP	7.3·10 ⁻²	1.3·10 ¹	2.9·10 ⁻²	2.5·10 ⁻²	9.0·10 ⁻²
		MAETP	1.5·10 ¹	1.4·10 ¹	1.3·10 ¹	5.1·10 ⁻¹	1.8
		FSETP	8.5·10 ⁻²	1.5·10 ¹	3.3·10 ⁻²	2.9·10 ⁻²	1.0·10 ⁻¹
		MSETP	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
Penta-chlorobenzene	608-93-5	FAETP	3.7·10 ⁻¹	5.1·10 ¹	2.4·10 ⁻¹	5.9·10 ⁻¹	1.1
		MAETP	1.7·10 ²	1.7·10 ²	1.7·10 ²	2.8·10 ¹	5.4·10 ¹
		FSETP	5.2·10 ⁻¹	7.2·10 ¹	3.3·10 ⁻¹	8.3·10 ⁻¹	1.6
		MSETP	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
Hexachloro-benzene	118-74-1	FAETP	1.3	1.5·10 ²	1.1	3.2	4.3
		MAETP	2.4·10 ³	2.4·10 ³	2.4·10 ³	7.2·10 ²	9.6·10 ²
		FSETP	4.3	4.9·10 ²	3.6	1.0·10 ¹	1.4·10 ¹
		MSETP	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
2-Chlorophenol	95-57-8	FAETP	1.3·10 ¹	1.6·10 ³	6.7·10 ⁻³	7.9	3.1·10 ¹
		MAETP	1.2·10 ¹	1.3·10 ¹	4.6·10 ¹	6.8·10 ⁻²	2.6·10 ⁻¹
		FSETP	1.0·10 ¹	1.3·10 ³	5.3·10 ⁻³	6.3	2.4·10 ¹
		MSETP	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
2,4-Dichloro-phenol	120-83-2	FAETP	1.4	1.7·10 ²	2.9·10 ⁻⁴	2.5	9.2
		MAETP	1.3	2.5·10 ⁻¹	3.7	7.0·10 ⁻³	2.7·10 ⁻²
		FSETP	5.5·10 ⁻¹	6.8·10 ¹	1.1·10 ⁻⁴	1.0	3.6
		MSETP	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
2,4,5-Tri-chlorophenol	95-95-4	FAETP	1.5·10 ¹	1.6·10 ³	5.4·10 ⁻²	2.8·10 ¹	9.9·10 ¹
		MAETP	5.3·10 ¹	6.4·10 ¹	1.2·10 ²	1.3 4.6	
		FSETP	1.7·10 ¹	1.9·10 ³	6.4·10 ⁻²	3.3·10 ¹	1.2·10 ²
		MSETP	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	4.5·10 ¹	6.1·10 ⁻¹	5.3	2.9

Substance Name	CAS No.	Type	Initial emission compartment				
			air	fresh water	sea water	agricult. soil	indust. soil
Halogenated aromatics							
2,4,6-Tri-chlorophenol	88-6-2	FAETP	5.9	2.9·10 ²	2.4·10 ⁻⁴	1.2	4.8
		MAETP	3.9	1.6	7.6	8.2·10 ⁻³	3.2·10 ⁻²
		FSETP	5.7	2.9·10 ²	2.3·10 ⁻⁴	1.2	4.7
		MSETP	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
2,3,4,6-Tetra-chlorophenol	58-90-2	FAETP	8.0·10 ¹	5.2·10 ³	1.3·10 ⁻³	3.2·10 ¹	1.2·10 ²
		MAETP	1.3·10 ²	9.1·10 ¹	2.2·10 ²	6.2·10 ⁻¹	2.5
		FSETP	8.7·10 ¹	5.7·10 ³	1.4·10 ⁻³	3.5·10 ¹	1.3·10 ²
		MSETP	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
Penta-chlorophenol	87-86-5	FAETP	1.1·10 ¹	7.1·10 ²	1.2·10 ⁻⁵	3.3·10 ⁻¹	1.3
		MAETP	4.0·10 ¹	1.2·10 ¹	7.8·10 ¹	5.9·10 ⁻³	2.7·10 ⁻²
		FSETP	2.4·10 ¹	1.6·10 ³	2.7·10 ⁻⁵	7.4·10 ⁻¹	3.0
		MSETP	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
Benzylchloride	100-44-7	FAETP	7.6·10 ⁻¹	2.0·10 ²	1.1·10 ⁻²	9.2·10 ⁻¹	3.2
		MAETP	2.1	1.2	7.8	8.2·10 ⁻²	2.9·10 ⁻¹
		FSETP	1.1·10 ⁻¹	2.9·10 ¹	1.7·10 ⁻³	1.3·10 ⁻¹	4.7·10 ⁻¹
		MSETP	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
3-Chloroaniline	108-42-9	FAETP	1.0·10 ²	2.5·10 ³	3.7·10 ⁻⁶	7.4·10 ¹	2.5·10 ²
		MAETP	2.3·10 ¹	1.1·10 ¹	5.9·10 ¹	3.2·10 ⁻¹	1.2
		FSETP	9.3·10 ¹	2.3·10 ³	3.4·10 ⁻⁶	6.8·10 ¹	2.3·10 ²
		MSETP	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
4-Chloroaniline	106-47-8	FAETP	2.0	3.1·10 ³	1.1·10 ⁻²	1.7·10 ²	4.9·10 ²
		MAETP	1.7	1.4·10 ¹	9.6·10 ¹	7.7·10 ⁻¹	2.2
		FSETP	1.8	2.7·10 ³	9.7·10 ⁻³	1.5·10 ²	4.2·10 ²
		MSETP	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
3,4-Dichloro-aniline	95-76-1	FAETP	1.7·10 ³	1.9·10 ⁴	1.2·10 ⁻³	1.8·10 ³	4.0·10 ³
		MAETP	1.7·10 ³	2.8·10 ³	3.3·10 ³	2.7·10 ²	6.0·10 ²
		FSETP	2.1·10 ³	2.4·10 ⁴	1.5·10 ⁻³	2.3·10 ³	5.0·10 ³
		MSETP	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
1-Chloro-4-nitrobenzene	100-00-5	FAETP	1.1·10 ¹	8.6·10 ²	1.9	1.5·10 ²	1.5·10 ²
		MAETP	3.9·10 ²	3.7·10 ²	3.7·10 ²	1.2·10 ²	1.2·10 ²
		FSETP	1.0·10 ¹	7.7·10 ²	1.7	1.3·10 ²	1.3·10 ²
		MSETP	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 Name	CAS No.	Type	Initial emission compartment				
			air	fresh water	sea water	agricult. soil	indust. soil
Halogenated aromatics							
Pentachloro nitrobenzene	82-68-8	FAETP	4.7·10 ¹	4.0·10 ³	1.1·10 ¹	1.5·10 ¹	5.8·10 ¹
		MAETP	6.0·10 ³	2.8·10 ³	5.6·10 ³	3.0·10 ¹	1.2·10 ²
		FSETP	1.3·10 ¹	1.1·10 ³	3.1	4.3	1.7·10 ¹
		MSETP	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
2,3,7,8-TCDD	1746-1-6	FAETP	2.1·10 ⁶	1.7·10 ⁸	1.3·10 ⁵	1.2·10 ⁵	4.9·10 ⁵
		MAETP	3.0·10 ⁸	4.5·10 ⁷	5.0·10 ⁸	4.5·10 ⁴	1.8·10 ⁵
		FSETP	6.8·10 ⁶	5.6·10 ⁸	4.3·10 ⁵	4.0·10 ⁵	1.6·10 ⁶
		MSETP	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							
Acephate	30560-19-1	FAETP	7.9·10 ¹	1.1·10 ³	6.0·10 ⁻⁸	5.1·10 ¹	1.6·10 ²
		MAETP	1.9·10 ¹	1.5·10 ¹	3.7·10 ¹	6.7·10 ⁻¹	2.1
		FSETP	4.0·10 ¹	5.6·10 ²	3.1·10 ⁻⁸	2.6·10 ¹	8.1·10 ¹
		MSETP	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	5.3·10 ⁻¹⁰	1.7	1.3
		HTP	3.1	2.1	5.1·10 ⁻⁴	2.2·10 ¹	3.1·10 ⁻¹
Aldicarb	116-6-3	FAETP	5.1·10 ⁴	4.4·10 ⁵	1.2·10 ⁻¹	9.6·10 ⁴	9.6·10 ⁴
		MAETP	8.2·10 ³	7.4·10 ³	1.5·10 ⁴	1.6·10 ³	1.6·10 ³
		FSETP	4.1·10 ⁴	3.5·10 ⁵	9.8·10 ⁻²	7.6·10 ⁴	7.6·10 ⁴
		MSETP	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
Aldrin	309-00-2	FAETP	2.7	1.2·10 ⁴	1.3	2.8·10 ²	2.9·10 ²
		MAETP	6.1·10 ¹	2.1·10 ²	8.0·10 ³	3.2·10 ¹	3.3·10 ¹
		FSETP	2.4·10 ⁻¹	1.0·10 ³	1.1·10 ⁻¹	2.4·10 ¹	2.5·10 ¹
		MSETP	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
Anilazine	101-5-3	FAETP	1.4·10 ¹	1.1·10 ³	1.1·10 ⁻⁷	2.1·10 ⁻¹	8.6·10 ⁻¹
		MAETP	8.3	2.5·10 ⁻¹	2.0·10 ¹	5.0·10 ⁻⁵	2.0·10 ⁻⁴
		FSETP	8.8·10 ⁻¹	7.0·10 ¹	6.8·10 ⁻⁹	1.4·10 ⁻²	5.5·10 ⁻²
		MSETP	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
Atrazine	1912-24-9	FAETP	3.6·10 ²	5.0·10 ³	8.3·10 ⁻³	3.4·10 ²	9.3·10 ²
		MAETP	2.8·10 ²	4.8·10 ²	6.0·10 ²	3.4·10 ¹	9.1·10 ¹
		FSETP	3.1·10 ²	4.3·10 ³	7.2·10 ⁻³	3.0·10 ²	8.0·10 ²
		MSETP	3.1·10 ²	5.4·10 ²	6.6·10 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
Azinphos-ethyl	2642-71-9	FAETP	2.9·10 ²	2.7·10 ⁵	4.1·10 ⁻²	2.8·10 ³	3.7·10 ³
		MAETP	1.6·10 ²	1.0·10 ³	5.9·10 ³	1.1·10 ¹	1.4·10 ¹
		FSETP	2.1·10 ²	2.0·10 ⁵	3.0·10 ⁻²	2.0·10 ³	2.7·10 ³
		MSETP	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

Substance Name	CAS No.	Type	Initial emission compartment				
			air	fresh water	sea water	agricult. soil	indust. soil
Pesticides							
Azinphos-methyl	86-50-0	FAETP	4.2·10 ²	5.2·10 ⁴	1.1·10 ⁻⁴	1.9·10 ²	8.0·10 ²
		MAETP	2.0·10 ²	3.5·10 ¹	1.0·10 ³	1.4·10 ⁻¹	5.8·10 ⁻¹
		FSETP	2.2·10 ²	2.7·10 ⁴	5.6·10 ⁻⁵	1.0·10 ²	4.1·10 ²
		MSETP	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
Benomyl	17804-35-2	FAETP	3.0·10 ¹	6.8·10 ³	8.9·10 ⁻⁸	4.6	1.8·10 ¹
		MAETP	2.1·10 ¹	8.6	1.5·10 ²	5.8·10 ⁻³	2.3·10 ⁻²
		FSETP	3.9	8.8·10 ²	1.1·10 ⁻⁸	5.9·10 ⁻¹	2.4
		MSETP	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
Bentazone	25057-89-0	FAETP	5.6	5.1·10 ¹	7.4·10 ⁻⁹	8.3	1.1·10 ¹
		MAETP	6.2·10 ⁻¹	2.2·10 ⁻¹	1.2	3.6·10 ⁻²	4.8·10 ⁻²
		FSETP	4.5	4.1·10 ¹	6.0·10 ⁻⁹	6.7	8.8
		MSETP	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
Bifenthrin	82657-4-3	FAETP	8.2·10 ²	2.4·10 ⁵	5.5·10 ⁻²	1.0·10 ²	4.1·10 ²
		MAETP	1.0·10 ³	2.1·10 ²	8.9·10 ³	1.1·10 ⁻¹	4.5·10 ⁻¹
		FSETP	2.4·10 ³	7.2·10 ⁵	1.6·10 ⁻¹	3.1·10 ²	1.2·10 ³
		MSETP	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
Captafol	2425-6-1	FAETP	2.0·10 ⁴	5.4·10 ⁵	5.0·10 ⁻⁵	2.7·10 ⁴	8.3·10 ⁴
		MAETP	2.7·10 ⁴	8.0·10 ⁴	9.4·10 ⁴	4.0·10 ³	1.2·10 ⁴
		FSETP	3.0·10 ⁴	7.7·10 ⁵	7.3·10 ⁻⁵	3.9·10 ⁴	1.2·10 ⁵
		MSETP	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
Captan	133-06-2	FAETP	1.6·10 ¹	2.1·10 ³	6.5·10 ⁻⁷	4.0·10 ⁻¹	4.7
		MAETP	1.0·10 ¹	1.0·10 ⁻¹	4.0·10 ¹	6.9·10 ⁻⁵	8.1·10 ⁻⁴
		FSETP	1.4·10 ⁻¹	1.8·10 ¹	5.7·10 ⁻⁹	3.5·10 ⁻³	4.1·10 ⁻²
		MSETP	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
Carbaryl	63-25-2	FAETP	1.1·10 ²	4.5·10 ³	1.9·10 ⁻⁶	2.3·10 ¹	1.2·10 ²
		MAETP	1.2·10 ¹	1.4	2.4·10 ¹	7.4·10 ⁻³	4.0·10 ⁻²
		FSETP	3.2·10 ¹	1.3·10 ³	5.5·10 ⁻⁷	6.7	3.6·10 ¹
		MSETP	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
Carbendazim	10605-21-7	FAETP	3.0·10 ³	3.8·10 ⁴	2.4·10 ⁻⁸	2.0·10 ³	6.1·10 ³
		MAETP	7.2·10 ²	5.8·10 ²	1.3·10 ³	3.0·10 ¹	9.3·10 ¹
		FSETP	3.0·10 ³	3.9·10 ⁴	2.4·10 ⁻⁸	2.0·10 ³	6.2·10 ³
		MSETP	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

Substance Name	CAS No.	Type	Initial emission compartment				
			air	fresh water	sea water	agricult. soil	indust. soil
Pesticides							
Carbofuran	1563-66-2	FAETP	9.0·10 ²	1.3·10 ⁴	1.8·10 ⁻⁴	5.8·10 ²	1.8·10 ³
		MAETP	1.5·10 ²	4.4·10 ¹	3.0·10 ²	2.0	6.2
		FSETP	5.2·10 ²	7.6·10 ³	1.1·10 ⁻⁴	3.4·10 ²	1.1·10 ³
		MSETP	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
Chlordane	57-74-9	FAETP	2.7·10 ²	9.0·10 ⁴	3.1·10 ¹	9.4·10 ¹	3.7·10 ²
		MAETP	6.1·10 ⁴	8.9·10 ³	4.7·10 ⁵	3.0·10 ¹	1.2·10 ²
		FSETP	2.7·10 ¹	9.1·10 ³	3.2	9.5	3.8·10 ¹
		MSETP	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
Chlorfenvinphos	470-90-6	FAETP	3.2·10 ¹	1.1·10 ³	5.6·10 ⁻⁵	1.6·10 ¹	5.9·10 ¹
		MAETP	1.1·10 ¹	5.7	2.8·10 ¹	8.5·10 ⁻²	3.1·10 ⁻¹
		FSETP	2.7·10 ¹	9.4·10 ²	4.8·10 ⁻⁵	1.4·10 ¹	5.0·10 ¹
		MSETP	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
Chloridazon	1698-60-8	FAETP	2.6·10 ⁻²	3.1·10 ¹	3.5·10 ⁻³	1.8	3.9
		MAETP	2.2·10 ⁻¹	1.2	8.0	8.1·10 ⁻²	1.8·10 ⁻¹
		FSETP	2.0·10 ⁻²	2.5·10 ¹	2.7·10 ⁻³	1.4	3.1
		MSETP	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
Chlorothalonil	1897-45-6	FAETP	2.5	3.7·10 ²	1.4·10 ⁻¹	1.0	3.7
		MAETP	5.1·10 ¹	4.0·10 ¹	3.6·10 ¹	1.7	6.0
		FSETP	1.8	2.6·10 ²	9.5·10 ⁻²	7.3·10 ⁻¹	2.6
		MSETP	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
Chlorpropham	101-21-3	FAETP	2.3	8.3·10 ¹	2.8·10 ⁻⁵	1.8	6.4
		MAETP	6.4·10 ⁻¹	3.5·10 ⁻¹	2.0	8.4·10 ⁻³	3.0·10 ⁻²
		FSETP	2.0	7.1·10 ¹	2.4·10 ⁻⁵	1.6 5.5	
		MSETP	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
Chlorpyriphos	2921-88-2	FAETP	5.2·10 ²	6.4·10 ⁵	2.3·10 ⁻¹	3.6·10 ²	1.4·10 ³
		MAETP	6.2·10 ¹	2.4·10 ²	2.2·10 ³	1.4·10 ⁻¹	5.8·10 ⁻¹
		FSETP	3.3·10 ²	4.1·10 ⁵	1.5·10 ⁻¹	2.3·10 ²	9.3·10 ²
		MSETP	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
Coumaphos	56-72-4	FAETP	2.4·10 ⁵	2.0·10 ⁷	1.1·10 ²	1.0·10 ⁶	3.1·10 ⁶
		MAETP	3.4·10 ⁵	3.0·10 ⁶	3.6·10 ⁶	1.5·10 ⁵	4.6·10 ⁵
		FSETP	3.5·10 ⁵	2.9·10 ⁷	1.5·10 ²	1.5·10 ⁶	4.4·10 ⁶
		MSETP	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

Substance Name	CAS No.	Type	Initial emission compartment				
			air	fresh water	sea water	agricult. soil	indust. soil
Pesticides							
Cyanazine	21725-46-2	FAETP	1.9·10 ³	5.4·10 ⁴	2.5·10 ⁻⁶	8.1·10 ²	3.0·10 ³
		MAETP	6.3·10 ²	1.9·10 ²	1.3·10 ³	2.8	1.0·10 ¹
		FSETP	1.5·10 ³	4.3·10 ⁴	1.9·10 ⁻⁶	6.3·10 ²	2.3·10 ³
		MSETP	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
Cypermethrin	52315-7-8	FAETP	8.4·10 ⁴	7.9·10 ⁶	2.4	2.0·10 ⁵	6.9·10 ⁵
		MAETP	1.9·10 ⁴	1.0·10 ⁴	1.6·10 ⁵	3.0·10 ²	1.0·10 ³
		FSETP	1.5·10 ⁵	1.4·10 ⁷	4.3	3.6·10 ⁵	1.3·10 ⁶
		MSETP	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
Cyromazine	66215-27-8	FAETP	3.5·10 ³	2.6·10 ⁴	8.1·10 ⁻⁷	6.5·10 ³	6.5·10 ³
		MAETP	9.2·10 ²	1.0·10 ³	1.6·10 ³	2.5·10 ²	2.5·10 ²
		FSETP	2.8·10 ³	2.1·10 ⁴	6.5·10 ⁻⁷	5.2·10 ³	5.2·10 ³
		MSETP	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
2,4-D	94-75-7	FAETP	3.9·10 ¹	4.0·10 ²	1.1·10 ⁻¹⁰	2.9·10 ¹	8.2·10 ¹
		MAETP	5.3	2.3	1.0·10 ¹	1.7·10 ⁻¹	4.6·10 ⁻¹
		FSETP	2.9·10 ¹	3.0·10 ²	8.5·10 ⁻¹¹	2.2·10 ¹	6.1·10 ¹
		MSETP	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
DDT	50-29-3	FAETP	3.2·10 ²	2.9·10 ⁴	1.5·10 ¹	8.7·10 ¹	3.4·10 ²
		MAETP	8.6·10 ⁴	4.4·10 ³	1.9·10 ⁵	4.3·10 ¹	1.7·10 ²
		FSETP	3.5·10 ²	3.1·10 ⁴	1.6·10 ¹	9.4·10 ¹	3.7·10 ²
		MSETP	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
Deltamethrin	52918-63-5	FAETP	1.8·10 ³	6.5·10 ⁵	3.2	2.4·10 ¹	9.6·10 ¹
		MAETP	3.5·10 ³	9.8·10 ²	3.6·10 ⁴	6.0·10 ⁻²	2.4·10 ⁻¹
		FSETP	2.7·10 ³	9.8·10 ⁵	4.8	3.6·10 ¹	1.5·10 ²
		MSETP	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
Demeton	8065-48-3	FAETP	2.3·10 ¹	2.2·10 ⁴	1.7·10 ⁻²	8.0·10 ²	2.6·10 ³
		MAETP	9.1	9.6·10 ¹	5.5·10 ²	3.5	1.1·10 ¹
		FSETP	1.6·10 ¹	1.6·10 ⁴	1.2·10 ⁻²	5.7·10 ²	1.8·10 ³
		MSETP	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
Desmetryn	1014-69-3	FAETP	6.8	1.9·10 ²	4.1·10 ⁻⁶	3.0	1.1·10 ¹
		MAETP	2.6	1.5	5.4	2.4·10 ⁻²	8.8·10 ⁻²
		FSETP	4.1	1.2·10 ²	2.4·10 ⁻⁶	1.8	6.6
		MSETP	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

Substance Name	CAS No.	Type	Initial emission compartment				
			air	fresh water	sea water	agricult. soil	indust. soil
Pesticides							
Diazinon	333-41-5	FAETP	2.3·10 ²	1.1·10 ⁵	6.4·10 ⁻²	1.3·10 ³	4.6·10 ³
		MAETP	1.2·10 ²	6.4·10 ²	2.8·10 ³	7.8	2.7·10 ¹
		FSETP	1.6·10 ²	7.7·10 ⁴	4.6·10 ⁻²	9.3·10 ²	3.3·10 ³
		MSETP	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
		Dichlorprop	7547-66-2	FAETP	9.9·10 ⁻²	5.3	1.6·10 ⁻¹²
MAETP	6.2·10 ⁻²			1.5·10 ⁻²	1.2·10 ⁻¹	3.6·10 ⁻⁵	1.4·10 ⁻⁴
FSETP	5.3·10 ⁻²			2.8	8.3·10 ⁻¹³	6.9·10 ⁻³	2.7·10 ⁻²
MSETP	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
Dichlorvos	62-73-7			FAETP	5.1·10 ²	1.2·10 ⁵	1.1·10 ⁻²
		MAETP	4.1·10 ²	1.2·10 ¹	2.4·10 ³	4.1·10 ⁻²	1.6·10 ⁻¹
		FSETP	2.3·10 ¹	5.5·10 ³	5.1·10 ⁻⁴	3.3	1.3·10 ¹
		MSETP	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
		Dieldrin	60-57-1	FAETP	2.0·10 ²	7.9·10 ⁴	1.6·10 ¹
MAETP	5.2·10 ³			9.0·10 ³	5.9·10 ⁴	8.1·10 ¹	3.1·10 ²
FSETP	2.0·10 ¹			8.2·10 ³	1.7	6.3·10 ¹	2.4·10 ²
MSETP	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
Dimethoate	60-51-5			FAETP	1.3·10 ¹	1.7·10 ²	7.4·10 ⁻⁶
		MAETP	1.6	7.5·10 ⁻¹	3.4	3.9·10 ⁻²	1.2·10 ⁻¹
		FSETP	9.3	1.3·10 ²	5.5·10 ⁻⁶	6.6	2.0·10 ¹
		MSETP	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
		Dinoseb	88-85-7	FAETP	1.0·10 ⁴	3.2·10 ⁵	1.1·10 ⁻¹
MAETP	4.6·10 ³			5.9·10 ³	1.3·10 ⁴	3.9·10 ²	1.1·10 ³
FSETP	2.9·10 ³			8.8·10 ⁴	2.9·10 ⁻²	5.6·10 ³	1.6·10 ⁴
MSETP	1.5·10 ³			2.2·10 ³	5.0·10 ³	1.5·10 ²	4.3·10 ²
TETP	9.7·10 ¹			3.4·10 ⁻¹	1.0·10 ⁻³	5.9·10 ²	4.2·10 ²
HTP	3.6·10 ³			1.6·10 ²	6.3·10 ⁻¹	5.6·10 ²	9.7·10 ¹
Dinoterb	1420-7-1			FAETP	2.9·10 ³	2.3·10 ⁵	4.2·10 ⁻²
		MAETP	7.3·10 ³	5.4·10 ³	1.2·10 ⁴	8.7	3.6·10 ¹
		FSETP	1.3·10 ³	1.0·10 ⁵	1.9·10 ⁻²	1.5·10 ²	5.9·10 ²
		MSETP	2.1·10 ³	2.0·10 ³	4.5·10 ³	3.1	1.3·10 ¹
		TETP	3.4	1.3·10 ⁻²	5.1·10 ⁻⁵	9.9	9.9
		HTP	1.7·10 ²	2.5	2.9·10 ⁻³	3.6·10 ⁻¹	1.2·10 ⁻¹
		Disulfothon	298-4-4	FAETP	2.7·10 ¹	6.4·10 ⁴	1.3·10 ⁻²
MAETP	2.0·10 ¹			1.2·10 ²	1.5·10 ³	1.4·10 ⁻¹	5.6·10 ⁻¹
FSETP	9.2			2.2·10 ⁴	4.6·10 ⁻³	2.5·10 ¹	9.9·10 ¹
MSETP	5.7			3.5·10 ¹	4.2·10 ²	4.0·10 ⁻²	1.6·10 ⁻¹
TETP	4.3·10 ⁻²			1.2·10 ⁻³	2.1·10 ⁻⁵	1.1·10 ¹	1.1·10 ¹
HTP	2.9·10 ²			3.4·10 ²	1.5	1.7·10 ²	2.0

Substance Name	CAS No.	Type	Initial emission compartment				
			air	fresh water	sea water	agricult. soil	indust. soil
Pesticides							
Diuron	330-54-1	FAETP	5.3·10 ²	9.4·10 ³	1.9·10 ⁻³	3.5·10 ²	1.1·10 ³
		MAETP	1.1·10 ²	5.5·10 ¹	2.4·10 ²	2.1	6.8
		FSETP	5.0·10 ²	8.9·10 ³	1.8·10 ⁻³	3.3·10 ²	1.1·10 ³
		MSETP	1.6·10 ²	7.8·10 ¹	3.4·10 ²	3.0	9.8
		TETP	8.7	1.7·10 ⁻³	3.2·10 ⁻⁵	2.3·10 ¹	1.9·10 ¹
		HTP	2.1·10 ²	5.3·10 ¹	1.9·10 ⁻¹	1.3·10 ³	7.2
DNOC	534-51-1	FAETP	3.4	1.1·10 ²	2.1·10 ⁻⁸	1.2	4.5
		MAETP	1.3	3.4·10 ⁻¹	2.6	3.6·10 ⁻³	1.4·10 ⁻²
		FSETP	5.7·10 ⁻¹	1.9·10 ¹	3.6·10 ⁻⁹	2.0·10 ⁻¹	7.5·10 ⁻¹
		MSETP	3.0·10 ⁻¹	8.0·10 ⁻²	6.1·10 ⁻¹	8.5·10 ⁻⁴	3.3·10 ⁻³
		TETP	2.4·10 ⁻¹	8.5·10 ⁻⁷	1.5·10 ⁻⁹	5.2·10 ⁻¹	4.9·10 ⁻¹
		HTP	1.6·10 ²	5.9·10 ¹	1.5·10 ⁻³	2.8·10 ²	2.8
Endosulfan	115-29-7	FAETP	4.5·10 ¹	2.8·10 ⁴	2.1·10 ⁻²	2.2	9.0
		MAETP	1.9·10 ¹	1.1·10 ¹	3.2·10 ²	1.4·10 ⁻³	5.5·10 ⁻³
		FSETP	9.8	6.0·10 ³	4.5·10 ⁻³	4.8·10 ⁻¹	1.9
		MSETP	1.2	7.7·10 ⁻¹	2.2·10 ¹	9.0·10 ⁻⁵	3.6·10 ⁻⁴
		TETP	3.6·10 ⁻²	1.8·10 ⁻³	1.6·10 ⁻⁵	2.7	2.8
		HTP	6.7	1.7·10 ¹	4.2·10 ⁻²	2.6·10 ⁻¹	1.6·10 ⁻²
Endrin	72-20-8	FAETP	1.1·10 ³	7.0·10 ⁵	6.1	2.1·10 ⁴	7.1·10 ⁴
		MAETP	4.9·10 ⁴	3.4·10 ⁵	2.7·10 ⁶	1.0·10 ⁴	3.5·10 ⁴
		FSETP	3.4·10 ²	2.1·10 ⁵	1.9	6.4·10 ³	2.2·10 ⁴
		MSETP	3.5·10 ³	2.5·10 ⁴	2.0·10 ⁵	7.5·10 ²	2.5·10 ³
		TETP	4.9·10 ¹	3.5·10 ⁻¹	3.8·10 ⁻¹	4.2·10 ³	3.6·10 ³
		HTP	1.2·10 ³	6.0·10 ³	1.6·10 ³	8.4·10 ³	7.5·10 ²
Ethoprophos	13194-48-4	FAETP	2.4·10 ³	1.5·10 ⁵	1.0	1.1·10 ⁴	3.0·10 ⁴
		MAETP	7.1·10 ²	3.5·10 ³	6.6·10 ³	2.6·10 ²	7.2·10 ²
		FSETP	1.9·10 ³	1.2·10 ⁵	7.9·10 ⁻¹	8.8·10 ³	2.4·10 ⁴
		MSETP	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
Fenitrothion	122-14-5	FAETP	2.5·10 ³	2.4·10 ⁵	9.9·10 ⁻³	7.6·10 ²	3.0·10 ³
		MAETP	1.5·10 ³	6.7·10 ²	5.6·10 ³	2.3	8.9
		FSETP	1.4·10 ³	1.4·10 ⁵	5.5·10 ⁻³	4.2·10 ²	1.7·10 ³
		MSETP	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
Fentin acetate	900-95-8	FAETP	4.3·10 ³	2.7·10 ⁵	8.7·10 ⁻²	3.8·10 ²	1.5·10 ³
		MAETP	2.1·10 ⁴	3.2·10 ³	4.0·10 ⁴	6.8	2.7·10 ¹
		FSETP	6.9·10 ³	4.3·10 ⁵	1.4·10 ⁻¹	6.2·10 ²	2.5·10 ³
		MSETP	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
Fentin chloride	639-58-7	FAETP	1.8·10 ³	1.7·10 ⁵	1.8·10 ¹	2.5·10 ²	9.9·10 ²
		MAETP	4.7·10 ⁴	1.9·10 ⁴	4.0·10 ⁴	9.5·10 ¹	3.7·10 ²
		FSETP	3.0·10 ³	2.8·10 ⁵	2.9·10 ¹	4.1·10 ²	1.6·10 ³
		MSETP	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

Substance Name	CAS No.	Type	Initial emission compartment				
			air	fresh water	sea water	agricult. soil	indust. soil
Pesticides							
Fentin hydroxide	76-87-9	FAETP	4.2·10 ³	2.7·10 ⁵	2.9·10 ⁻²	3.8·10 ²	1.5·10 ³
		MAETP	2.0·10 ⁴	3.1·10 ³	4.0·10 ⁴	6.1	2.4·10 ¹
		FSETP	6.8·10 ³	4.3·10 ⁵	4.7·10 ⁻²	6.2·10 ²	2.5·10 ³
		MSETP	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
Fenthion	55-38-9	FAETP	2.5·10 ³	9.1·10 ⁵	2.6·10 ⁻¹	3.5·10 ³	1.4·10 ⁴
		MAETP	1.6·10 ³	3.6·10 ³	2.3·10 ⁴	1.5·10 ¹	5.7·10 ¹
		FSETP	1.8·10 ³	6.6·10 ⁵	1.9·10 ⁻¹	2.5·10 ³	9.9·10 ³
		MSETP	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
Folpet	133-7-3	FAETP	4.1·10 ²	8.2·10 ⁴	1.6·10 ¹	4.5·10 ³	1.3·10 ⁴
		MAETP	2.3·10 ³	1.2·10 ⁴	2.1·10 ⁴	7.1·10 ²	2.1·10 ³
		FSETP	5.6·10 ²	1.1·10 ⁵	2.2·10 ¹	6.2·10 ³	1.8·10 ⁴
		MSETP	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
Glyphosate	1071-83-6	FAETP	2.2·10 ¹	1.4·10 ³	2.1·10 ⁻¹¹	9.2·10 ⁻¹	3.7
		MAETP	1.7·10 ¹	4.2	3.3·10 ¹	2.8·10 ⁻³	1.1·10 ⁻²
		FSETP	2.1·10 ¹	1.3·10 ³	2.0·10 ⁻¹¹	9.0·10 ⁻¹	3.6
		MSETP	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
Heptachlor	76-44-8	FAETP	1.4	1.8·10 ⁴	3.9·10 ⁻²	2.3	8.9
		MAETP	2.9	1.2·10 ¹	1.1·10 ³	2.4·10 ⁻²	9.5·10 ⁻²
		FSETP	2.0	2.6·10 ⁴	5.5·10 ⁻²	3.2	1.3·10 ¹
		MSETP	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
Heptenophos	23560-59-0	FAETP	1.2·10 ²	2.2·10 ⁴	1.3·10 ⁻³	3.1·10 ¹	1.2·10 ²
		MAETP	7.8·10 ¹	1.1·10 ¹	4.5·10 ⁻²	2.6·10 ⁻²	1.0·10 ⁻¹
		FSETP	1.5·10 ¹	2.8·10 ³	1.7·10 ⁻⁴	3.8	1.5·10 ¹
		MSETP	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
Iprodione	36734-19-7	FAETP	2.8	1.6·10 ²	3.8·10 ⁻⁹	2.3·10 ⁻¹	1.9
		MAETP	3.2·10 ⁻¹	1.5·10 ⁻²	7.2·10 ⁻¹	2.2·10 ⁻⁵	1.8·10 ⁻⁴
		FSETP	2.3·10 ⁻¹	1.3·10 ¹	3.1·10 ⁻¹⁰	1.9·10 ⁻²	1.6·10 ⁻¹
		MSETP	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
Isoproturon	34123-59-6	FAETP	1.9·10 ²	1.9·10 ³	2.9·10 ⁻⁵	1.7·10 ²	4.0·10 ²
		MAETP	3.2·10 ¹	2.0·10 ¹	5.9·10 ¹	1.8	4.2
		FSETP	7.1·10 ¹	7.1·10 ²	1.1·10 ⁻⁵	6.3·10 ¹	1.5·10 ²
		MSETP	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

Substance Name	CAS No.	Type	Initial emission compartment				
			air	fresh water	sea water	agricult. soil	indust. soil
Pesticides							
Lindane	58-89-9	FAETP	5.2·10 ¹	6.5·10 ³	1.1·10 ⁻¹	9.7·10 ¹	3.7·10 ²
		MAETP	5.2·10 ¹	8.7·10 ¹	2.3·10 ²	1.4 5.3	
		FSETP	1.4·10 ¹	1.7·10 ³	3.0·10 ⁻²	2.5·10 ¹	9.7·10 ¹
		MSETP	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
Linuron	330-55-2	FAETP	4.0·10 ¹	3.1·10 ⁴	6.0·10 ⁻²	6.9·10 ²	2.4·10 ³
		MAETP	2.7·10 ¹	5.6·10 ²	1.3·10 ³	1.2·10 ¹	4.4·10 ¹
		FSETP	3.9·10 ¹	3.1·10 ⁴	6.0·10 ⁻²	6.9·10 ²	2.4·10 ³
		MSETP	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
Malathion	121-74-6	FAETP	1.8·10 ³	2.1·10 ⁵	1.8·10 ⁻²	1.6·10 ²	6.5·10 ²
		MAETP	1.4·10 ³	7.7·10 ²	5.1·10 ³	6.6·10 ⁻¹	2.6
		FSETP	1.1·10 ³	1.2·10 ⁵	1.1·10 ⁻²	9.5·10 ¹	3.8·10 ²
		MSETP	7.8·10 ²	4.3·10 ²	2.8·10 ³	3.7·10 ⁻¹	1.5
		TETP	2.0·10 ⁻²	1.1·10 ⁻⁵	2.0·10 ⁻⁷	7.6·10 ⁻²	7.5·10 ⁻²
		HTP	3.5·10 ⁻²	2.4·10 ⁻¹	8.4·10 ⁻⁴	2.6·10 ⁻²	9.5·10 ⁻⁴
MCPA	94-74-6	FAETP	1.1	2.7·10 ¹	5.3·10 ⁻¹³	4.6·10 ⁻¹	1.7
		MAETP	2.8·10 ⁻¹	3.6·10 ⁻²	5.6·10 ⁻¹	6.2·10 ⁻⁴	2.2·10 ⁻³
		FSETP	7.0·10 ⁻¹	1.8·10 ¹	3.6·10 ⁻¹³	3.1·10 ⁻¹	1.1
		MSETP	3.5·10 ⁻¹	4.4·10 ⁻²	6.9·10 ⁻¹	7.6·10 ⁻⁴	2.7·10 ⁻³
		TETP	4.3·10 ⁻²	1.4·10 ⁻¹¹	2.2·10 ⁻¹⁴	9.4·10 ⁻²	8.6·10 ⁻²
		HTP	1.5·10 ¹	1.5·10 ¹	3.7·10 ⁻²	1.0·10 ²	9.7·10 ⁻¹
Mecoprop	7085-19-0	FAETP	3.7·10 ¹	3.8·10 ²	3.8·10 ⁻¹⁰	3.0·10 ¹	7.8·10 ¹
		MAETP	4.1	6.7·10 ⁻¹	8.0	5.3·10 ⁻²	1.4·10 ⁻¹
		FSETP	2.5·10 ¹	2.5·10 ²	2.5·10 ⁻¹⁰	2.0·10 ¹	5.3·10 ¹
		MSETP	5.3	8.7·10 ⁻¹	1.1·10 ¹	6.9·10 ⁻²	1.8·10 ⁻¹
		TETP	1.8	1.1·10 ⁻⁸	1.8·10 ⁻¹¹	4.7	3.3
		HTP	1.2·10 ²	2.0·10 ²	8.4·10 ⁻¹	7.4·10 ²	4.2·10 ¹
Metamitron	41394-5-2	FAETP	9.3·10 ⁻¹	2.3·10 ¹	6.8·10 ⁻¹⁰	4.1·10 ⁻¹	1.5
		MAETP	2.5·10 ⁻¹	6.3·10 ⁻²	4.9·10 ⁻¹	1.1·10 ⁻³	4.1·10 ⁻³
		FSETP	4.9·10 ⁻¹	1.2·10 ¹	3.5·10 ⁻¹⁰	2.2·10 ⁻¹	7.9·10 ⁻¹
		MSETP	1.9·10 ⁻¹	5.0·10 ⁻²	3.8·10 ⁻¹	8.9·10 ⁻⁴	3.2·10 ⁻³
		TETP	1.9·10 ⁻²	8.5·10 ⁻¹⁰	1.4·10 ⁻¹¹	4.2·10 ⁻²	3.8·10 ⁻²
		HTP	8.8·10 ⁻¹	1.6·10 ⁻¹	3.2·10 ⁻⁵	6.5	1.2·10 ⁻²
Metazachlor	67129-8-2	FAETP	7.4	1.5·10 ²	3.0·10 ⁻⁶	3.9	1.4·10 ¹
		MAETP	2.2	1.3	4.4	3.3·10 ⁻²	1.1·10 ⁻¹
		FSETP	5.3	1.1·10 ²	2.2·10 ⁻⁶	2.8	9.8
		MSETP	2.6	1.5	5.2	3.9·10 ⁻²	1.4·10 ⁻¹
		TETP	7.4·10 ⁻²	1.4·10 ⁻⁶	3.0·10 ⁻⁸	1.7·10 ⁻¹	1.5·10 ⁻¹
		HTP	6.8	1.7	2.4·10 ⁻³	4.9·10 ¹	1.6·10 ⁻¹
Metha-benzthiazuron	18691-97-9	FAETP	7.0·10 ¹	1.1·10 ³	9.2·10 ⁻⁵	4.4·10 ¹	1.4·10 ²
		MAETP	2.5·10 ¹	2.5·10 ¹	4.8·10 ¹	1.0	3.2
		FSETP	7.6·10 ¹	1.2·10 ³	1.0·10 ⁻⁴	4.8·10 ¹	1.5·10 ²
		TETP	4.5·10 ⁻¹	2.0·10 ⁻⁵	6.0·10 ⁻⁷	1.1	8.8·10 ⁻¹
		HTP	7.1	2.6	8.2·10 ⁻³	5.1·10 ¹	3.6·10 ⁻¹

Substance Name	CAS No.	Type	Initial emission compartment				
			air	fresh water	sea water	agricult. soil	indust. soil
Pesticides							
Methomyl	16752-77-5	FAETP	1.4·10 ⁴	1.4·10 ⁵	8.5·10 ⁻³	1.4·10 ⁴	2.8·10 ⁴
		MAETP	3.9·10 ³	4.2·10 ³	6.9·10 ³	4.4·10 ²	8.9·10 ²
		FSETP	1.0·10 ⁴	1.0·10 ⁵	6.3·10 ⁻³	1.1·10 ⁴	2.1·10 ⁴
		MSETP	5.0·10 ³	5.4·10 ³	8.9·10 ³	5.7·10 ²	1.1·10 ³
		TETP	1.2·10 ²	2.2·10 ⁻³	7.5·10 ⁻⁵	3.0·10 ²	2.2·10 ²
		HTP	6.2	3.3	1.4·10 ⁻³	4.3·10 ¹	6.9·10 ⁻¹
		Methylbromide	74-83-9	FAETP	3.3·10 ⁻²	1.9·10 ¹	2.3·10 ⁻³
MAETP	4.1			3.5	2.4	3.1	3.1
FSETP	1.7·10 ⁻²			1.0·10 ¹	1.2·10 ⁻³	7.2·10 ⁻²	7.3·10 ⁻²
MSETP	1.1			9.6·10 ⁻¹	2.0	8.3·10 ⁻¹	8.3·10 ⁻¹
TETP	1.3·10 ⁻²			1.1·10 ⁻²	9.1·10 ⁻⁴	3.6·10 ⁻¹	3.7·10 ⁻¹
HTP	3.5·10 ²			3.0·10 ²	2.5·10 ¹	2.6·10 ²	2.6·10 ²
Metobromuron	3060-89-7			FAETP	4.9·10 ¹	4.3·10 ²	1.6·10 ⁻³
		MAETP	4.2·10 ¹	6.4·10 ¹	7.3·10 ¹	1.4·10 ¹	1.4·10 ¹
		FSETP	4.8·10 ¹	4.2·10 ²	1.6·10 ⁻³	9.2·10 ¹	9.2·10 ¹
		MSETP	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
		Metolachlor	51218-45-2	FAETP	1.5·10 ³	3.8·10 ⁴	7.0·10 ⁻²
MAETP	3.8·10 ²			5.8·10 ²	1.3·10 ³	3.0·10 ¹	9.1·10 ¹
FSETP	1.3·10 ³			3.4·10 ⁴	6.2·10 ⁻²	1.7·10 ³	5.2·10 ³
MSETP	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
Mevinphos	7786-34-7			FAETP	9.3·10 ³	5.9·10 ⁵	6.9·10 ⁻⁵
		MAETP	5.4·10 ³	5.7·10 ²	1.1·10 ⁴	3.4·10 ⁻¹	1.4
		FSETP	1.2·10 ³	7.4·10 ⁴	8.8·10 ⁻⁶	4.4·10 ¹	1.8·10 ²
		MSETP	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
		Oxamyl	23135-22-0	FAETP	5.6·10 ¹	6.5·10 ²	4.5·10 ⁻⁷
MAETP	1.4			1.8·10 ⁻¹	2.8	8.4·10 ⁻³	3.4·10 ⁻²
FSETP	2.5·10 ¹			3.0·10 ²	2.1·10 ⁻⁷	1.3·10 ¹	5.5·10 ¹
MSETP	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
Oxydemethon-methyl	301-12-2			FAETP	2.4·10 ³	7.0·10 ⁴	3.0·10 ⁻⁴
		MAETP	5.0·10 ²	1.4·10 ²	1.0·10 ³	2.0	7.3
		FSETP	5.3·10 ²	1.6·10 ⁴	6.8·10 ⁻⁵	2.2·10 ²	8.1·10 ²
		MSETP	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
		Parathion-ethyl	56-38-2	FAETP	2.8·10 ³	1.2·10 ⁶	2.0·10 ⁻¹
MAETP	3.1·10 ³			5.3·10 ³	4.1·10 ⁴	2.3	9.2
FSETP	1.9·10 ³			8.0·10 ⁵	1.4·10 ⁻¹	3.4·10 ²	1.3·10 ³
MSETP	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

Substance Name	CAS No.	Type	Initial emission compartment				
			air	fresh water	sea water	agricult. soil	indust. soil
Pesticides							
Parathion-methyl	298-00-0	FAETP	$9.9 \cdot 10^2$	$2.9 \cdot 10^5$	$1.2 \cdot 10^{-1}$	$1.1 \cdot 10^3$	$4.4 \cdot 10^3$
		MAETP	$7.2 \cdot 10^2$	$1.5 \cdot 10^3$	$8.1 \cdot 10^3$	5.9	$2.3 \cdot 10^1$
		FSETP	$6.0 \cdot 10^1$	$1.8 \cdot 10^4$	$7.4 \cdot 10^{-3}$	$6.8 \cdot 10^1$	$2.6 \cdot 10^2$
		MSETP	$3.0 \cdot 10^1$	$6.2 \cdot 10^1$	$3.4 \cdot 10^2$	$2.5 \cdot 10^{-1}$	$9.8 \cdot 10^{-1}$
		TETP	5.7	$3.4 \cdot 10^{-2}$	$7.1 \cdot 10^{-4}$	$8.1 \cdot 10^1$	$7.9 \cdot 10^1$
		HTP	$5.3 \cdot 10^1$	$1.0 \cdot 10^2$	$5.4 \cdot 10^{-1}$	$2.4 \cdot 10^1$	1.7
Permethrin	52645-53-1	FAETP	$1.6 \cdot 10^4$	$5.0 \cdot 10^6$	$1.0 \cdot 10^1$	$9.2 \cdot 10^2$	$3.7 \cdot 10^3$
		MAETP	$3.1 \cdot 10^4$	$2.7 \cdot 10^4$	$2.8 \cdot 10^5$	5.5	$2.2 \cdot 10^1$
		FSETP	$2.1 \cdot 10^4$	$6.7 \cdot 10^6$	$1.3 \cdot 10^1$	$1.2 \cdot 10^3$	$4.8 \cdot 10^3$
		MSETP	$2.3 \cdot 10^4$	$2.0 \cdot 10^4$	$2.2 \cdot 10^5$	4.2	$1.7 \cdot 10^1$
		TETP	$2.6 \cdot 10^1$	$3.9 \cdot 10^{-1}$	$1.7 \cdot 10^{-2}$	$2.5 \cdot 10^2$	$2.5 \cdot 10^2$
		HTP	$8.5 \cdot 10^{-1}$	$2.3 \cdot 10^1$	$2.6 \cdot 10^{-1}$	$1.1 \cdot 10^1$	$2.1 \cdot 10^{-2}$
Phoxim	14816-18-3	FAETP	$4.4 \cdot 10^{-1}$	$2.6 \cdot 10^3$	$3.3 \cdot 10^{-2}$	4.4	7.9
		MAETP	1.6	5.0	$3.0 \cdot 10^2$	$3.1 \cdot 10^{-1}$	$5.5 \cdot 10^{-1}$
		FSETP	$7.1 \cdot 10^{-2}$	$4.3 \cdot 10^2$	$5.4 \cdot 10^{-3}$	$7.2 \cdot 10^{-1}$	1.3
		MSETP	$2.1 \cdot 10^{-1}$	$6.7 \cdot 10^{-1}$	$4.1 \cdot 10^1$	$4.1 \cdot 10^{-2}$	$7.2 \cdot 10^{-2}$
		TETP	$1.7 \cdot 10^{-2}$	$1.5 \cdot 10^{-2}$	$1.3 \cdot 10^{-3}$	4.7	3.8
		HTP	$9.7 \cdot 10^{-1}$	$1.2 \cdot 10^1$	$2.9 \cdot 10^{-1}$	$2.5 \cdot 10^1$	$3.8 \cdot 10^{-1}$
Pirimicarb	23103-98-2	FAETP	$2.4 \cdot 10^3$	$3.6 \cdot 10^4$	$8.9 \cdot 10^{-4}$	$1.7 \cdot 10^3$	$5.2 \cdot 10^3$
		MAETP	$4.1 \cdot 10^2$	$1.6 \cdot 10^2$	$8.6 \cdot 10^2$	7.3	$2.3 \cdot 10^1$
		FSETP	$2.4 \cdot 10^3$	$3.6 \cdot 10^4$	$9.0 \cdot 10^{-4}$	$1.7 \cdot 10^3$	$5.3 \cdot 10^3$
		MSETP	$6.2 \cdot 10^2$	$2.4 \cdot 10^2$	$1.3 \cdot 10^3$	$1.1 \cdot 10^1$	$3.5 \cdot 10^1$
		TETP	$4.6 \cdot 10^1$	$9.3 \cdot 10^{-4}$	$1.7 \cdot 10^{-5}$	$1.2 \cdot 10^2$	$9.4 \cdot 10^1$
		HTP	3.4	1.7	$1.3 \cdot 10^{-3}$	$2.6 \cdot 10^1$	$2.9 \cdot 10^{-1}$
Propachlor	1918-16-7	FAETP	$2.0 \cdot 10^1$	$1.2 \cdot 10^3$	$5.0 \cdot 10^{-4}$	$1.7 \cdot 10^1$	$6.4 \cdot 10^1$
		MAETP	7.1	2.4	$2.7 \cdot 10^1$	$4.2 \cdot 10^{-2}$	$1.6 \cdot 10^{-1}$
		FSETP	$1.1 \cdot 10^1$	$6.7 \cdot 10^2$	$2.7 \cdot 10^{-4}$	9.4	$3.4 \cdot 10^1$
		MSETP	6.5	2.3	$2.5 \cdot 10^1$	$4.0 \cdot 10^{-2}$	$1.5 \cdot 10^{-1}$
		TETP	$5.4 \cdot 10^{-1}$	$8.1 \cdot 10^{-4}$	$1.3 \cdot 10^{-5}$	2.5	2.3
		HTP	$1.2 \cdot 10^1$	1.6	$2.6 \cdot 10^{-3}$	$1.5 \cdot 10^1$	$1.4 \cdot 10^{-1}$
Propoxur	114-26-1	FAETP	$2.5 \cdot 10^4$	$2.6 \cdot 10^5$	$1.2 \cdot 10^{-4}$	$2.0 \cdot 10^4$	$5.4 \cdot 10^4$
		MAETP	$1.8 \cdot 10^3$	$5.0 \cdot 10^2$	$3.4 \cdot 10^3$	$3.9 \cdot 10^1$	$1.0 \cdot 10^2$
		FSETP	$1.8 \cdot 10^4$	$1.8 \cdot 10^5$	$8.2 \cdot 10^{-5}$	$1.4 \cdot 10^4$	$3.8 \cdot 10^4$
		MSETP	$1.8 \cdot 10^3$	$5.2 \cdot 10^2$	$3.6 \cdot 10^3$	$4.0 \cdot 10^1$	$1.1 \cdot 10^2$
		TETP	$7.0 \cdot 10^2$	$3.1 \cdot 10^{-4}$	$3.2 \cdot 10^{-6}$	$1.8 \cdot 10^3$	$1.3 \cdot 10^3$
		HTP	$3.7 \cdot 10^1$	1.3	$3.9 \cdot 10^{-4}$	$2.7 \cdot 10^2$	$2.7 \cdot 10^{-1}$
Pyrazophos	13457-18-6	FAETP	$1.8 \cdot 10^2$	$4.9 \cdot 10^4$	$2.3 \cdot 10^{-3}$	$2.5 \cdot 10^2$	$9.9 \cdot 10^2$
		MAETP	$9.4 \cdot 10^1$	$1.2 \cdot 10^2$	$1.1 \cdot 10^3$	$6.8 \cdot 10^{-1}$	2.6
		FSETP	$1.7 \cdot 10^2$	$4.5 \cdot 10^4$	$2.0 \cdot 10^{-3}$	$2.3 \cdot 10^2$	$9.0 \cdot 10^2$
		MSETP	$8.9 \cdot 10^1$	$1.2 \cdot 10^2$	$1.1 \cdot 10^3$	$6.5 \cdot 10^{-1}$	2.5
		TETP	2.3	$1.7 \cdot 10^{-3}$	$2.9 \cdot 10^{-5}$	$3.0 \cdot 10^1$	$2.9 \cdot 10^1$
		HTP	$2.5 \cdot 10^1$	$5.3 \cdot 10^1$	$2.3 \cdot 10^{-1}$	$5.1 \cdot 10^1$	1.2
Simazine	122-34-9	FAETP	$2.1 \cdot 10^3$	$2.7 \cdot 10^4$	$4.5 \cdot 10^{-3}$	$2.3 \cdot 10^3$	$5.6 \cdot 10^3$
		MAETP	$2.8 \cdot 10^2$	$1.4 \cdot 10^2$	$6.7 \cdot 10^2$	$1.3 \cdot 10^1$	$3.1 \cdot 10^1$
		FSETP	$1.8 \cdot 10^3$	$2.3 \cdot 10^4$	$3.8 \cdot 10^{-3}$	$2.0 \cdot 10^3$	$4.8 \cdot 10^3$
		MSETP	$4.1 \cdot 10^2$	$2.1 \cdot 10^2$	$1.0 \cdot 10^3$	$1.9 \cdot 10^1$	$4.6 \cdot 10^1$
		TETP	8.8	$1.0 \cdot 10^{-3}$	$1.9 \cdot 10^{-5}$	$2.9 \cdot 10^1$	$2.1 \cdot 10^1$
		HTP	$3.3 \cdot 10^1$	9.7	$1.6 \cdot 10^{-2}$	$2.1 \cdot 10^2$	2.2

Substance Name	CAS No.	Type	Initial emission compartment				
			air	fresh water	sea water	agricult. soil	indust. soil
Pesticides							
2,4,5-T	93-76-5	FAETP	8.5·10 ⁻¹	1.7·10 ¹	1.7·10 ⁻¹⁰	4.4·10 ⁻¹	1.5
		MAETP	2.0·10 ⁻¹	6.1·10 ⁻²	4.0·10 ⁻¹	1.6·10 ⁻³	5.5·10 ⁻³
		FSETP	6.1·10 ⁻¹	1.2·10 ¹	1.2·10 ⁻¹⁰	3.2·10 ⁻¹	1.1
		MSETP	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
		Thiram	137-26-8	FAETP	2.7·10 ³	9.8·10 ⁴	2.6·10 ⁻²
MAETP	2.2·10 ²			7.4·10 ¹	4.2·10 ²	6.5·10 ⁻¹	4.2
FSETP	9.8·10 ²			3.5·10 ⁴	9.5·10 ⁻³	2.5·10 ²	1.6·10 ³
MSETP	1.8·10 ¹			6.6	3.7·10 ¹	5.7·10 ⁻²	3.6·10 ⁻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
Tolclophos-methyl	57018-4-9			FAETP	1.5·10 ⁻¹	5.0·10 ²	2.9·10 ⁻²
		MAETP	1.4	4.4	1.4·10 ²	1.3·10 ⁻¹	3.9·10 ⁻¹
		FSETP	1.6·10 ⁻¹	5.3·10 ²	3.1·10 ⁻²	3.3	9.9
		MSETP	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
		Tri-allaat	2303-17-5	FAETP	6.1·10 ¹	4.9·10 ⁴	1.1
MAETP	1.5·10 ²			7.8·10 ²	3.3·10 ³	8.4·10 ⁻¹	3.4
FSETP	2.2·10 ¹			1.7·10 ⁴	4.1·10 ⁻¹	1.8·10 ¹	7.0·10 ¹
MSETP	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
Triazophos	24017-47-8			FAETP	3.3·10 ³	1.7·10 ⁵	7.9·10 ⁻²
		MAETP	8.5·10 ²	1.5·10 ³	4.9·10 ³	5.3·10 ¹	1.7·10 ²
		FSETP	3.0·10 ³	1.6·10 ⁵	7.4·10 ⁻²	5.4·10 ³	1.8·10 ⁴
		MSETP	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
		Tributyltinoxide	56-35-9	FAETP	7.7·10 ³	4.5·10 ⁵	3.0
MAETP	3.1·10 ⁵			2.1·10 ⁵	5.7·10 ⁵	5.6·10 ²	2.2·10 ³
FSETP	1.0·10 ⁴			6.1·10 ⁵	4.1	1.5·10 ³	5.7·10 ³
MSETP	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
Trichlorfon	52-68-6			FAETP	1.3·10 ⁴	4.1·10 ⁵	5.3·10 ⁻⁶
		MAETP	1.8·10 ³	8.3·10 ¹	3.6·10 ³	6.7·10 ⁻¹	3.7
		FSETP	2.4·10 ³	7.6·10 ⁴	9.9·10 ⁻⁷	6.1·10 ²	3.4·10 ³
		MSETP	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
		Trifluarin	1582-9-8	FAETP	9.9	2.7·10 ⁴	1.8
MAETP	1.0·10 ²			4.2·10 ²	8.3·10 ³	1.2	4.5
FSETP	8.1			2.2·10 ⁴	1.4	3.3·10 ¹	1.3·10 ²
MSETP	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

Substance Name	CAS No.	Type	Initial emission compartment				
			air	fresh water	sea water	agricult. soil	indust. soil
Pesticides							
Zineb	12122-67-7	FAETP	$9.4 \cdot 10^2$	$2.8 \cdot 10^4$	$3.6 \cdot 10^{-3}$	$3.7 \cdot 10^2$	$1.4 \cdot 10^3$
		MAETP	$4.1 \cdot 10^2$	$2.5 \cdot 10^2$	$8.1 \cdot 10^2$	3.5	$1.3 \cdot 10^1$
		FSETP	$7.4 \cdot 10^2$	$2.2 \cdot 10^4$	$2.9 \cdot 10^{-3}$	$3.0 \cdot 10^2$	$1.1 \cdot 10^3$
		MSETP	$4.5 \cdot 10^2$	$2.7 \cdot 10^2$	$8.9 \cdot 10^2$	3.8	$1.4 \cdot 10^1$
		TETP	7.2	$1.3 \cdot 10^{-3}$	$2.8 \cdot 10^{-5}$	$1.6 \cdot 10^1$	$1.5 \cdot 10^1$
		HTP	4.8	1.7	$8.2 \cdot 10^{-4}$	$2.0 \cdot 10^1$	$1.0 \cdot 10^{-1}$

The toxicity potentials calculated with USES-LCA can be compared with the toxicity potentials previously calculated with USES 1.0 (Guinée *et al.*, 1996a). Distinction is made between:

- 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 according to the continental scale in USES-LCA, although air speed and water flow are still minimised to prevent substance flow across the system boundaries (Huijbregts, 1999a);
- USES-LCA, containing the toxicity potentials calculated by the adapted USES 2.0 model and using up-to-date substance-specific input data.

Table 3.3 compares the results of the toxicity potentials for 10 chemicals calculated with USES 1.0 OLD, USES 1.0 NEW and USES-LCA for the initial emission compartments air, fresh water, industrial soil and agricultural soil. Fresh water and marine sediment ecotoxicity potentials, marine aquatic toxicity potentials and toxicity potentials after emission to the continental seawater compartment are not included in the comparison, because USES 1.0 does not calculate RCRs for the sediment compartment and lacks a seawater compartment. Differences between USES 1.0 OLD and USES 1.0 NEW are typically several orders of magnitude. Comparison of toxicity potentials as calculated by USES-LCA with the USES 1.0 NEW toxicity potentials also gives differences up to several orders of magnitude.

Table 3.3 Toxicity potentials of 10 substances calculated with ‘USES 1.0 NEW’, ‘USES 1.0 OLD’ and USES-LCA for the initial emission compartments air, fresh water, agricultural soil and industrial soil.

Substance	Type	Air			Fresh water			Agricultural soil			Industrial soil		
		USES 1.0 OLD	USES 1.0 NEW	USES-LCA	USES 1.0 OLD	USES 1.0 NEW	USES-LCA	USES 1.0 OLD	USES 1.0 NEW	USES-LCA	USES 1.0 OLD	USES 1.0 NEW	USES-LCA
1,4-Dichloro-benzene	FAETP	0.01	0.04	0.002	1	1	1	0.0004	0.03	0.01	0.001	0.04	0.01
	TETP	8.5	1.0	0.01	5.1	1.0	0.01	2600	100	1.0	1	1	1
	HTP	1	1	1	0.7	1.3	1.1	0.1	1.9	2.9	0.1	1.0	0.7
Hexachloro-benzene	FAETP	4.3	19	1.3	160	160	150	3.3	7.3	3.2	3.9	13	4.3
	TETP	400000	450	0.3	310000	420	0.3	3100000	850	3.5	370000	310	3.0
	HTP	4400	84000000	3200000	7300	16000000	5600000	14000	12000000	33000000	4000	5700000	1300000
Pentachloro-phenol	FAETP	100	30	11	420	500	710	49	0.003	0.3	75	0.01	1.3
	TETP	2400000	350	2.3	2200000	13	0.0003	13000000	1700	4.8	1800000	0.1	4.8
	HTP	200	5400	5.1	200	220	7.2	250	0.7	0.2	150	1.9	0.04
2,3,7,8-TCDD	FAETP	7.2·10 ⁶	4.2·10 ⁶	2.1·10 ⁶	1.6·10 ⁶	1.4·10 ⁸	1.7·10 ⁸	1.6·10 ⁶	2.4·10 ²	1.2·10 ⁵	2.1·10 ⁶	9.4·10 ²	4.9·10 ⁵
	TETP	2.6·10 ⁸	1.6·10 ⁶	1.2·10 ⁴	6.5·10 ⁸	5.2·10 ⁴	5.9·10 ²	6.5·10 ⁸	6.0·10 ⁶	2.7·10 ⁴	5.1·10 ⁸	3.6·10 ²	2.7·10 ⁴
	HTP	2.6·10 ¹⁰	6.5·10 ¹⁰	1.9·10 ⁹	3.2·10 ⁹	4.2·10 ⁹	8.6·10 ⁸	6·10 ¹⁰	5.4·10 ⁸	1.3·10 ⁹	1.2·10 ¹⁰	1.4·10 ⁷	1.0·10 ⁷
Dichloromethane	FAETP	0.0004	0.01	0.00003	0.02	0.1	0.01	0.0004	0.001	0.0002	0.0004	0.01	0.0002
	TETP	0.08	0.01	0.000004	0.08	0.01	0.000004	7.2	0.5	0.0003	0.08	0.01	0.0003
	HTP	11	8.5	2.0	12	8.0	1.8	12	7.8	2.4	11	7.9	1.3
Atrazine	FAETP	92	280	360	360	11000	5000	50	0.2	340	73	0.8	930
	TETP	6900	370	2.0	6500	0.3	0.0008	190000	1600	6.6	5500	1.0	4.4
	HTP	920	20	4.5	890	50	4.6	790	8.6	21	730	0.06	0.9
Lindane	FAETP	2200	160	52	41000	9900	6500	23	0.7	97	68	2.4	370
	TETP	16000000	850	1.8	2800000	120	0.2	59000000	13000	23	490000	13	22
	HTP	6100	52	280	32000	540	120	2600	42	62	190	0.8	9.0
Lead	FAETP	1.2	0.5	2.4	40	17	9.6	4·10 ⁻⁹	6·10 ⁻¹¹	6.5	1·10 ⁻⁹	2·10 ⁻¹⁰	6.5
	TETP	11000	10	16	2·10 ⁻⁷	4·10 ⁻¹⁶	5·10 ⁻²¹	40000	39	33	0.0003	3·10 ⁻¹⁴	33
	HTP	67000	7.8	470	260	28	12	480	26	3300	0.0002	3·10 ⁻¹⁰	290
Benzo[a]pyrene	FAETP	320	300	88	10000	11000	250000	2.9	0.01	130	8.8	0.05	530
	TETP	64000000	2000	0.2	81000	1.0	0.003	230000000	8300	23	1800000	0.3	23
	HTP	3700	n.c	n.c	1700	n.c	n.c	11000	n.c	n.c	100	n.c	n.c
Benzene	FAETP	0.001	0.0005	0.00008	1.0	0.09	0.09	0.0001	0.0005	0.0007	0.0004	0.0005	0.0007
	TETP	0.06	0.0006	0.00002	0.04	0.0006	0.00001	53	53	0.2	0.02	0.0006	0.003
	HTP	29	1800	1900	22	1800	1800	5.2	5500	15000	9.4	1700	1600

Discussion

This discussion consists of two parts. In the first part, the differences between the toxicity potentials calculated with USES 1.0 OLD, USES 1.0 NEW and USES-LCA are discussed. In the second part, the validity of the toxicity potentials calculated with USES-LCA is discussed.

Comparison with previous toxicity potentials

Table 3.3 shows the results of the comparison of the three calculation procedures mentioned above. Differences up to several orders of magnitude between USES 1.0 NEW and USES 1.0 OLD are caused by a different selection of input data. The use of up-to-date substance-specific degradation rates and toxicity data in the USES 1.0 NEW calculations are the main causes of the differences found (Huijbregts, 1999a). The most important explanations for the differences found between toxicity potentials calculated by USES-LCA and the USES 1.0 NEW are discussed in more detail below (quantitative differences mentioned below are not presented separately in the results):

- 1 In USES-LCA a much larger part of the total area is covered with water than in USES 1.0. Within USES-LCA, emission to air will generally result in a relatively smaller flux of the emitted substance to the fresh water compartment and soil compartments compared to USES 1.0, resulting in smaller fresh water AETPs (up to 2 orders of magnitude) and smaller TETPs (up to 1 order of magnitude).
- 2 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). One side effect of this change is the very low mass flow of the chemical from the soil to the water compartment. In USES-LCA this artificial model change is not needed which results in larger AETPs after initial emissions to industrial soil and larger AETPs and HTPs after emissions to agricultural soil (up to 2 orders of magnitude for the selected organic substances and 9.5 orders of magnitude for Lead).
- 3 TETP-values are calculated very differently in USES-LCA compared to USES 1.0. In USES 1.0, TETPs are calculated by 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 all soil compartments into account. As a result, TETPs after initial emission to air, fresh water, agricultural soil are generally much lower in USES-LCA compared to USES 1.0 NEW (up to 3.5 orders of magnitude). In contrast, for initial emission to the industrial soil of extremely non-volatile substances the TETPs are much higher in USES-LCA compared to USES 1.0 (up to 3 orders of magnitude for the selected organic substances and 18 orders of magnitude for Lead).

- 4 Introduction of pH-dependency in the model calculations affects the toxicity potentials. Toxicity potentials of Pentachlorophenol are changed up to 3 orders of magnitude.
- 5 Human ingestion of soil affects the HTP of persistent substances after direct emission to industrial/urban soil. For example regarding Lead, the increase is 1.5 orders of magnitude.
- 6 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 1.5 orders of magnitude for HTPs after release to fresh water or seawater.
- 7 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 1.5 orders of magnitude for the HTPs of the 10 selected substances.

Validity of toxicity potentials

As has been shown in the model comparison, USES-LCA leads to substantial differences in toxicity potentials, compared to earlier estimates. An important question, however, is whether the outcomes of USES-LCA give a reliable approximation of reality. As already has been argued, it is expected that the structure of USES-LCA is closer to reality than USES 1.0, because artificial changes in environmental parameters are not needed in USES-LCA and additional model features, such as the inclusion of human ingestion of soil, are introduced in the model calculations. From this perspective it is expected that the results of USES-LCA are more realistic than the results of USES 1.0. However, as long as validation of multi-media fate model results is practically impossible (Ragas *et al.*, 1999), and toxicity potentials are not based on actual risks (Owens, 1997), fundamental uncertainties are large in USES-LCA. This should be subject of further research. Here, the validity of the new toxicity potentials is assessed tentatively by a critical discussion of the assumptions concerning the model structure, input data, and application in LCA case studies.

Model structure

One implicit assumption is that the model sufficiently covers all relevant compartments and environmental processes. However, a groundwater compartment is not implemented as a full compartment and a terrestrial vegetation compartment is not included. A preliminary assessment including a terrestrial vegetation compartment on the continental scale (Severinsen and Jager, 1997), however, indicates that terrestrial

vegetation does not have a large impact on the toxicity potentials (Huijbregts, 1999a). Furthermore, the global scale in USES-LCA is divided in three large zones and no differentiation within the types of soil and water compartments is implemented. Dividing the world in more boxes, as in the global distribution model developed by Wania and Mackay (1995), may improve the calculations to some extent. Moreover, USES-LCA does not take differences between seawater and fresh water uptake capacity into account. In particular, the inclusion of ionic strength effects on the adsorption of dissociating organic substances and metals will improve the current model structure (Johnson and Westhall, 1990; Bayens *et al.*, 1998).

Apart from the general model simplifications, USES-LCA may be less suitable to use for metals, chemicals that are transformed into stable or more toxic metabolites, and dissociating substances. Firstly, the use of USES-LCA for metals is debatable. No attempt is made to take metal speciation into account in the assessment. Furthermore, metal bioavailability may differ for calculated exposure levels and PNECs. In addition, the use of bioconcentration and bioaccumulation factors for metals, in particular essential metals, in the human exposure assessment may be invalid, because uptake is only partially related to the concentration in the environment (Chapman *et al.*, 1996). Chemicals that are transformed into stable or more toxic metabolites in the environment also form a problem. Although the fate and toxicity of these transformation products should be taken into account in the computation of the toxicity potentials, this is not possible in USES-LCA. A third group of substances, which is difficult to assess in USES-LCA, are dissociating substances, such as chlorophenols. In a first approximation, the apparent solubility K_{ow} and K_{oc} were estimated following Bockting *et al.* (1993) and Shiu *et al.* (1994), and uptake of dissociating pesticides by plants was estimated on the basis of results of Briggs *et al.* (1987). These approximations cause substantial uncertainty in the toxicity potentials of these substances.

LCA-specific alterations to USES 2.0 in the model structure may also have a significant impact on the validity of the model results. An important assumption in USES-LCA is that all life cycle emissions take place on the continental scale, which represents Western Europe. This is a gross simplification of reality because part of the emissions of many product life cycles takes place outside Western Europe. Another problem is that all emissions are assumed to be homogeneously distributed over Western Europe, impeding computation of region- or country-specific toxicity potentials. A spatially explicit fate model for Europe, recently developed by Klepper and Den Hollander (1999), may be used to calculate region-specific toxicity potentials. It should, however, be noted that the introduction of spatial differentiation requires spatially distributed emission estimates which are currently in most cases unavailable for LCA studies. Another arbitrary choice in the calculation of toxicity potentials is that aggregation of aquatic RCRs takes place on the basis of volumes of the compartments involved, and aggregation of terrestrial and sediment RCRs on the basis of compartment weights. Other weighting methods, for instance on the basis of species density per compartment, may result in different marine AETPs, marine SETPs, and TETPs.

Substance-specific data

Although much effort has been put in obtaining relevant input data for the model calculations, still a number of shortcomings can be noted. The effects assessment is seriously hampered by a lack of relevant data. The inhalatory HLVs used here are in most cases derived by applying route-to-route extrapolation, although this extrapolation procedure is not very reliable (Vermeire *et al.*, 1998). Due to a lack of ecotoxicity data about 50% of the terrestrial PNECs and 100% of the sediment PNECs were based on aquatic PNECs (Huijbregts, 1999a, b). Furthermore, as argued before, worst-case estimates should be avoided in the calculation of toxicity potentials. However, safety factors in the derivation of PNECs and HLVs may be considered as worst-case approaches (Emans *et al.*, 1993; ECETOC, 1995). Thus, in principle, PNECs and HLVs derived with safety factors should be replaced by realistic estimates. However, adjustment of these safety factors by more reasonable estimates was not considered as a feasible option in this work. Finally, 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. This problem is addressed for lead, atrazine and 2,3,7,8-TCDD in a separate paper (Huijbregts *et al.*, 2000b).

Application of toxicity potentials in LCAs

Although the current calculation of impact scores is relatively straightforward, it has some serious limitations. Firstly, it presumes that there is a single overall endpoint per impact category. This may be true for terrestrial ecotoxicity, sediment ecotoxicity and aquatic ecotoxicity, because only effect parameters that exclusively affect 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 simple weighting procedure for human toxicity does not fulfil the ISO requirements on life cycle impact assessment (ISO, 1998a). This limitation may be overcome by dividing human toxicity in several subcategories. Burke *et al.* (1996), for instance, proposed to divide substances causing human toxicity in three categories which are (1) irreversible effects, (2) reversible but life-threatening effects, and (3) reversible and not life-threatening effects. Expert-based weighting factors of these three impact categories for human toxicity are set to 100, 10 and 1, respectively. Aggregation may also be established with the concept of Disability Adjusted Life Years (DALYs), as described in detail by Hofstetter (1998). Other limitations concerning the application of toxicity potentials, such as the assumption of linearity between emissions and potential effects (Owens, 1997) and disregarding interactions between substances, are far more difficult

to deal with, because solving these limitations requires much more knowledge than currently available.

Conclusions

The use of the nested global multi-media fate, exposure and effects model USES-LCA has improved the calculation of toxicity potentials in comparison with previous research. Apart from the improved model structure, much effort was spent to prevent the use of estimation routines or worst-case default estimates for input data in the model calculations for 181 substances. Differences of several orders of magnitude were found between the new toxicity potentials and previously calculated ones. Although method and input data were both improved, uncertainties in the model structure of USES-LCA may still be large, as results have not been validated. Apart from validation, the following issues should be addressed in future research:

- Model improvements in USES-LCA, such as the inclusion of a ground water module, are needed;
- The simple compartment aggregation procedure on the basis of volumes for marine aquatic ecotoxicity and on the basis of mass' for marine sediment and terrestrial ecotoxicity, may be replaced by a more suitable aggregation procedure perhaps based on other compartment characteristics, such as species density;
- An uncertainty (importance) analysis should be performed to operationalise data uncertainty in the computation of toxicity potentials and to focus further research on parameters which contribute dominantly to the uncertainty in toxicity potentials.

Notes

USES-LCA is available in Excel[®] format and may be obtained via the corresponding author. Substance-specific data underlying the calculations can be found on webpage <http://www.leidenuniv.nl/interfac/cml/lca2/>

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§ 3.2 Parameter uncertainty and human variability

Toxicity potentials are standard values used in life cycle assessment (LCA) to enable a comparison of toxic impacts between substances. This paper presents the results of an uncertainty assessment of toxicity potentials that were calculated with the global nested multi-media fate, exposure and effects model USES-LCA. The variance in toxicity potentials resulting from input parameter uncertainties and human variability was quantified by means of Monte Carlo analysis with Latin Hypercube sampling. For Atrazine, 2,3,7,8-TCDD and Lead, variation, expressed by the ratio of the 97.5%-ile and the 2.5%-ile, ranges from about 1.5 to 6 orders of magnitude. The major part of this variation originates from a limited set of substance-specific input parameters, i.e. parameters that describe transport mechanisms, substance degradation, indirect exposure routes and no-effect concentrations. Considerable correlations were found between the toxicity potentials of one substance, in particular within one impact category. The uncertainties and correlations reported in the present study may have a significant impact on the outcome of LCA case studies.

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Introduction

Toxicity potentials are substance-specific, quantitative representations of potential impacts per unit emission of a toxic substance. In environmental life cycle assessments of products (LCAs), these potentials are used as weighting factors to determine the relative contribution of a substance to toxicity related impact categories, such as human toxicity. Huijbregts *et al.* (2000a) calculated toxicity potentials for 181 substances with the global nested multi-media fate, exposure and effects model USES-LCA, which is based on the Uniform System for the Evaluation of Substances 2.0 (USES 2.0), developed by RIVM *et al.* (1998). The calculation of toxicity potentials with USES-LCA is outlined by Huijbregts *et al.* (2000a).

Although the nested model structure of USES-LCA is better suited for the calculation of toxicity potentials previously used (Huijbregts *et al.*, 2000a), the calculated toxicity potentials may still suffer from large uncertainties. LCAs may give rise to incorrect decisions when uncertainty and variability are not properly accounted for (Huijbregts, 1998a, b). According to the ISO guidelines (ISO, 1997a, b, 1998a, b), an uncertainty analysis is obliged for an environmental comparison of products. However, it is unclear from these ISO guidelines how the uncertainty and variability in toxicity potentials should be assessed and how these uncertainty estimates should be implemented in LCA case studies.

Huijbregts *et al.* (2000a) show that toxicity potentials differ up to several orders of magnitude due to changes in model structure. This paper assesses the effect of parameter uncertainty and human variability on toxicity potentials, using Monte Carlo simulation. As an example, the results for the chemicals Atrazine, 2,3,7,8-TCDD and Lead are presented. Furthermore, uncertainty importance of parameters is assessed, identifying the parameters that introduce the largest spread in the toxicity potentials. Finally, the results of the uncertainty analysis are discussed including the possible implications for LCA case studies.

Analysis of uncertainty and variability

Model outcomes can be uncertain or variable for several reasons, which may have implications for the way the uncertainty or variability is dealt with (Huijbregts, 1998a; Ragas *et al.*, 1999). For this reason, it is important to distinguish between different types of uncertainty and variability, and to determine if and how each type of uncertainty or variability should be dealt with. Huijbregts (1998a) developed a general framework to account for uncertainty and variability in LCA. This framework distinguishes the following types of uncertainty and variability:

- 1 parameter uncertainty, such as a lack of knowledge about emission estimates per unit process or environmental degradation rates;
- 2 model uncertainty, such as the assumption of linear relationships in an LCA inventory analysis or the assumption that the boxes in the fate model of USES-LCA are physically and chemically homogeneous;
- 3 uncertainty due to choices, such as the choice between several allocation methods in

an LCA inventory analysis or the choice of weighting factors to sum RCRs of different scales in USES-LCA;

- 4 spatial variability, such as regional differences in emission estimates or the organic carbon content of the soil;
- 5 temporal variability, such as differences in yearly emission inventories or wind speed;
- 6 variability between subjects/sources, such as different characteristics between humans or different emissions between factories.

Huijbregts (1998a) concluded that in LCAs the quantification of (1) parameter uncertainty, (6) variability between objects/sources and in some cases (3) uncertainty due to choices might be feasible. In contrast, the feasibility of dealing with spatial and temporal variability is limited, because in LCAs spatial and temporal variability are not accounted for during the inventory analysis. The emissions of a certain substance, which usually take place at different times and places for the unit processes involved, are in practice summed up in the inventory. Consequently, it is impossible to match the spatial and temporal variability of the USES-LCA parameters, such as wind speed, with the inventory data.

USES-LCA has three types of input parameters:

- 1 substance-independent parameters, such as human characteristics (e.g. body weight and food intake rates) and environmental characteristics (e.g. area of the system and soil depth);
- 2 substance-specific parameters, such as physical and chemical parameters (e.g. degradation rates and octanol-water partitioning coefficient) and no-effect parameters (e.g. human limit values);
- 3 LCA-specific decision parameters, such as the specific weighting factors for the aggregation of impact-specific RCRs.

This assessment focuses on the quantification of parameter uncertainty in substance-specific parameters and variability in human characteristics.

The uncertainty propagation was performed by means of Monte Carlo analysis with Latin Hypercube sampling (LHS) in Crystal Ball™ 4.0e (Decisioneering Inc., 1998). LHS is referred to as 'stratified sampling' because the uncertainty distribution of each input parameter is divided into a specified number of intervals (*strata*), each with equal probability (McKay *et al.*, 1979; Iman and Conover, 1980). From each interval a value is selected randomly, following the specific distribution of that interval. In this way it is possible to obtain relatively easily a representative image of the complete parameter domain. Each LHS experiment consisted of 5.000 iterations which is assumed to produce a representative picture of the complete uncertainty distribution of the model outcome. Crystal Ball™ 4.0e is also equipped with a tool that calculates the uncertainty importance of each parameter. It calculates the Spearman rank correlation coefficient between each input parameter and each toxicity potential. If a parameter and a toxicity potential have a high correlation coefficient, this implies that the uncertainty in this parameter has a relatively large impact on the uncertainty in the toxicity potential. In the current assessment, the relative contribution of each uncertain parameter to the uncertainty of the toxicity potentials is approximated by the square value of the rank correlation coefficient r normalised to 100%.

To save time and money in collecting data for defining density distributions, only the most important parameters are to be considered in detail (Burmaster and Anderson, 1994; USEPA, 1997a). Those parameters were identified by a preliminary uncertainty importance analysis. In the preliminary analysis the uncertainty distributions of all parameters were estimated only roughly with the aim to determine what input parameters contribute most to the uncertainty of the output parameters. The parameters that appeared to contribute insignificantly to the output uncertainty were replaced by their most likely values. From the preliminary analysis it appeared that uncertainty in substance-specific input parameters from the reference substance will not contribute significantly to the uncertainty of LCA toxicity potentials (Thissen, 1999). Consequently, only substance-specific input parameters of the substances under study (Tables 3.4 to 3.6) and human characteristics (Table 3.7) were specified in more detail. Where QSAR-estimates were used to estimate substance-specific input data, the uncertainty distribution represents the uncertainty of the QSAR-estimate itself, for instance the uncertainty in the correlation between the biotransfer factor for milk (BAF_{milk}) and the octanol-water partition coefficient (K_{ow}). In the LHS, this uncertainty is combined with the uncertainty related to the primary parameter itself, such as the K_{ow} . For input parameters with only one or two values available, the geometric standard deviation (GSD) of the uncertainty distribution was assigned a default value. Default values were obtained from chemicals with more than two values available for these substance-specific input parameters. If data were available, dependencies between input parameters were considered, for instance between solubility and the octanol-water partition coefficient.

Predicted No Effect Concentrations (PNECs) were derived either using statistical extrapolation, assessment factors, or equilibrium partitioning, depending on the availability of toxicity data (Aldenberg and Slob, 1993; Crommentuijn *et al.*, 1997a, b; European Commission, 1996; FAO/WHO, 1993; Health Council of the Netherlands, 1996; Huijbregts, 1999a; Liem *et al.*, 1993; Slooff, 1992; USEPA, 1999). The extrapolation constant needed in the statistical extrapolation method of Aldenberg and Slob (1993) and the ecotoxicological assessment factors (Jager *et al.*, 1997) were considered uncertain in the ecotoxicological effects assessment. If necessary, Human Limit Values (HLVs) were derived with help of assessment factors (Health Council of the Netherlands, 1996; USEPA, 1999), in which the interspecies extrapolation factor from animals to humans was considered uncertain (Baird *et al.*, 1996; Health Council of the Netherlands, 1996; Vermeire *et al.*, 1998). Uncertainty in toxicity data was not taken into account, because the potential deviation of the No Observed Effect Concentration (NOEC) or the No Observed Adverse Effect Level (NOAEL) from the true threshold concentration or level cannot be quantified (Slob and Pieters, 1999).

To simplify the implementation of the uncertain toxicity potentials in LCA case studies, the sampled distributions were fitted to standard uncertainty distributions, such as Normal, Lognormal and Gamma distributions. The Anderson-Darling test was used as a measure of fit (Vose, 1996). As these uncertainty distributions are to be used in LCA case studies, it is vital to know the correlations between the toxicity potentials. The toxicity potentials of one

substance may be correlated, because they all stem from the same uncertain substance-specific parameters. Crystal Ball™ was used for the calculation of Spearman rank correlation coefficients between the toxicity potentials of each substance.

Table 3.4 Substance-specific input parameters for Atrazine. The numbers in *italic* were derived by QSAR-estimates, which are part of USES-LCA, whereas the other numbers are based on experimental data.

Parameter	Units	Distribution ^m	Reference
<i>Fate analysis</i>			
Octanol-water partition coefficient	m ³ .m ⁻³	L {347, 1.6}	a
Water solubility (25 °C) ⁿ	mg.l ⁻¹	L {35.2, 1.3}	a
Vapour pressure (25 °C) ^o	Pa	L {4.0.10 ⁻⁵ , 8.1}	a, b
Melting point	°C	U {171, 177}	a, b
Organic carbon-water partition coefficient ^p	m ³ .m ⁻³	L {155, 2.2}	c
Constant of Junge equation	Pa.m	L {0.4, 1.8}	a
Hydroxyl radical reaction rate in air	cm ³ .molec ⁻¹ . sec ⁻¹	L {1.5.10 ⁻¹⁰ , 1.4}	a, d
Half-life in water	d	L {700, 1.8}	a
Half-life in soil	d	L {70, 1.8}	a
Half-life in aerobic sediment	d	L {70, 1.8}	a
Half-life in anaerobic sediment	d	L {280, 3.2}	a, e
<i>Exposure assessment</i>			
Fish bioconcentration factor	l.kg ⁻¹	L {8.3, 3.9}	a
Leaf - air partition coefficient	m ³ .m ⁻³	L {6.4.10 ⁷ , 2.8}	f
Plant conductance	-	T {1.10 ⁻⁴ , 1.2.10 ⁻³ , 5.10 ⁻³ }	g
Root - pore water concentration factor	l.kg _{swwt} ⁻¹	L {1.9, 1.6}	h
Leaf - soil concentration factor	kg _{swwt} .kg _{swwt} ⁻¹	L {0.26, 1.4}	i
Biotransfer factor for milk	d.kg _{food} ⁻¹	L {7.9.10 ⁻⁶ , 6.2}	b, j
Biotransfer factor for meat	d.kg _{food} ⁻¹	L {8.7.10 ⁻⁶ , 8.4}	b, j
Purification factor for drinking water	-	T {0, 0.15, 0.65}	b
Respirable fraction of inhaled substance	-	U {0, 1}	b
Bioavailability for human inhalation	-	U {0, 0.75}	b
Bioavailability for human oral uptake	-	U {0, 1}	b
<i>Effects assessment</i>			
Interspecies assessment factor (rat - human)	-	L {4, 6}	k
Statistical extrapolation constant for the aquatic PNEC	-	L {1.68, 1.3}	l
Statistical extrapolation constant for the terrestrial species PNEC	-	L {1.75, 1.4}	l
Statistical extrapolation constant for the terrestrial processes PNEC	-	L {1.92, 1.9}	l
Acute LC50 to chronic NOEC assessment factor for ecotoxicological input data	-	L {5, 3.2}	b

^a Mackay *et al.* (1997); ^b Jager *et al.* (1997); ^c Bockting *et al.* (1993); ^d Atkinson (1988); ^e Howard *et al.* (1991); ^f Polder *et al.* (1998); ^g Riederer (1995); ^h Polder *et al.* (1995); ⁱ Dowdy and McKone (1997); ^j Travis and Arms (1988); ^k Vermeire *et al.* (1998); ^l Aldenberg and Slob (1993); ^m L = lognormal distribution (geometric mean and geometric standard deviation between brackets); U = uniform distribution (minimum and maximum values between brackets); T = triangular distribution (minimum, most likely and maximum values between brackets); ⁿ Water solubility was correlated with the octanol-water partition coefficient with a correlation coefficient of -0.96 on log-scale (Jager *et al.*, 1997); ^o Vapour pressure was correlated with the octanol-water partition coefficient with a correlation coefficient of -0.87 on log-scale (Jager *et al.* 1997); ^p The organic carbon-water partition coefficient was correlated with the octanol-water partition coefficient with a correlation coefficient of 0.83 on log-scale (personal assessment).

Table 3.5 Substance-specific input parameters for 2,3,7,8-TCDD.

Parameter	Units	Distribution ^r	Reference
<i>Fate analysis</i>			
Octanol-water partition coefficient	m ³ .m ⁻³	L {8.1·10 ⁶ , 1.5}	a
Water solubility (25 °C) ^s	mg.l ⁻¹	L {4.1·10 ⁻⁵ , 4.2}	a
Vapour pressure (25 °C) ^t	Pa	L {2.7·10 ⁻⁷ , 8.1}	a, b, c
Melting point	°C	U {302, 307}	a, b, c
Organic carbon-water partition coefficient ^u	m ³ .m ⁻³	L {2.9·10 ⁶ , 3.1}	a
Constant of Junge equation	Pa.m	L {0.4, 1.8}	b
Hydroxyl radical reaction rate in air (-10 °C)	cm ³ .molec ⁻¹ . sec ⁻¹	L {4.0·10 ⁻¹³ , 1.4}	d, e
Hydroxyl radical reaction rate in air (12 °C)	cm ³ .molec ⁻¹ . sec ⁻¹	L {6.6·10 ⁻¹³ , 1.4}	d, e
Hydroxyl radical reaction rate in air (25 °C)	cm ³ .molec ⁻¹ . sec ⁻¹	L {8.6·10 ⁻¹³ , 1.4}	d, e
Half-life in water	d	L {620, 1.5}	a, f
Half-life in soil	d	L {3200, 3.4}	a
Half-life in aerobic sediment	d	L {620, 1.5}	a, f
Half-life in anaerobic sediment	d	L {1750, 1.8}	a, f
<i>Exposure assessment</i>			
Fish bioconcentration factor	l.kg ⁻¹	L {12300, 2.5}	a
Leaf – air partition coefficient	m ³ .m ⁻³	L {3.2·10 ⁷ , 1.8}	g, h
Plant conductance	-	T {1·10 ⁻⁴ , 1.0·10 ⁻³ , 5·10 ⁻³ }	i, j
Photodegradation upon plant tissue	d	L {6.2, 10.5}	h, j
Root – pore water concentration factor	l.kg _{wwt} ⁻¹	L {780, 1.6}	k
Leaf – soil concentration factor	kg _{wwt} .kg _{wwt} ⁻¹	L {2.7·10 ⁻² , 2.8}	l
Biotransfer factor for milk	d.kg _{food} ⁻¹	L {8.0·10 ⁻³ , 1.1}	m
Biotransfer factor for meat	d.kg _{food} ⁻¹	L {0.11, 1.7}	m
Purification factor for drinking water	-	T {0, 0.15, 0.65}	b
Respirable fraction of inhaled substance	-	U {0, 1}	b
Bioavailability for human inhalation	-	U {0, 0.75}	b
Bioavailability for human oral uptake	-	T {0, 0.5, 1}	b, n
<i>Effects assessment</i>			
Interspecies assessment factor (monkey – human)	-	L {2.2, 1.5}	o, p
Extrapolation factor to the most sensitive species for ecotoxicological input data ^v	-	1 + L {6.3, 5.0}	b
Lab to field assessment factor for ecotoxicological input data	-	L {1, 3.3}	b, q

^a McKone *et al.* (1995); ^b Jager *et al.* (1997); ^c Mackay *et al.* (1992); ^d Atkinson (1988); ^e Brubaker and Hites (1997); ^f Howard *et al.* (1991); ^g Polder *et al.* (1998); ^h McGrady and Maggard (1993); ⁱ Riederer (1995); ^j Trapp and Matthies (1995); ^k Polder *et al.* (1995); ^l Dowdy and McKone (1997); ^m Dowdy *et al.* (1996); ⁿ WHO (1989); ^o Health Council of the Netherlands (1996); ^p Baird *et al.* (1996); ^q Emans *et al.* (1993); ^r L = lognormal distribution (geometric mean and geometric standard deviation between brackets); U = uniform distribution (minimum and maximum values between brackets); T = triangular distribution (minimum, most likely and maximum values between brackets); ^s Water solubility was correlated with the octanol-water partition coefficient with a correlation coefficient of -0.96 on log-scale (Jager *et al.*, 1997); ^t Vapour pressure was correlated with the octanol-water partition coefficient with a correlation coefficient of -0.87 on log-scale (Jager *et al.*, 1997); ^u The organic carbon-water partition coefficient was correlated with the octanol-water partition coefficient with a correlation coefficient of 0.83 on log-scale (personal assessment); ^v Because the extrapolation factor to the most sensitive species can never be smaller than 1, the assessment factor minus 1 is taken as lognormally distributed.

Table 3.6 Substance-specific input parameters for Lead.

Parameter	Units	Distribution ^m	Reference
<i>Fate analysis</i>			
Melting point	°C	U {324-330}	a, b
Solid-water partition coefficient in soils	L.kg ⁻¹	L {4.3·10 ³ , 2.5}	c, d
Solid-water partition coefficient in sediments	L.kg ⁻¹	L {1.4·10 ⁵ , 2.5}	e, f
Solid-water partition coefficient in suspended matter	L.kg ⁻¹	L {4.7·10 ⁵ , 2.0}	c, e
Aerosol collection efficiency	-	T {5·10 ⁴ , 1·10 ⁵ , 2·10 ⁵ }	g
Fraction of aerosol bounded substance	-	T {0.9, 0.95, 1}	g
<i>Exposure assessment</i>			
Fish bioconcentration factor	L.kg ⁻¹	L {500, 3.2}	h
Root - soil concentration factor	kg _{swt} .kg _{swt} ⁻¹	T{2·10 ⁻³ , 6·10 ⁻³ , 1·10 ⁻¹ }	i
Leaf - soil concentration factor	kg _{swt} .kg _{swt} ⁻¹	T{1.2·10 ⁻⁵ , 1.2·10 ⁻⁴ , 1.2·10 ⁻² }	i
Biotransfer factor for milk	d.kg _{food} ⁻¹	T{1.4·10 ⁻⁴ , 2.6·10 ⁻⁴ , 4.5·10 ⁻⁴ }	j
Biotransfer factor for meat	d.kg _{food} ⁻¹	T{2·10 ⁻⁴ , 1·10 ⁻³ , 2·10 ⁻³ }	j
Purification factor for drinking water	-	T {0, 0.15, 0.65}	b
Respirable fraction of inhaled substance	-	U {0, 1}	b
Bioavailability for human inhalation	-	T {0.2, 0.5, 0.62}	k
Bioavailability for human oral uptake	-	T {0.01, 0.1, 0.14}	k
<i>Effects assessment</i>			
Statistical extrapolation constant for the aquatic PNEC	-	L {1.66, 1.2}	l
Statistical extrapolation constant for the terrestrial species PNEC	-	L {1.73, 1.4}	l
Statistical extrapolation constant for the terrestrial processes PNEC	-	L {1.66, 1.2}	l

^a West (1985); ^b Jager *et al.* (1997); ^c Bockting *et al.* (1992); ^d De Groot *et al.* (1998); ^e Van den Hoop and Crommentuijn (1998); ^f Mahony *et al.* (1996); ^g Crommentuijn *et al.* (1997a); ^h Mennes *et al.* (1998); ⁱ Bockting and Van den Berg (1992); ^j Ng (1982); ^k Owen (1990); ^l Aldenberg and Slob (1993); ^m L = lognormal distribution (geometric mean and geometric standard deviation between brackets); U = uniform distribution (minimum and maximum values between brackets); T = triangular distribution (minimum, most likely and maximum values between brackets).

Table 3.7 Human characteristics.

Parameter name	Unit	Distribution ^d	Reference
Daily intake of drinking water	m ³ .d ⁻¹	L {1.4·10 ⁻² , 1.2}	a, b
Daily intake of fish	kg _{swt} .d ⁻¹	L {1.3·10 ⁻² , 3.6}	a, b, c
Daily intake of leaf crops (incl. fruit and cereals)	kg _{swt} .d ⁻¹	L {7.6·10 ⁻¹ , 1.2}	a, b, c
Daily intake of root crops	kg _{swt} .d ⁻¹	L {1.8·10 ⁻¹ , 1.2}	a, b, c
Daily intake of meat	kg.d ⁻¹	L {2.6·10 ⁻¹ , 1.2}	a, b, c
Daily intake of dairy products	kg.d ⁻¹	L {2.8·10 ⁻¹ , 1.2}	a, b, c
Daily intake of soil particles	kg _{swt} .d ⁻¹	L {5.0·10 ⁻⁵ , 4.6}	a, b
Inhalation rate	m ³ .d ⁻¹	L {13, 1.2}	a, b
Body weight	kg	L {61, 1.2}	a, b

^a Huijbregts *et al.* (2000a); ^b USEPA (1997b); ^c ECETOC (1994); ^d L = lognormal distribution (geometric mean and geometric standard deviation between brackets)

Results

For each substance, 30 frequency plots were produced, representing the uncertainty distributions of the 30 toxicity potentials. It turned out that a lognormal distribution fits best the uncertainty distributions of the majority of the toxicity potentials. Table 3.8 lists some statistical characteristics of the uncertainty distributions. The uncertainty in the toxicity potentials of the three substances, defined as the ratio of the 97.5th and 2.5th percentile, ranges from about 1.5 to 6 orders of magnitude. Ecotoxicity potentials of 2,3,7,8-TCDD show the largest uncertainty, together with the Aquatic and Sediment Ecotoxicity Potentials for the fresh water environment (FAETP and FSETP) after release to seawater and the Terrestrial EcoToxicity Potentials (TETP) of Atrazine (3.5 to 6 orders of magnitude). Uncertainty in the other AETPs and SETPs of Atrazine and the ecotoxicity potentials of Lead varies from about 1.5 to 2.5 orders of magnitude. The uncertainty in Human Toxicity Potentials (HTP) ranges from 1.5 to 4.5 orders of magnitude. Table 3.8 also indicates that for every substance the uncertainty in TETPs is much lower after emission to air, agricultural soil or industrial soil in comparison to the uncertainty after emission to fresh water or seawater. Furthermore, the uncertainty in the marine and fresh water AETPs and SETPs, except for the fresh water AETPs and SETPs after release to seawater, tend to be lower after initial emission to air, fresh water or seawater than after emission to agricultural soil or industrial soil. Finally, for each substance the uncertainty in HTPs after emission to sea water and industrial soil is generally higher compared to the HTPs after emission to air, surface water or agricultural soil.

SETPs and AETPs of Atrazine generally show high correlations (≥ 0.6). Furthermore, TETPs of Atrazine are correlated, which is also true for the HTPs (≥ 0.7). For 2,3,7,8-TCDD high correlations exist between all ecotoxicity potentials (≥ 0.8). Moreover, correlations between HTPs after emission to fresh water and seawater are high, just as the correlations between the HTP after emission to air and the other HTPs of 2,3,7,8-TCDD. For Lead, high correlations are found between toxicity potentials within each ecotoxicological impact category (≥ 0.7). In addition, fresh water and marine AETPs are highly correlated for Lead, which is also the case for the fresh water and marine SETPs (≥ 0.8). Finally, correlations between HTPs after emission to fresh water and seawater and correlations between HTPs after emission to air and agricultural soil are high for Lead (≥ 0.9).

The results of the uncertainty importance analysis are listed in Tables 3.9 to 3.11. They show the relative contribution of each uncertain parameter to the uncertainty of the toxicity potentials. In all cases, more than 95% of the variance is caused by a limited set of parameters. As can be seen in Tables 3.9 to 3.11, parameters involved in describing chemical transport, degradation in water and soil, and defining the uncertainty in the no-effect levels, are dominant sources of uncertainty. Furthermore, substance-specific parameters used to define indirect human exposure routes, such as fish bioconcentration factors, may cause a significant spread in the HTPs. Finally, the spread in HTPs after emission to fresh water and seawater is partly caused by variation in daily fish intake, and the variation in daily soil particle intake influences the HTP after emission to industrial soils to a large extent.

Substance	TP	Air			Fresh air			Seawater			Agricultural soil			Industrial soil		
		GM	GSD	UF	GM	GSD	UF	GM	GSD	UF	GM	GSD	UF	GM	GSD	UF
Atrazine	A _{fw}	2.9·10 ²	2.6	4.2·10 ¹	5.7·10 ³	2.2	2.0·10 ¹	8.4·10 ⁻³	7.0	2.0·10 ³	3.9·10 ²	3.0	7.4·10 ¹	9.1·10 ²	2.5	3.6·10 ¹
	A _m	4.3·10 ²	2.9	6.6·10 ¹	1.0·10 ³	2.7	5.0·10 ¹	1.2·10 ³	2.6	4.2·10 ¹	7.1·10 ¹	3.5	1.4·10 ²	1.6·10 ²	3.0	7.4·10 ¹
	S _{fw}	2.5·10 ²	2.6	4.2·10 ¹	4.9·10 ³	2.2	2.0·10 ¹	7.1·10 ⁻³	6.8	1.8·10 ³	3.3·10 ²	3.0	7.4·10 ¹	7.7·10 ²	2.5	3.6·10 ¹
	S _m	3.9·10 ²	2.7	5.0·10 ¹	9.2·10 ²	2.5	3.6·10 ¹	1.1·10 ³	2.4	3.1·10 ¹	6.3·10 ¹	3.5	1.4·10 ²	1.5·10 ²	2.8	5.7·10 ¹
	T	2.8	25	2.9·10 ⁵	1.0·10 ⁻³	34	1.0·10 ⁶	9.4·10 ⁻⁵	35	1.1·10 ⁶	1.1·10 ¹	24	2.5·10 ⁵	8.7	24	2.5·10 ⁵
2,3,7,8-TCDD	H	1.7	6.6	1.7·10 ³	2.9	6.7	1.8·10 ³	5.4·10 ⁻³	12	1.9·10 ⁴	9.1	6.7	1.7·10 ³	5.0·10 ⁻¹	7.1	2.3·10 ³
	A _{fw}	1.3·10 ⁶	7.7	3.0·10 ³	7.9·10 ⁷	7.6	2.8·10 ³	3.5·10 ⁴	19	1.0·10 ⁵	2.9·10 ⁵	11	1.2·10 ⁴	1.1·10 ⁶	10	1.1·10 ⁴
	A _m	1.4·10 ⁸	7.3	2.5·10 ³	1.8·10 ⁷	9.3	6.3·10 ³	2.3·10 ⁸	7.2	2.3·10 ³	9.5·10 ⁴	15	4.1·10 ⁴	3.7·10 ⁵	15	4.1·10 ⁴
	S _{fw}	4.1·10 ⁶	7.7	3.0·10 ³	2.5·10 ⁸	7.6	2.8·10 ³	1.0·10 ⁵	19	1.0·10 ⁵	9.1·10 ⁵	11	1.2·10 ⁴	3.5·10 ⁶	10	1.2·10 ⁴
	S _m	3.5·10 ⁸	7.1	2.1·10 ³	5.8·10 ⁷	8.8	5.1·10 ³	7.9·10 ⁸	7.1	2.1·10 ³	2.8·10 ⁵	14	3.1·10 ⁴	1.1·10 ⁶	13	2.3·10 ⁴
Lead	T	3.1·10 ⁴	11	1.3·10 ⁴	5.2·10 ⁻²	38	1.6·10 ⁶	7.3·10 ²	34	1.0·10 ⁶	7.4·10 ⁴	11	1.2·10 ⁴	7.2·10 ⁴	10	1.1·10 ⁴
	H	1.7·10 ⁹	4.4	3.5·10 ²	2.5·10 ⁸	7.1	2.1·10 ³	1.6·10 ⁸	7.9	3.1·10 ³	3.3·10 ⁹	4.7	4.4·10 ²	3.9·10 ⁷	7.5	2.7·10 ³
	A _{fw}	3.6	2.3	2.7·10 ¹	1.4·10 ¹	2.3	2.7·10 ¹	1.1·10 ⁻²²	3.9	2.0·10 ²	9.7	2.3	2.7·10 ¹	9.7	2.3	2.7·10 ¹
	A _m	1.0·10 ⁴	2.3	2.7·10 ¹	1.7·10 ³	2.4	3.0·10 ¹	1.7·10 ⁴	2.3	2.7·10 ¹	1.2·10 ³	2.4	3.0·10 ¹	1.2·10 ³	2.4	3.0·10 ¹
	S _{fw}	2.1·10 ¹	2.8	5.4·10 ¹	8.0·10 ¹	2.8	5.4·10 ¹	6.1·10 ⁻²²	3.2	1.0·10 ²	5.5·10 ¹	2.8	5.4·10 ¹	5.5·10 ¹	2.8	5.4·10 ¹
H ^a	S _m	2.4·10 ⁴	2.8	5.4·10 ¹	3.9·10 ³	2.8	5.4·10 ¹	3.8·10 ⁴	2.8	5.4·10 ¹	2.7·10 ³	2.8	5.4·10 ¹	2.7·10 ³	2.8	5.4·10 ¹
	T	1.8·10 ¹	2.3	2.7·10 ¹	7.9·10 ⁻²²	3.1	8.6·10 ¹	7.3·10 ⁻²¹	3.1	8.6·10 ¹	3.7·10 ¹	2.3	2.7·10 ¹	3.7·10 ¹	2.3	2.7·10 ¹
	H ^a	2.2·10 ³	2.0	1.7·10 ¹	9.3	5.4	7.4·10 ²	4.8·10 ¹	6.4	1.4·10 ³	1.7·10 ⁴	2.1	1.9·10 ¹	3.0·10 ²	4.5	3.9·10 ²

TP = Toxicity Potential; A_{fw} = Fresh water Aquatic EcoToxicity Potential; A_m = Marine Aquatic EcoToxicity Potential; S_{fw} = Fresh water Sediment EcoToxicity Potential; S_m = Marine Sediment EcoToxicity Potential; T = Terrestrial EcoToxicity Potential; H = Human Toxicity Potential; a Characteristics of a lognormal distribution are given for the HTPs after emission to air and agricultural soil of lead. However, the Gamma distribution shows the best fit for these two HTPs. The Gamma distribution characteristics of the HTP_{air} of lead are 'location = 1.7·10², scale = 1.4·10³, and shape = 1.9', the characteristics of the HTP_{agri. soil} of lead are 'location = 1.0·10³, scale = 1.1·10⁴, and shape = 1.8'.

Table 3.8 Geometric mean (GM), geometric standard deviation (GSD), and uncertainty factor (UF), defined as the ratio of the 97.5th and 2.5th percentile value, of the lognormal uncertainty distributions of the toxicity potentials of Atrazine, 2,3,7,8-TCDD and Lead.

Table 3.9 Uncertainty importance of relevant input parameters (> 1%), expressed in percentage contribution to the uncertainty in the toxicity potentials of Atrazine. Human characteristics are in *italic*.

Substance	Air			Fresh air			Seawater			Agricultural soil			Industrial soil		
	A _{fw}	A _m	T	A _{fw}	A _m	T	A _{fw}	A _m	T	A _{fw}	A _m	T	A _{fw}	A _m	T
Fate analysis	1.5														
Hydroxyl radical reaction rate in air		25.8			37.8		1.6	33.1	1.3	2.0					
Half-life in water			4.0			1.9			1.9		15.7			27.6	
Half-life in soil	4.6						22.9		16.6		9.9	8.6	5.0	4.2	5.1
Octanol-water partition coefficient		5.4	2.2		16.8						14.3	12.4		7.4	6.0
Solubility		4.8	2.0		14.7		20.5		14.6		13.3	11.3		6.9	5.4
Vapour pressure	4.3	9.0	3.1		22.7		29.6		22.3		10.6	9.4		5.2	4.4
Organic carbon-water partition coefficient		3.3				1.3	18.1				20.7	17.4	3.0	11.0	8.3
															2.5
Exposure assessment															
Purification factor for drinking water									5.3						5.5
Fish bioconcentration factor									1.2						1.3
Daily intake of fish									1.0						1.1
										26.4					
										22.6					
Effect assessment															
Statistical extrapolation constant for the ecotoxicological PNECs	85.2	49.4	84.0		97.0	60.0	41.7	6.0	65.0	40.9	29.8	24.1	88.6	63.2	43.3
Acute LC50 to chronic NOEC assessment factor for ecotoxicological input data			2.4			1.2			1.2				2.7		2.8
Interspecies assessment factor (rat - human)									90.2				89.1		86.4
Total explained uncertainty importance	95.6	97.7	97.7	95.2	97.0	97.8	97.9	97.7	98.1	98.8	98.4	98.6	99.0	96.3	97.2
														98.5	96.6
															96.8

A_{fw} = Fresh water Aquatic EcoToxicity Potential; A_m = Marine Aquatic Ecotoxicity Potential; T = Terrestrial EcoToxicity Potential; H = Human Toxicity Potential; ^a Sediment ecotoxicity potentials for the fresh water and marine environment give similar results as their corresponding aquatic ecotoxicity potentials (results not shown).

Table 3.11 Uncertainty importance of relevant input parameters (> 1%), expressed in percentage contribution to the uncertainty in the toxicity potentials of Lead. Human characteristics are in *italic*.

Toxicity potentials ^a					Air			Fresh air			Seawater			Agricultural soil			Industrial soil			
	A _{fw}	A _m	T	H	A _{fw}	A _m	T	H	A _{fw}	A _m	T	H	A _{fw}	A _m	T	H	A _{fw}	A _m	T	H
Fate analysis																				
Solid-water partition coefficient in suspended matter	71.7				74.7		41.1	16.7	71.8		41.1	13.0	73.1		73.1					
Solid-water partition coefficient in soils			56.0	49.0			32.9				32.9		2.0	1.2	56.2	48.7	2.0	1.2	56.2	11.7
Solid-water partition coefficient in sediments		81.1				80.9				81.2					79.9			79.9		
Exposure assessment																				
Root – soil concentration factor				31.2																33.6
Leaf – soil concentration factor				11.3																11.7
Fish bioconcentration factor				1.2				37.7					40.2							1.0
Daily intake of root crops				3.3																3.3
Daily intake of fish				1.2				43.7					45.5							
Daily intake of soil particles																				84.9
Effect assessment																				
Statistical extrapolation constant for the ecotoxicological PNECs	26.4	17.0	42.2		23.6	17.0	22.9		26.5	16.9	24.4		23.2	16.9	42.0		23.2	16.9	42.0	
Total explained uncertainty importance	98.1	98.1	98.2	97.2	98.3	97.9	98.4	98.1	98.3	98.1	98.4	98.5	98.3	98.0	98.2	97.3	98.3	98.0	98.2	97.6

A_{fw} = Fresh water Aquatic EcoToxicity Potential; S_{fw} = Fresh water Sediment EcoToxicity Potential; T = Terrestrial EcoToxicity Potential; H = Human Toxicity Potential; ^a Aquatic and sediment ecotoxicity potentials for the marine environment give similar results as their corresponding ecotoxicity potentials for the fresh water environment (results not shown).

Discussion

Toxicity potentials

The results show that significant differences in uncertainty estimates can be found between different (a) substances, (b) impact categories and (c) initial emission compartments, ranging from about 1.5 to 6 orders of magnitude for the three substances evaluated. Differences between substances and impact categories are mainly caused by the differences in input parameter uncertainties, particularly for the effect assessment. Toxicity potentials for Lead, for instance, show relatively low uncertainty. The reason is that the HLV of Lead is based on epidemiological data precluding the application of an interspecies assessment factor, and the PNECs are based on a large set of NOECs, decreasing the uncertainty in ecotoxicological extrapolation to a large extent. Systematic differences in uncertainty also exist between toxicity potentials of the same impact category and substance, but emitted to different compartments. Emission to a compartment which does not (dominantly) contribute to a specific impact category, generally leads to larger uncertainty estimates, as the emitted substance has to be transported to another compartment. If the parameters involved in describing these transport mechanisms are very uncertain, the uncertainty in the predicted environmental concentration of the secondary compartment(s) also increases (Cowan *et al.*, 1995), which in turn further increases the uncertainty of the toxicity potentials.

The results show that correlations between the toxicity potentials of one substance, in particular within one impact category, are in most cases high. This can be explained by the fact that the uncertainty in the toxicity potentials of one impact category is caused by the same uncertain substance-specific input parameters of each substance (Table 3.9 to 3.11). Moreover, correlations between toxicity potentials of different ecotoxicological impact categories may be high. The latter correlations are typically found, if the aquatic PNEC is used to calculate the terrestrial and/or sediment PNEC by using the equilibrium partition method.

It must, however, be stressed that several sources of variability and uncertainty have not been quantified in this study. As pointed out before, temporal and spatial variability is very difficult to quantify in an LCA and was therefore neglected. Hertwich *et al.* (1999) showed that the influence of spatial and temporal variation in landscape parameters is limited when compared to the effect of uncertain substance-specific parameters. Uncertainty due to choices and model uncertainties were also disregarded in this study. As pointed out by Huijbregts *et al.* (2000a), important choices, such as the choice of weighting factors for the ecotoxicological impact categories, may have an important impact on the outcome. Other weighting methods, for instance on the basis of species density per compartment, may result in other toxicity potentials for the ecotoxicological impact categories. The impact of uncertainty due to choices can be assessed with a scenario analysis (Huijbregts, 1998b). This should be subject of further research. Uncertainties in the model descriptions may also influence the calculation of toxicity potentials to a large extent. Model uncertainties may be large in multi-media fate and exposure models (Ragas *et al.*, 1999) and the effect assessment (Power and McCarthy, 1997; Smith and Cairns Jr., 1993; Forbes and Forbes,

1993). Huijbregts *et al.* (2000a) tentatively assessed the impact of model uncertainties on the toxicity potentials by comparing the outcome of the models USES-LCA and USES 1.0. Comparing the results of Huijbregts *et al.* (2000a) and this study reveals that uncertainty in model structure is the dominant source of uncertainty in the toxicity potentials of Lead, except for the toxicity potentials after emission to fresh water. In contrast, uncertainty in the toxicity potentials of 2,3,7,8-TCDD and Atrazine, except for the AETPs after emission to the soil compartments, are dominantly caused by parameter uncertainty and human variability. This suggests that the dominant source of uncertainty depends on the nature of the substance under study and on the initial emission compartment chosen.

LCA case studies

The research presented in this article is primarily concerned with the implications of using uncertainty estimates for toxicity potentials as input in LCA case studies. Although the uncertainty in toxicity potentials may be considerable, it is important to keep in mind that in LCAs in most cases only relative differences are important, for instance between product systems or product improvement options. Large absolute uncertainty estimates do not necessarily have a large influence on LCA outcomes (Huijbregts, 1998b). The influence of toxicity potential uncertainties on LCA outcomes can only be assessed by performing an uncertainty analysis for an LCA case study, including the uncertainty in other LCA phases, such as the inventory analysis and other characterisation factors. This is currently under study.

Conclusions

Uncertainty in the toxicity potentials of Atrazine, 2,3,7,8-TCDD and Lead ranges from about 1.5 to 6 orders of magnitude. This uncertainty is caused by a limited set of parameters, which are involved in describing chemical transport, degradation in water and soil and in deriving no-effect levels. Furthermore, parameters describing indirect human exposure routes may cause a significant spread in the Human Toxicity Potentials. Correlations between toxicity potentials of one substance can be high, in particular within one impact category. If the uncertain toxicity potentials are used as input in an uncertainty analysis of LCA case studies, it is vital to take these correlations into account.

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§ 3.3 Export of potential impact over time and space

Toxicity potentials are scaling factors used in life cycle assessment (LCA) indicating their relative importance in terms of potential toxic impacts. This paper presents the results of an uncertainty assessment of toxicity potentials for 181 substances that were calculated with the global nested multi-media fate, exposure and effects model USES-LCA. The variance in toxicity potentials resulting from choices in the modelling procedure was quantified by means of scenario analysis. A first scenario analysis showed to what extent potential impacts in the relatively short term are obscured by the inclusion of impacts on the very long term. Toxicity potentials representing potential impacts over time horizons of 20, 100 and 500 years were compared with toxicity potentials representing potential impacts over an infinite time horizon. Time horizon dependent differences up to 6.5 orders of magnitude were found for metal toxicity potentials, while for toxicity potentials of organic substances under study, differences remain within 0.5 orders of magnitude. The second scenario analysis addressed to what extent potential impacts on the continental scale are obscured by the inclusion of impacts on the global scale. Exclusion of potential impacts on the global scale changed the toxicity potentials of metals and volatile persistent halogenated organics up to 2.3 orders of magnitude. These scenario analyses also provide the basis for determining exports to future generations and outside the emission area.

Introduction

Toxicity potentials are substance-specific, quantitative measures of potential impacts per unit emission of a toxic substance that can be used as weighting factors in the aggregation of emissions coming from life cycle inventories. Huijbregts *et al.* (2000a) calculated toxicity potentials for 181 substances with the global nested multi-media fate, exposure and effects model USES-LCA, which is based on the Uniform System for the Evaluation of Substances 2.0 (USES 2.0), developed by RIVM *et al.* (1998).

Although USES-LCA may be better suited for the calculation of toxicity potentials than methods previously used, the calculated toxicity potentials may still contain large uncertainties. For instance, the variance in toxicity potentials resulting from input parameter uncertainties and human variability for Atrazine, 2,3,7,8-TCDD and Lead, expressed by the ratio of the 97.5%-ile and the 2.5%-ile, ranges from about 1.5 to 6 orders of magnitude (Huijbregts *et al.*, 2000b).

The relevance of (value) choices in the modelling procedure has, however, so far not been assessed in USES-LCA. In this respect an important choice in the calculations may be the choice for a certain time horizon. For instance, the global warming potential of a pollutant used in the impact assessment of greenhouse gases may differ more than one order of magnitude depending on the time horizon chosen (Albritton *et al.*, 1996). In the calculation of toxicity potentials, an infinite time horizon is generally used (Guinée *et al.*, 1996; Hertwich *et al.*, 1998; Huijbregts *et al.*, 2000a). However, by using an infinite time horizon potential impacts occurring over a shorter period of time may be obscured in the impact assessment of product systems.

Another important choice may be the decision whether or not to include potential impacts exported from the continental scale to the global scale. Huijbregts *et al.* (2000a) included potential impacts on the global scales in the calculation of toxicity potentials by way of scale-specific weighting factors. However, including exposure that occurs on the global scale may fully dominate the potential impacts, obscuring those on the continental scale.

This paper assesses the influence of export of potential impact over time and space in the calculation of toxicity potentials. Toxicity potentials using time horizons of 20, 100 and 500 years and toxicity potentials excluding impacts on the global scale are calculated. Then, these potentials are compared with toxicity potentials calculated by Huijbregts *et al.* (2000a), which relate to potential impacts over an infinite time horizon and the global scale.

Analysis of scenario uncertainty

Toxicity potentials

USES-LCA calculates toxicity potentials for the six impact categories fresh water aquatic ecotoxicity, marine aquatic ecotoxicity, fresh water sediment ecotoxicity, marine sediment ecotoxicity, terrestrial ecotoxicity and human toxicity, after initial emission to the compartments air, fresh water, seawater, industrial soil and agricultural soil,

respectively. Thus, ultimately, 30 toxicity potentials can be calculated for each substance; one for each combination of six impact categories and five emission compartments.

Time horizon dependency

For the calculation of time horizon-dependent toxicity potentials the time-integrated exposure over the time period T considered is of interest (Figure 3.2).

Figure 3.2 Graphical interpretation of the time-integrated exposure γ_e over time horizon T in compartment e after an emission pulse Δm_i released to compartment i at $t = 0$, superimposed to a background level $m_{b,e}$ in compartment e .

The time-integrated exposure at time T to a pulse emission Δm , released at time $t = 0$ and added to the steady state situation m_b at $t = 0$, is (Heijungs, 1995)

$$\gamma_T = \int_0^T (m(t) - m_b) dt$$

Because

$$m(t) = m_b + e^{tA} \cdot \Delta m$$

the first equation can be rewritten as

$$\gamma_T = \int_0^T (e^{tA} \cdot \Delta m) dt$$

which is equal to

$$\gamma_T = (e^{TA} - I) \cdot A^{-1} \cdot \Delta m$$

where γ_T is the vector of time-integrated exposure from 0 to T (hr.kg), $m(t)$ is the vector of mass m at time t (kg), m_b is the vector of steady state mass situation m_b (kg), A is the matrix of coefficients which determines the fate of a substance (hr^{-1}), I is the identity matrix (dimensionless), and Δm is the vector of emission pulse m at $t=0$ (kg). As the term $(e^{TA} - I) \cdot A^{-1}$, needed in the integrated exposure calculations, is also applied in dynamic mass-balance models (Brandes *et al.*, 1996; Heijungs, 1999), outcomes of dynamic mass-balance modelling can be used directly in the assessment of time horizon dependent toxicity potentials.

Dynamic calculations in USES-LCA are performed by implementing a routine that numerically solves the mass balance equations of the fate part of USES-LCA. The dynamic module of the fate model Simplebox 2.0 is used for this purpose (Brandes *et al.*, 1996). It has been chosen to calculate toxicity potentials for the time horizons 20, 100 and 500 years, following the time horizons used in the calculation of global warming potentials (Albritton *et al.*, 1996). It is believed that these three time horizons provide a practical range for policy applications.

Exclusion of the global scale

USES-LCA has two spatial scales (continental and global) and three climate zones, reflecting arctic, moderate and tropic climatic zones of the Northern hemisphere. Huijbregts *et al.* (2000a) aggregated potential impacts on the continental scale and the global scale by way of scale-specific weighting factors. Potential impacts in the marine aquatic compartments were aggregated on the basis of the compartment's volume, and potential impacts in the marine sediment and terrestrial compartments were both aggregated on the basis of the compartment's mass. For humans, the human population present at a certain scale has been used as a weighting factor. For the impact categories related to the fresh water aquatic and sediment compartment no weighting factors were needed, as these compartments are only identified at the continental scale.

Excluding potential impacts on the global scale in the calculation of toxicity potentials can be done by setting the weighting factors for the arctic, tropic and moderate zone of

the impact categories involved to zero. Similar to the assessment of export of potential impacts over time, inclusion or exclusion of potential impacts on the global scale can be seen as a (value) choice in the calculation of toxicity potentials.

Results and discussion

Export over time

Figures 3.3 to 3.6 compare the toxicity potentials calculated for the time horizons 20 years, 100 years and 500 years with the toxicity potentials calculated for an infinite time horizon. The time-integrated exposure to organic substances is in most cases virtually completed within 20 years. For persistent organic substances, such as endrin, the relative difference between toxicity potentials calculated for an infinite time horizon (Huijbregts *et al.*, 2000a) and a time horizon of 20 years is up to 0.5 orders of magnitude, while for the time horizons 100 years and 500 years relative differences with an infinite time horizon are negligible. Compared to the influence of parameter uncertainty on toxicity potentials (Huijbregts *et al.*, 2000b), time horizon dependent differences for these substances can be considered small.

On the other hand, time horizon dependent differences for metal toxicity potentials can be up to several orders of magnitude, indicating that there may be a large export of impacts to future generations. Therefore, the choice of a particular time horizon is important in the impact assessment of heavy metal emissions. Toxicity potentials related to the marine environment show a relatively high time horizon dependency due to the very long modelled residence times of most metals in the marine aquatic compartment and the upper layer of the marine sediment (Figure 3.3). For most of the metals, residence times in USES-LCA are in the same order of magnitude as reported by Goldberg (1965), the major exception being Be (Huijbregts, 2000). If the metal is emitted to one of the soil compartments, time horizon dependent differences of the marine toxicity potentials further increase. The reason is that run-off from the soil to the aquatic environment may take a very long time (> 1000 years) for metals strongly bound to the soil matrix (Cleven *et al.*, 1992; Guinée *et al.*, 1999).

Exposure to metals in the fresh water environment after emission to fresh water is almost completed in 20 years. This follows from efficient removal pathways, such as burial of metals in deep fresh water sediment and metal flow from the fresh water compartment to the sea water compartment. However, after emission to air and soil, fresh water toxicity potentials markedly increase over time, as metal run-off from the soil may cause exposure in the fresh water environment over a very long time (Figure 3.4). The slow run-off of metals to the aquatic environment and leaching of metals to deeper soil layers from the upper soil compartment, which is also shown in other fate models (Cleven *et al.*, 1992; Guinée *et al.*, 1999; Van de Meent, 1990; Moolenaar *et al.*, 1997), cause significant time horizon dependent differences in terrestrial ecotoxicity potentials (TETP) of metals (Figure 3.5). In this respect it should also be noted that USES-LCA

Figure 3.3 Comparison of marine aquatic and sediment ecotoxicity potentials for an infinite time horizon ($METP_{infinite}$) with marine aquatic and sediment ecotoxicity potentials for the time horizons 20 years (x), 100 years (o), and 500 years (+) ($METP_{finite}$).

Figure 3.4 Comparison of fresh water aquatic and sediment ecotoxicity potentials for an infinite time horizon ($FETP_{infinite}$) with fresh water aquatic and sediment ecotoxicity potentials for the time horizons 20 years (x), 100 years (o), and 500 years (+) ($FETP_{finite}$).

Figure 3.5 Comparison of terrestrial ecotoxicity potentials for an infinite time horizon ($TETP_{infinite}$) with terrestrial ecotoxicity potentials for the time horizons 20 years (x), 100 years (o), and 500 years (+) ($TETP_{finite}$).

Figure 3.6 Comparison of human toxicity potentials for an infinite time horizon ($HTP_{infinite}$) with human toxicity potentials for the time horizons 20 years (x), 100 years (o), and 500 years (+) (HTP_{finite}).

assumes a vertically mixed soil layer up to 1 m. If, however, a smaller soil depth is assumed ecologically relevant, the modelled residence time of metals in the soil may decrease substantially (De Vries and Bakker, 1998). In turn, this will lower all metal TETPs, in particular for the longer time horizons. It also decreases the time horizon dependent differences between the metal TETPs.

Finally, human toxicity potentials (HTPs) of metals may show substantial time horizon dependent differences (Figure 3.6). The actual time horizon dependency of HTPs follows from the dominant exposure route. If exposure via air or fresh water is the dominant exposure route, no substantial time horizon dependent differences in HTPs are found. If, however, the marine environment (via fish consumption) or the soil compartments (e.g. via crop consumption or direct soil ingestion) are important, differences between HTPs for an infinite time horizon and the time horizons 20, 100 and 500 years can be up to several orders of magnitude.

Export to the global scale

Figures 3.7 to 3.10 compare the toxicity potentials excluding and including impacts on the global scale.

Figure 3.7 Comparison of marine aquatic ecotoxicity potentials including the global scales ($MAETP_{continental + global}$) and marine aquatic ecotoxicity potentials excluding the global scales ($MAETP_{continental}$).

Figure 3.8 Comparison of marine sediment ecotoxicity potentials including the global scales ($MSETP_{continental + global}$) and marine sediment ecotoxicity potentials excluding the global scales ($MSETP_{continental}$).

Figure 3.9 Comparison of terrestrial ecotoxicity potentials including the global scales ($TETP_{continental + global}$) and terrestrial ecotoxicity potentials excluding the global scales ($TETP_{continental}$).

Figure 3.10 Comparison of human toxicity potentials including the global scales ($HTP_{\text{continental} + \text{global}}$) and human toxicity potentials excluding the global scales ($HTP_{\text{continental}}$).

As can be seen in the Figures 3.7 to 3.10, toxicity potentials of the majority of the substances are not affected by excluding potential impacts on the global scale. The reason is that organic substances which are not very persistent and volatile are not capable of moving from the continental to the global scale.

On the other hand, as shown in Figures 3.7 and 3.8, exclusion of potential impacts on the global scale decrease the Marine Aquatic EcoToxicity Potentials (MAETP) and Marine Sediment EcoToxicity Potentials (MSETP) of metals and persistent volatile halogenated organic substances up to 2.3 and 1.6 orders of magnitude, respectively. This is true for all initial emission compartments. It shows that the marine toxicity potentials of these substances are dominated by the time-integrated exposure at the global scale, reflecting that the oceanic compartment acts as a major sink for these persistent pollutants.

Figure 3.9 shows that potential impacts on the global scale substantially contribute to TETPs of persistent and volatile substances emitted to continental air, fresh water and seawater compartment. Exclusion of the global scale results for these substances in a decrease in TETPs up to 1.5 orders of magnitude. In contrast, TETPs of all direct emissions to agricultural and industrial soils are completely explained by potential impacts in the continental soil compartments. This means that after emission to continental soils transport of substances to soils on the global scale hardly occurs.

Finally, Figure 3.10 indicates that the HTPs of metals and persistent volatile halogenated organic substances may be up to 1.2 orders of magnitude lower compared to substances

not persistent and/or mobile enough to enter the global scale. Compared to the ecotoxicity potentials, excluding the global scale has a less pronounced effect on the HTPs. The reason is that the weighting factors in the HTP calculation are based on population numbers instead of the compartment's mass or volume. Therefore, for instance, exclusion of the arctic zone hardly influences the HTP outcomes, while this is not the case for the ecotoxicity potentials of metals and persistent volatile halogenated organic substances involved.

USES-LCA

USES-LCA calculations may suffer from substantial model uncertainties (Huijbregts *et al.*, 2000a; Ragas *et al.*, 1999). In this respect, model uncertainties related to the application of USES-LCA for metals are particularly important. Two important examples of uncertainty in the model structure and possible improvement options will be discussed below.

A major drawback of using box models, such as USES-LCA, is that they do not account for subcompartmental differences in fate and corresponding effects. Although for organic substances spatial variability may not be very important in the assessment of fate and effects compared to the influence of parameter uncertainties (Hertwich *et al.*, 1999), this may not be the case for metals. For instance, lack of reliable information about partition coefficients is an important source of uncertainty for toxicity potentials of lead (Huijbregts *et al.*, 2000b). Metal partitioning in turn strongly depends on environmental characteristics and may have a large influence on the residence time of metals particularly in the soil compartment (De Vries and Bakker, 1998). Therefore, moving to spatially explicit models (e.g. Klepper and Den Hollander, 1999; Van den Hout *et al.*, 1998; Stolwijk *et al.*, 1998) may be an improvement in the fate, exposure and effect assessment of metals. Moreover, in these spatially explicit models it may be easier to account for currently lacking site-dependent processes in USES-LCA, such as the site dependent slow conversion of reversibly adsorbed heavy metals into forms irreversibly adsorbed to the soil matrix (Harmsen, 1992; De Vries and Bakker, 1998) and corresponding uptake of metals by organisms (Peijnenburg *et al.*, 1997, 1999). Including these processes may substantially decrease all metal TETPs and toxicity potentials after emission to the soil and air compartments and TETPs of metals, and lower the time horizon dependent differences between these toxicity potentials. Further research in LCA context is recommended here.

The fate analysis of geochemically reactive metals in the marine environment, such as Be, also needs improvement. Goldberg (1965) reports an oceanic residence time of Be 3 orders of magnitude lower than calculated by USES-LCA (Huijbregts, 2000). The reason is that the ions of Be are expected to be rapidly hydrolysed at the pH of seawater and incorporated into minerals, such as ferro-manganese nodules (Goldberg, 1965; Riley, 1971), giving rise to a removal mechanism which has not been included in USES-LCA.

Conclusions

The dynamic USES-LCA calculations may give a first impression about the time horizon dependence of organic and inorganic pollutants over the time horizons 20, 100 and 500 years. It is shown that time horizon dependent differences can be up to several orders of magnitude for the metal toxicity potentials, while time horizon dependent differences remain within 0.5 order of magnitude for organic substances. Exclusion of potential impacts on the global scale changed the toxicity potentials of metals and volatile persistent halogenated organics. Differences up to 2.3 orders of magnitude are found for these types of substances. As the latter substances may substantially contribute to the potential impact of product systems, the (value) choice of the time and spatial horizon in the LCA impact assessment of toxic substances is an important one. It should, however, be stressed that uncertainties in the model structure of USES-LCA may be large, as results have not been validated. In particular, modelling of geochemical reactive metals in the marine environment and spatial dependency of metal behaviour needs improvement.

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Chapter 4

Life cycle impact assessment of acidifying and eutrophying substances

§ 4.1 Acidification and terrestrial eutrophication

Simple models are often used to assess the potential impact of acidifying and eutrophying substances released during the life cycle of products. As fate, background depositions and ecosystem sensitivity are not included in these models, environmental life cycle assessment of products (LCA) may produce incorrect results for these impact categories. This paper outlines the spatially explicit model RAINS-LCA which was developed for the calculation of acidification and terrestrial eutrophication potentials of ammonia (NH_3) and nitrogen oxide (NO_x) air emissions and of acidification potentials for sulfur dioxide (SO_2) air emissions for Europe and a number of European regions, taking fate, background depositions and effects into account. Two impact definitions are explored in the calculations: (1) the marginal change in the hazard index of all ecosystems in Europe; (2) the marginal change in the hazard index of ecosystems in Europe where the critical load is actually exceeded. The inclusion of fate, background depositions and ecosystem sensitivity results in a different ranking of substances compared to simpler model outcomes. In the context of acidification, emissions of nitrogen compounds are regarded about a factor 2 less important relative to sulfur compounds. Furthermore, using RAINS-LCA as opposed to simpler models, it was found that region-specific differences in terrestrial eutrophication and acidification potentials range up to 1.5 and 3.5 orders of magnitude, respectively. By means of scenario analysis, it was also shown that 'only above critical load' terrestrial eutrophication and acidification potentials for the years 1995 and 2010 differ up to 0.6 and 1 order of magnitude, respectively. These results imply that it is important to use region-specific and time-specific acidification and terrestrial eutrophication potentials, if it is expected that life cycle emissions of acidifying and eutrophying air pollutants are predominantly situated in a few (European) regions and/or within a specific year. Further improvements in RAINS-LCA may be established by including source-receptor matrices of the Northern Hemisphere instead of Europe and using the probability of species occurrence as a basis for the effect assessment.

Introduction

Life Cycle Assessment (LCA) is a tool for the assessment of the environmental impact of a product system (Consoli *et al.* 1993). In such an assessment, the entire life cycle of a product from resource extraction to waste disposal is considered. An important part of an LCA is assessing the potential impact of inventory results, also called impact assessment. In the impact assessment, it is determined first which extractions and emissions contribute to which impact categories. Impact categories reflect various environmental problems, such as global warming and ozone depletion. Next, the indicator result for each impact category is determined. This is done by multiplying the aggregated emission of each individual substance with a characterisation factor (also called 'potential' or 'equivalency factor') for each impact category to which it may potentially contribute (Heijungs *et al.* 1992).

$$S_u = \sum_i \sum_k \sum_x Q_{u,x,k,i} \times M_{x,k,i}$$

where S_u is the impact score for impact category u per functional unit (kg), $Q_{u,x,k,i}$ is the characterisation Factor of impact category u for the emission of substance x to compartment k (e.g. air, water, soil) in region i (dimensionless), and $M_{x,k,i}$ is the emission of substance x to compartment k (e.g. air, water, soil) in region i , per functional unit (kg).

Characterisation factors are substance-specific, quantitative representations of the additional environmental pressure per unit emission of a substance. Examples are the global warming potential (GWP) and the ozone depletion potential (ODP). They can also be used to calculate normalisation scores for the impact categories involved. Normalisation is an optional step in the weighting between impact categories. In normalisation, the impact score per functional unit is divided by the impact score of a reference situation (Udo de Haes 1996). Instead of using life cycle inventory emissions, total emissions per region in a certain year are used to calculate normalisation scores.

Among the environmental impacts typically assessed using LCA are acidification and eutrophication. They can cause direct toxicity to individual species, soil-mediated effects upon plant species, increased susceptibility to secondary stress factors and changes in competitive relationships between (plant) species, resulting in changes and loss of biodiversity (UBA 1996). Up until now, relatively simple models were used to assess the potential impact of acidifying and eutrophying substances (see Lindfors *et al.* 1995b). The impact indicator for acidification is the potential proton release (H^+), and for eutrophication, it is the potential share in biomass formation. These models introduce major uncertainty in LCAs due to the fact that fate, background depositions, and ecosystem sensitivity are not included in the computation of the impact factors. Recently, Potting *et al.* (1998) incorporated fate, background depositions and ecosystem sensitivity in the computation of acidification potentials by using the RAINS (Regional Air pollution INformation and Simulation) model (Alcamo *et al.* 1990). The marginal change in the area

of threatened ecosystems due to a marginal emission change served as an impact indicator for acidification. However, the use of other impact definitions may result in different sets of characterisation factors and therefore different results for an LCA .

To explore the effect of using other impact definitions, an adapted version of the RAINS model, called RAINS-LCA, was developed and applied to calculating potentials for acidifying and eutrophying air emissions, according to two new impact definitions. Initially, the impact indicator definitions and the input data for RAINS-LCA will be discussed. Then, the calculated acidification potentials, eutrophication potentials for the terrestrial environment and normalisation scores will be presented. Finally, the acidification potentials are compared with those calculated previously.

Characterisation factors

Hazard index: above and below critical loads

Instead of defining the impact indicator as the marginal change in square meters of threatened surface as Potting and colleagues do (1998), the marginal change in the hazard index of European ecosystems is taken as a definition of potential impacts for RAINS-LCA. The hazard index, also known as the PEC/PNEC ratio (Predicted (No) Environmental Concentration), has already been successfully applied in the calculation of toxicity potentials (Guinée and Heijungs 1993; Guinée *et al.* 1996, Hertwich *et al.* 1998; Huijbregts *et al.* 2000). PNECs for substances causing acidification and/or terrestrial eutrophication are also called 'critical loads' which can be defined as "a quantitative estimate of an exposure to one or more pollutants below which significant harmful effects on specified sensitive elements of the environment do not occur, according to present knowledge' (UBA 1996). By terrestrial eutrophication, we mean the deposition onto the terrestrial environment of compounds that promote biomass formation. The new impact indicator is not only concerned with the degree to which an environmental standard or critical load actually is exceeded, but also the degree to which it is filled up (Guinée *et al.* 1996). This means that marginal changes in the hazard index of all ecosystems are taken into account in the calculation of the impact indicator, using the ecosystem area as a weighting factor. The new impact indicator can be used for acidification potentials as well as terrestrial eutrophication potentials, as there are ecosystem-specific critical loads available for both impact categories in RAINS. First, the load of acid deposition is calculated by

$$L_{x,j} = \sum_i t_{x,i,j} \times E_{x,i}$$

where $L_{x,j}$ is the load in grid cell j due to emission of pollutant x in several regions i (equivalent.hectare⁻¹.year⁻¹), $t_{x,i,j}$ is the transfer coefficient, representing the deposition in grid cell j due to the emission of 1 kg pollutant x in region i (eq.ha⁻¹.kg⁻¹), and $E_{x,i}$ is the emission of substance x in region i (kg.year⁻¹).

This load can be compared with the critical load and weighted over ecosystems and regions to yield the definition of our hazard index.

$$I_{u,x} = \frac{\sum_j \sum_{e \in j} A_{e \in j} \times L_{j,x} / CL_{u,x,e \in j}}{\sum_j \sum_{e \in j} A_{e \in j}}$$

where $I_{u,x}$ is the hazard index of substance x related to impact category u (dimensionless); $A_{e \in j}$ is the area of European ecosystem e in grid cell j (km²), and $CL_{u,x,e \in j}$ is the critical load value of substance x in European ecosystem e situated in grid cell j and related to impact category u (eq.ha⁻¹.yr⁻¹).

Finally, the derivative of the hazard index with respect to the emission is found to be

$$dI_{u,x} = \sum_j \sum_{e \in j} A_{e \in j} \times t_{x,i,j} / CL_{u,x,e \in j}$$

in which $dI_{u,x}/dE_{x,i}$ is the marginal change in the hazard index of impact category u after a marginal emission change of substance x in region i (year.kg⁻¹).

To stress that characterisation factors are relative measures, a reference substance is introduced. The use of a reference substance follows the established use of carbon dioxide (CO₂), ethylene (C₂H₄), chlorofluorocarbon (CFC11) and 1,4-dichlorobenzene (1,4-DCB) as reference substances in the evaluation of global warming, photochemical ozone formation, stratospheric ozone depletion, and toxicity, respectively (Albritton, *et al.* 1996; Derwent *et al.* 1998; Solomon *et al.* 1995; Guinée *et al.* 1996). Acidification and terrestrial eutrophication potentials were calculated for 44 separate European regions using the following equation;

$$Q_{u,x,i} = \frac{dI_{u,x}/dE_{x,i}}{dI_{u,ref}/dE_{ref,ref}}$$

where $Q_{u,x,i}$ is the characterisation factor related to impact category u for substance x after emission to region i (reference-equivalents), $dI_{u,x}/dE_{x,i}$ is the marginal change in the hazard index of impact category u after a marginal emission change of substance x in region i (year.kg⁻¹), and $dI_{u,ref}/dE_{ref,ref}$ is the marginal change in the hazard index after a marginal emission change of the reference substance in a reference region (year.kg⁻¹). Emissions of sulfur dioxide (SO₂) and nitrogen oxide (NO_x) in Switzerland were selected

as references for the calculation of acidification and terrestrial eutrophication potentials, respectively.¹

After calculation of region-specific acidification and terrestrial eutrophication potentials, average potentials and normalisation scores were calculated for Europe, western Europe² and eastern Europe³. Average potentials were calculated by a weighted summation of the region-specific potentials involved, using total region-specific emissions related to the years 1995 and 2010 as weighting factors.

Hazard index: only above critical load

It is standard practice in the calculation of characterisation factors for many impact categories, such as human toxicity, ecotoxicity (Hertwich *et al.* 1998; Huijbregts *et al.* 2000), and photochemical ozone formation (Derwent *et al.* 1998), to use 'above and below threshold marginal changes'. However, one may argue that marginal changes in the hazard index are important only in areas where the critical loads are currently exceeded or will be exceeded in the future. A change in the hazard index in areas where critical loads are not exceeded may be considered as unimportant, because no actual risks are expected in these areas. Therefore, a second impact indicator was defined representing the marginal change in the hazard index of ecosystem areas only where the critical load is exceeded. Equation 4 was also used in the calculation of such 'only above critical load' characterisation factors, but now excluding ecosystem areas in the numerator where no actual risk is expected. Deposition patterns were used to determine in which ecosystems of Europe actual or future impacts are expected. The reference situation in the 'only above critical load' calculations is equal to the 'above and below critical load' reference value.

It should be stressed that this calculation procedure assumes that marginal changes in emissions produce no change in the protection status of an ecosystem. An important consequence of this calculation procedure is that the characterisation factors for acidification and terrestrial eutrophication become dependent on the current and future emission estimates. Emission data of two different years (1995 and two 2010 emission forecast scenarios) were chosen for the calculation of the marginal change in relative risk of threatened ecosystems.

RAINS-LCA

The RAINS-model has been developed at the International Institute for Applied System Analysis (IIASA) as a tool for the integrated assessment of alternative strategies to reduce impacts on acidification, terrestrial eutrophication, and photochemical ozone formation in Europe (Schöpp *et al.* 1999). As RAINS does not allow the calculation of the marginal change in the hazard index of European ecosystems, its structure was modified to

incorporate the equations listed above. The input data needed to run the modified model, called RAINS-LCA, are discussed in more detail below.

Emissions

RAINS contains annual emission estimates for 44 European regions. These emission estimates are needed for the calculation of 'only above critical load' potentials, European averaged potentials and normalisation scores. 1995 emission estimates (EMEP/MSC-W 1998) and an emission scenario for 2010 were chosen for this purpose. The 2010 emission projection is partly based on a cost-optimal allocation of emission reductions to simultaneously achieve expected policy targets for acidification, terrestrial eutrophication, and ozone exposure in the European Union (Amman *et al.* 1999). In addition, the emission projection builds on detailed forecasts of economic activities and application of emission control techniques in various sectors of the economy. Here, the economic activity 2010 forecast scenario, called the BaseLine scenario (BL), represents the 'business as usual' energy and agricultural activity projection. The projections in the BL scenario are mainly based on officially reported national energy and agricultural activity projections and on studies performed for the European Union (Amann *et al.* 1998). The second economic activity 2010 forecast scenario, called the New target Policy scenario (NP), represents an 'optimistic' energy and agricultural activity projection for 2010. The energy projection for the countries of the EU-15 meet the reduction targets of the Kyoto agreement, assuming no emission trading (Cofala *et al.*, 1999). For the non-EU countries, an 'Economic and Environmental Convergence' energy 2010 forecast, developed by Cofala *et al.* (1997), is used in the NP scenario. The optimistic agricultural activity projection assumes that uniformly for all countries and all animal categories, the total livestock numbers will be 10 percent lower than in the BL forecast (Amann *et al.*, 1999).

Transfer matrices

RAINS calculates total deposition of nitrogen and sulfur compounds on European grid elements (150-km resolution) with substance-specific region-to-grid source-receptor transfer matrices. These transfer matrices indicate which fraction of the emissions from the 44 regions in Europe deposit in which European grid elements. The transfer matrices are based on the results of a Lagrangian model (EMEP/MSC-W 1996). Model calculations are based on input data of actual meteorological conditions and emissions for the years 1985 through 1995. Following the approach developed by Posch (1996), separate calculations are performed for each of these years and finally averaged over the 11 years (Huijbregts 1999).

Critical loads and ecosystem areas

For about 1.3 million European ecosystems, critical loads for acidification and terrestrial eutrophication have been gathered by the Coordination Center for Effects (De Smet and Posch 1999, 13-27). The acidity critical loads refer to both terrestrial and fresh water ecosystems, while critical loads for eutrophication solely refer to terrestrial ecosystems. The full data set on critical loads is, however, not readily available in RAINS. Instead, a summary of the cumulative critical load distribution function for each 150x150 km² grid cell was used. For each grid cell, cumulative distribution functions of the maximum acidity critical loads for sulfur and nitrogen and the critical load for eutrophication, based on 29 percentile values, are available.⁴ Following the approach developed by Kåresen and Hirst (1999, 45-51), a true critical load function was approximated by taking the average values of the successive known percentile values (Figure 4.1).

Figure 4.1 A hypothetical example of a true critical load function (dashed line) and the approximation (solid line) of a grid cell. The circles indicate the available points of the cumulative density function (derived from Kåresen and Hirst, 1999).

This approximation procedure assumes that for every grid cell and impact category

$$\sum_{e \in j} \frac{A_{e \in j}}{CL_{e \in j}} \approx \sum_{n=1}^{n=29} \frac{((P_{n+1} - P_n)/100) \times \sum_{e \in j} A_{e \in j}}{((CL_{n+1} + CL_n)/2)}$$

in which corresponding variables equal those used in equations listed above, and P_n is the percentile value of the n^{th} point on the cumulative density curve (dimensionless), and CL_n is the critical load value of the n^{th} point on the cumulative density curve ($\text{eq.ha}^{-1}\text{.yr}^{-1}$).

Huijbregts (1999c) checked the validity of the approximation procedure by comparing the outcomes based on the full dataset with the approximated outcomes for grid cells situated in Sweden, the United Kingdom and Germany. These countries kindly submitted their detailed data set on critical loads and ecosystem areas. The approximation procedure showed deviations smaller than 5% compared to the exact outcomes for more than 95% of the analyzed grid cells. Maximum deviations never exceeded 20% (Huijbregts 1999).

Results

Tables 4.1 and 4.2 show the region-specific acidification potentials and Table 4.5 shows the European averages. The following differences between regions, scenarios and substances can be identified:

- The spread between the region-specific acidification potentials of NH_3 is the largest, followed by acidification potentials of SO_2 .⁵ Regional differentiation is the smallest for the acidification potentials of NO_x . Because the transport potential order is $\text{NH}_3 < \text{SO}_2 < \text{NO}_x$, it implies that the shorter the transport potential, the larger the regional differences found for the substance under consideration. Maximum regional differences between acidification potentials of the same substance are up to 3.5 orders of magnitude dependent on the substance and the chosen scenario. For the 'above and below critical load' scenario, the regional differences in acidification potentials of the same substance are caused by differences in the sensitivity of the environment, while for the 'only below critical load' scenarios, regional differences in the threatened ecosystem area play also a role. Regions with relatively high acidification potentials are the Kola/Karelia region in Russia and the Scandinavian countries, while the southern and southeastern European regions have relatively low acidification potentials;
- Depending on the substance and the region, differences between the 'only above critical load' acidification potentials of the years 1995 and 2010 for the same substance and region are up to 1 order of magnitude, while differences between the 2010 Baseline and New Policy scenario remain within 0.5 orders of magnitude. In particular, acidification potentials related to regions in southern and middle Europe are sensitive to the emission year chosen. This implies that in the areas with significant acid deposition from these regions, a relatively large number of ecosystems threatened due to acidification in 1995, will become protected in 2010;
- According to the RAINS-LCA model, in Europe, on average, the acidification potential of NH_3 is 2.5-3.2 times higher than the acidification potential of NO_x ; the acidification potential of NH_3 is 0.7-1.3 times higher than the acidification potential SO_2 ; and the acidification potential of SO_2 is 2.4-3.5 times higher than the acidification potential of NO_x .

Table 4.1 Acidification potentials of ammonia (NH₃), nitrogen oxide (NO_x), and sulfur dioxide (SO₂) for 22 West European regions (in Swiss SO₂-equivalents).

West European regions	Acidification potentials											
	Ammonia (NH ₃)			Nitrogen Oxide (NO _x)			Sulfur dioxide (SO ₂)					
	A&B	OA	OA	A&B	OA	OA	A&B	OA	OA	OA	OA	OA
		1995	2010BL	2010NP		1995	2010BL	2010NP		1995	2010BL	2010NP
Austria	1.3	6.0·10 ⁻¹	7.2·10 ⁻²	7.4·10 ⁻²	2.7·10 ⁻¹	8.6·10 ⁻²	1.9·10 ⁻²	1.9·10 ⁻²	1.0	5.2·10 ⁻¹	2.2·10 ⁻¹	2.2·10 ⁻¹
Belgium	1.0	5.0·10 ⁻¹	1.4·10 ⁻¹	1.4·10 ⁻¹	4.9·10 ⁻¹	1.8·10 ⁻¹	5.9·10 ⁻²	5.8·10 ⁻²	1.0	5.0·10 ⁻¹	1.8·10 ⁻¹	1.8·10 ⁻¹
Denmark	1.5	5.4·10 ⁻¹	2.7·10 ⁻¹	2.7·10 ⁻¹	8.8·10 ⁻¹	2.3·10 ⁻¹	1.1·10 ⁻¹	1.1·10 ⁻¹	1.8	7.2·10 ⁻¹	3.5·10 ⁻¹	3.5·10 ⁻¹
Finland	6.4	7.4·10 ⁻¹	4.6·10 ⁻¹	4.1·10 ⁻¹	1.9	1.9·10 ⁻¹	1.1·10 ⁻¹	1.0·10 ⁻¹	5.0	7.7·10 ⁻¹	5.1·10 ⁻¹	4.7·10 ⁻¹
France	2.0	3.9·10 ⁻¹	5.3·10 ⁻²	5.3·10 ⁻²	4.3·10 ⁻¹	1.2·10 ⁻¹	2.9·10 ⁻²	2.9·10 ⁻²	1.1	3.7·10 ⁻¹	9.2·10 ⁻²	9.2·10 ⁻²
Germany (new)	1.6	7.7·10 ⁻¹	1.6·10 ⁻¹	1.6·10 ⁻¹	5.7·10 ⁻¹	1.9·10 ⁻¹	5.3·10 ⁻²	5.3·10 ⁻²	1.2	5.2·10 ⁻¹	1.7·10 ⁻¹	1.7·10 ⁻¹
Germany (old)	1.4	7.6·10 ⁻¹	1.8·10 ⁻¹	1.9·10 ⁻¹	5.1·10 ⁻¹	1.9·10 ⁻¹	5.5·10 ⁻²	5.4·10 ⁻²	1.3	6.8·10 ⁻¹	2.2·10 ⁻¹	2.2·10 ⁻¹
Greece	1.3·10 ⁻¹	3.9·10 ⁻³	1.2·10 ⁻³	1.1·10 ⁻³	3.7·10 ⁻²	1.9·10 ⁻³	5.2·10 ⁻⁴	4.8·10 ⁻⁴	6.6·10 ⁻²	6.8·10 ⁻³	3.9·10 ⁻³	3.8·10 ⁻³
Ireland	7.9·10 ⁻¹	2.8·10 ⁻¹	9.7·10 ⁻²	9.4·10 ⁻²	3.4·10 ⁻¹	1.3·10 ⁻¹	6.0·10 ⁻²	5.9·10 ⁻²	5.7·10 ⁻¹	2.4·10 ⁻¹	1.0·10 ⁻¹	1.0·10 ⁻¹
Italy	5.9·10 ⁻¹	1.7·10 ⁻¹	2.3·10 ⁻²	2.3·10 ⁻²	1.3·10 ⁻¹	3.3·10 ⁻²	5.8·10 ⁻³	5.7·10 ⁻³	4.6·10 ⁻¹	1.6·10 ⁻¹	3.4·10 ⁻²	3.4·10 ⁻²
Luxembourg	1.5	5.1·10 ⁻¹	9.2·10 ⁻²	9.3·10 ⁻²	5.0·10 ⁻¹	1.9·10 ⁻¹	4.5·10 ⁻²	4.5·10 ⁻²	1.3	5.9·10 ⁻¹	1.5·10 ⁻¹	1.5·10 ⁻¹
Netherlands	1.0	5.4·10 ⁻¹	2.1·10 ⁻¹	2.1·10 ⁻¹	5.1·10 ⁻¹	1.9·10 ⁻¹	7.3·10 ⁻²	7.2·10 ⁻²	9.2·10 ⁻¹	4.6·10 ⁻¹	1.9·10 ⁻¹	1.9·10 ⁻¹
Norway	6.0	2.6	1.8	1.8	1.2	3.6·10 ⁻¹	2.2·10 ⁻¹	2.2·10 ⁻¹	3.8	1.7	1.1	1.1
Portugal	2.8·10 ⁻¹	1.2·10 ⁻²	3.0·10 ⁻³	3.0·10 ⁻³	8.0·10 ⁻²	1.1·10 ⁻²	2.6·10 ⁻³	2.6·10 ⁻³	1.8·10 ⁻¹	1.4·10 ⁻²	3.4·10 ⁻³	3.3·10 ⁻³
Spain	2.7·10 ⁻¹	3.2·10 ⁻²	5.3·10 ⁻³	5.3·10 ⁻³	1.0·10 ⁻¹	1.9·10 ⁻²	3.7·10 ⁻³	3.6·10 ⁻³	2.2·10 ⁻¹	5.0·10 ⁻²	1.1·10 ⁻²	1.1·10 ⁻²
Sweden	4.4	1.3	5.3·10 ⁻¹	5.2·10 ⁻¹	1.3	2.6·10 ⁻¹	1.4·10 ⁻¹	1.3·10 ⁻¹	3.8	1.2	7.1·10 ⁻¹	6.9·10 ⁻¹
Switzerland	1.3	5.6·10 ⁻¹	1.1·10 ⁻¹	1.1·10 ⁻¹	2.8·10 ⁻¹	9.9·10 ⁻²	1.8·10 ⁻²	1.9·10 ⁻²	1.0	4.5·10 ⁻¹	1.1·10 ⁻¹	1.1·10 ⁻¹
United Kingdom	1.5	7.9·10 ⁻¹	3.1·10 ⁻¹	2.9·10 ⁻¹	4.3·10 ⁻¹	1.8·10 ⁻¹	8.4·10 ⁻²	8.2·10 ⁻²	8.6·10 ⁻¹	4.6·10 ⁻¹	2.3·10 ⁻¹	2.2·10 ⁻¹
Baltic sea	x	x	x	x	1.1	1.8·10 ⁻¹	8.8·10 ⁻²	8.5·10 ⁻²	2.2	5.5·10 ⁻¹	2.7·10 ⁻¹	2.6·10 ⁻¹
North sea	x	x	x	x	5.3·10 ⁻¹	1.9·10 ⁻¹	8.5·10 ⁻²	8.4·10 ⁻²	9.9·10 ⁻¹	4.5·10 ⁻¹	2.2·10 ⁻¹	2.2·10 ⁻¹
Atlantic ocean	x	x	x	x	1.6·10 ⁻¹	4.6·10 ⁻²	1.8·10 ⁻²	1.8·10 ⁻²	2.7·10 ⁻¹	8.3·10 ⁻²	3.4·10 ⁻²	3.3·10 ⁻²
Mediterranean sea	x	x	x	x	1.5·10 ⁻²	1.9·10 ⁻³	4.6·10 ⁻⁴	4.5·10 ⁻⁴	2.5·10 ⁻²	3.5·10 ⁻³	7.4·10 ⁻⁴	7.3·10 ⁻⁴

x = Potential is not calculated; A&B = Scenario in which 'above and below critical load' marginal changes in the hazard index are summed; OA_1995 = Scenario in which 'only above critical load' marginal changes in the hazard index are summed, taking 1995 emissions as a starting point; OA_2010BL = Scenario in which 'only above critical load' marginal changes in the hazard index are summed, taking 2010 baseline forecast emissions as a starting point; OA_2010NP = Scenario in which 'only above critical load' marginal changes in the hazard index are summed, taking 2010 new policy forecast emissions as a starting point.

Table 4.2 Acidification potentials of ammonia (NH₃), nitrogen oxide (NO_x), and sulfur dioxide (SO₂) for 22 East European regions (in Swiss SO₂-equivalents).

East European regions	Acidification potentials											
	Ammonia (NH ₃)			Nitrogen Oxide (NO _x)			Sulfur dioxide (SO ₂)					
	A&B	OA	OA	A&B	OA	OA	A&B	OA	OA	A&B	OA	OA
		1995	2010BL		1995	2010BL		1995	2010BL		1995	2010BL
			2010NP			2010NP						2010NP
Albania	1.6·10 ⁻¹	5.6·10 ⁻³	1.7·10 ⁻³	1.6·10 ⁻³	4.9·10 ⁻²	1.0·10 ⁻³	1.3·10 ⁻¹	1.7·10 ⁻²	9.9·10 ⁻³	9.6·10 ⁻³		
Belarus	2.0	3.1·10 ⁻¹	1.6·10 ⁻¹	7.4·10 ⁻²	9.2·10 ⁻¹	3.2·10 ⁻²	2.2	2.8·10 ⁻¹	1.9·10 ⁻¹	6.3·10 ⁻²		
Bosnia-Herzegovina	2.3·10 ⁻¹	2.5·10 ⁻²	8.3·10 ⁻³	7.8·10 ⁻³	1.0·10 ⁻¹	4.6·10 ⁻³	2.5·10 ⁻¹	5.8·10 ⁻²	3.6·10 ⁻²	3.5·10 ⁻²		
Bulgaria	3.9·10 ⁻¹	1.0·10 ⁻²	3.5·10 ⁻³	3.0·10 ⁻³	1.1·10 ⁻¹	1.9·10 ⁻³	2.0·10 ⁻¹	1.8·10 ⁻²	1.1·10 ⁻²	9.8·10 ⁻³		
Croatia	3.1·10 ⁻¹	5.0·10 ⁻²	1.5·10 ⁻²	1.4·10 ⁻²	1.6·10 ⁻¹	8.9·10 ⁻³	3.9·10 ⁻¹	1.3·10 ⁻¹	7.4·10 ⁻²	7.3·10 ⁻²		
Czech Republic	1.4	8.3·10 ⁻¹	8.5·10 ⁻²	8.5·10 ⁻²	4.5·10 ⁻¹	3.5·10 ⁻²	1.2	6.1·10 ⁻¹	1.9·10 ⁻¹	1.9·10 ⁻¹		
Estonia	3.0	2.2·10 ⁻¹	1.2·10 ⁻¹	1.1·10 ⁻¹	1.5	5.9·10 ⁻²	4.1	3.1·10 ⁻¹	1.9·10 ⁻¹	1.7·10 ⁻¹		
Hungary	6.2·10 ⁻¹	1.9·10 ⁻¹	8.0·10 ⁻²	7.6·10 ⁻²	3.1·10 ⁻¹	2.2·10 ⁻²	1.0	5.4·10 ⁻¹	4.2·10 ⁻¹	4.2·10 ⁻¹		
Latvia	2.5	1.5·10 ⁻¹	7.9·10 ⁻²	6.8·10 ⁻²	1.2	4.7·10 ⁻²	2.4	2.5·10 ⁻¹	1.5·10 ⁻¹	1.3·10 ⁻¹		
Lithuania	1.7	1.6·10 ⁻¹	7.3·10 ⁻²	6.1·10 ⁻²	9.8·10 ⁻¹	8.6·10 ⁻²	1.9	2.6·10 ⁻¹	1.4·10 ⁻¹	1.2·10 ⁻¹		
Macedonia	1.8·10 ⁻¹	5.8·10 ⁻³	2.0·10 ⁻³	1.9·10 ⁻³	5.2·10 ⁻²	1.3·10 ⁻³	1.5·10 ⁻¹	1.8·10 ⁻²	1.1·10 ⁻²	1.1·10 ⁻²		
Moldavia	5.9·10 ⁻¹	3.7·10 ⁻²	1.3·10 ⁻²	1.0·10 ⁻²	3.4·10 ⁻¹	2.0·10 ⁻²	6.8·10 ⁻¹	7.1·10 ⁻²	4.1·10 ⁻²	3.5·10 ⁻²		
Poland	1.7	5.0·10 ⁻¹	8.2·10 ⁻²	9.1·10 ⁻²	5.9·10 ⁻¹	1.1·10 ⁻¹	1.3	4.3·10 ⁻¹	1.5·10 ⁻¹	1.5·10 ⁻¹		
Romania	4.5·10 ⁻¹	3.4·10 ⁻²	1.3·10 ⁻²	1.1·10 ⁻²	2.0·10 ⁻¹	1.9·10 ⁻²	4.6·10 ⁻¹	8.2·10 ⁻²	5.0·10 ⁻²	4.7·10 ⁻²		
Russia (Kalinigrad region)	2.3	2.0·10 ⁻¹	7.9·10 ⁻²	7.4·10 ⁻²	8.9·10 ⁻¹	4.6·10 ⁻²	1.9	3.0·10 ⁻¹	1.5·10 ⁻¹	1.3·10 ⁻¹		
Russia (Kola, Karelia)	1.0·10 ¹	7.5·10 ⁻¹	2.3·10 ⁻¹	2.3·10 ⁻¹	2.0	7.2·10 ⁻¹	7.2	2.3	4.2·10 ⁻¹	4.5·10 ⁻¹		
Russia (St. Petersburg region)	6.0	1.6·10 ⁻¹	7.4·10 ⁻²	6.1·10 ⁻²	1.9	8.1·10 ⁻²	5.2	2.5·10 ⁻¹	1.3·10 ⁻¹	1.2·10 ⁻¹		
Russia (Remaining)	3.7	2.3·10 ⁻²	1.0·10 ⁻²	6.8·10 ⁻³	1.1	5.5·10 ⁻³	3.0	3.4·10 ⁻²	1.7·10 ⁻²	1.3·10 ⁻²		
Slovakia	1.1	4.4·10 ⁻¹	1.7·10 ⁻¹	1.6·10 ⁻¹	3.5·10 ⁻¹	2.6·10 ⁻²	1.5	8.6·10 ⁻¹	6.6·10 ⁻¹	6.6·10 ⁻¹		
Slovenia	6.8·10 ⁻¹	1.3·10 ⁻¹	2.8·10 ⁻²	2.8·10 ⁻²	1.7·10 ⁻¹	9.4·10 ⁻³	5.7·10 ⁻¹	1.8·10 ⁻¹	7.7·10 ⁻²	7.7·10 ⁻²		
Ukraine	9.4·10 ⁻¹	5.5·10 ⁻²	2.2·10 ⁻²	1.8·10 ⁻²	5.6·10 ⁻¹	7.9·10 ⁻³	1.1	5.4·10 ⁻²	2.9·10 ⁻²	2.3·10 ⁻²		
Yugoslavia	2.8·10 ⁻¹	2.3·10 ⁻²	8.0·10 ⁻³	7.5·10 ⁻³	1.3·10 ⁻¹	4.9·10 ⁻³	3.4·10 ⁻¹	8.7·10 ⁻²	5.7·10 ⁻²	5.5·10 ⁻²		

See Table 4.1 for abbreviations

Table 4.3 Terrestrial eutrophication potentials of ammonia (NH₃) and nitrogen oxide (NO_x) for 22 West European regions (in Swiss NO_x-equivalents).

West European regions	Terrestrial eutrophication potentials							
	Ammonia (NH ₃)				Nitrogen Oxide (NO _x)			
	A&B	OA 1995	OA 2010BL	OA 2010NP	A&B	OA 1995	OA 2010BL	OA 2010NP
Austria	4.2	3.6	2.4	2.3	8.9·10 ⁻¹	6.3·10 ⁻¹	4.8·10 ⁻¹	4.6·10 ⁻¹
Belgium	2.9	2.5	2.2	2.2	1.2	9.3·10 ⁻¹	7.8·10 ⁻¹	7.8·10 ⁻¹
Denmark	2.5	1.3	9.3·10 ⁻¹	8.7·10 ⁻¹	1.6	6.9·10 ⁻¹	5.5·10 ⁻¹	5.1·10 ⁻¹
Finland	1.5·10 ¹	6.4	3.6	2.8	3.5	9.9·10 ⁻¹	7.5·10 ⁻¹	6.2·10 ⁻¹
France	6.4	6.0	5.3	5.3	1.3	1.1	8.9·10 ⁻¹	8.9·10 ⁻¹
Germany (new)	4.6	3.8	3.5	3.4	1.5	1.0	9.2·10 ⁻¹	9.0·10 ⁻¹
Germany (old)	3.7	3.1	2.6	2.6	1.3	9.4·10 ⁻¹	7.9·10 ⁻¹	7.7·10 ⁻¹
Greece	1.5	4.3·10 ⁻¹	3.9·10 ⁻¹	2.4·10 ⁻¹	2.7·10 ⁻¹	9.1·10 ⁻²	8.2·10 ⁻²	6.6·10 ⁻²
Ireland	1.0	4.2·10 ⁻¹	2.9·10 ⁻¹	2.9·10 ⁻¹	5.2·10 ⁻¹	2.8·10 ⁻¹	2.1·10 ⁻¹	2.1·10 ⁻¹
Italy	2.8	2.1	1.4	1.4	6.0·10 ⁻¹	4.1·10 ⁻¹	2.9·10 ⁻¹	2.8·10 ⁻¹
Luxembourg	4.4	4.0	3.4	3.3	1.4	1.1	9.5·10 ⁻¹	9.5·10 ⁻¹
Netherlands	2.3	1.8	1.6	1.6	1.1	7.5·10 ⁻¹	6.3·10 ⁻¹	6.2·10 ⁻¹
Norway	6.2	1.2	3.4·10 ⁻¹	3.1·10 ⁻¹	1.6	3.8·10 ⁻¹	2.5·10 ⁻¹	2.2·10 ⁻¹
Portugal	2.4	1.6	1.2	1.1	4.9·10 ⁻¹	3.1·10 ⁻¹	2.3·10 ⁻¹	2.1·10 ⁻¹
Spain	2.0	1.1	6.7·10 ⁻¹	6.5·10 ⁻¹	5.2·10 ⁻¹	3.3·10 ⁻¹	2.2·10 ⁻¹	2.2·10 ⁻¹
Sweden	5.7	2.0	1.3	1.2	2.1	6.8·10 ⁻¹	5.1·10 ⁻¹	4.5·10 ⁻¹
Switzerland	5.0	4.7	3.8	3.8	1.0	8.4·10 ⁻¹	6.6·10 ⁻¹	6.6·10 ⁻¹
United Kingdom	1.7	7.9·10 ⁻¹	4.9·10 ⁻¹	4.8·10 ⁻¹	7.6·10 ⁻¹	4.4·10 ⁻¹	3.5·10 ⁻¹	3.4·10 ⁻¹
Baltic sea	x	x	x	x	2.1	8.4·10 ⁻¹	6.9·10 ⁻¹	6.2·10 ⁻¹
North sea	x	x	x	x	1.1	6.5·10 ⁻¹	5.4·10 ⁻¹	5.2·10 ⁻¹
N.E. Atlantic ocean	x	x	x	x	4.0·10 ⁻¹	2.6·10 ⁻¹	2.1·10 ⁻¹	2.1·10 ⁻¹
Mediterranean sea	x	x	x	x	1.2·10 ⁻¹	6.4·10 ⁻²	3.5·10 ⁻²	3.3·10 ⁻²

See Table 4.1 for abbreviations

Tables 4.3 and 4.4 show the region-specific terrestrial eutrophication potentials and Table 4.5 shows the European averages. The following differences between regions and substances can be identified:

- A larger spread between the region-specific terrestrial eutrophication potentials of NH₃ is found compared to the terrestrial eutrophication potentials of NO_x, because the transport potential of NO_x is larger compared to NH₃. Maximum regional differences between terrestrial eutrophication potentials are up to 1.5 orders of magnitude, depending on the substance and the scenario chosen. For the 'above and below critical load' scenario, the regional differences in terrestrial eutrophication potentials of the same substance are caused by differences in the sensitivity of the environment, while for the 'only below critical load' scenarios regional differences in threatened ecosystem area also important. Regions with relatively high terrestrial eutrophication potentials are Scandinavia, the Baltic regions and regions in mid-western Europe, while Ireland, the United Kingdom and the southern and southeastern European regions have relatively low terrestrial eutrophication potentials;

Table 4.4 Terrestrial eutrophication potentials of ammonia (NH₃) and nitrogen oxide (NO_x) for 22 East European regions (in Swiss NO_x-equivalents).

East European regions	Terrestrial eutrophication potentials							
	Ammonia (NH ₃)				Nitrogen Oxide (NO _x)			
	A&B	OA 1995	OA 2010BL	OA 2010NP	A&B	OA 1995	OA 2010BL	OA 2010NP
Albania	2.8	1.1	9.3·10 ⁻¹	8.7·10 ⁻¹	5.0·10 ⁻¹	2.1·10 ⁻¹	1.8·10 ⁻¹	1.6·10 ⁻¹
Belarus	4.5	1.8	1.6	1.5	2.0	6.3·10 ⁻¹	6.0·10 ⁻¹	5.4·10 ⁻¹
Bosnia-Herzegovina	2.9	2.3	1.4	1.4	6.1·10 ⁻¹	3.8·10 ⁻¹	2.7·10 ⁻¹	2.6·10 ⁻¹
Bulgaria	2.8	1.3	1.3	9.6·10 ⁻¹	5.6·10 ⁻¹	2.3·10 ⁻¹	2.2·10 ⁻¹	1.8·10 ⁻¹
Croatia	1.5	9.8·10 ⁻¹	6.7·10 ⁻¹	6.4·10 ⁻¹	6.7·10 ⁻¹	4.1·10 ⁻¹	3.1·10 ⁻¹	3.0·10 ⁻¹
Czech Republic	4.2	3.5	3.0	3.0	1.3	9.1·10 ⁻¹	8.0·10 ⁻¹	7.7·10 ⁻¹
Estonia	8.7	4.2	3.7	3.3	3.3	1.1	9.9·10 ⁻¹	8.6·10 ⁻¹
Hungary	2.2	1.4	1.1	1.0	1.0	5.8·10 ⁻¹	4.9·10 ⁻¹	4.6·10 ⁻¹
Latvia	7.3	3.9	3.8	3.5	2.6	9.1·10 ⁻¹	8.3·10 ⁻¹	7.3·10 ⁻¹
Lithuania	4.9	2.6	2.5	2.4	2.2	7.8·10 ⁻¹	7.2·10 ⁻¹	6.5·10 ⁻¹
Macedonia	2.3	1.0	8.5·10 ⁻¹	7.8·10 ⁻¹	4.7·10 ⁻¹	2.4·10 ⁻¹	2.0·10 ⁻¹	1.8·10 ⁻¹
Moldavia	1.6	5.1·10 ⁻¹	5.1·10 ⁻¹	4.6·10 ⁻¹	9.1·10 ⁻¹	2.9·10 ⁻¹	3.0·10 ⁻¹	2.6·10 ⁻¹
Poland	6.1	4.8	4.6	4.5	1.6	9.0·10 ⁻¹	8.3·10 ⁻¹	7.9·10 ⁻¹
Romania	2.3	9.4·10 ⁻¹	8.8·10 ⁻¹	8.2·10 ⁻¹	7.5·10 ⁻¹	3.1·10 ⁻¹	2.9·10 ⁻¹	2.6·10 ⁻¹
Russia (Kalingrad region)	6.7	2.4	2.2	2.1	2.0	7.8·10 ⁻¹	7.1·10 ⁻¹	6.5·10 ⁻¹
Russia (Kola, Karelia)	1.6·10 ¹	1.9	1.6	1.4	3.2	2.8·10 ⁻¹	2.6·10 ⁻¹	2.2·10 ⁻¹
Russia (St. Petersburg region)	1.4·10 ¹	6.0	5.7	4.9	3.8	1.1	9.9·10 ⁻¹	8.6·10 ⁻¹
Russia (Remaining)	8.4	1.6	2.0	1.7	2.3	4.1·10 ⁻¹	5.1·10 ⁻¹	4.2·10 ⁻¹
Slovakia	4.0	3.0	2.3	2.2	1.1	6.7·10 ⁻¹	5.7·10 ⁻¹	5.4·10 ⁻¹
Slovenia	2.8	2.0	9.8·10 ⁻¹	9.6·10 ⁻¹	6.4·10 ⁻¹	4.5·10 ⁻¹	3.1·10 ⁻¹	3.1·10 ⁻¹
Ukraine	3.0	1.3	1.3	1.1	1.5	3.7·10 ⁻¹	4.3·10 ⁻¹	3.6·10 ⁻¹
Yugoslavia	2.8	1.8	1.3	1.2	7.0·10 ⁻¹	3.8·10 ⁻¹	3.0·10 ⁻¹	2.7·10 ⁻¹

See Table 4.1 for abbreviations

- Depending on the substance and the region, differences between the 'only above critical load' terrestrial eutrophication potentials of the years 1995 and 2010 for the same substance and region are up to 0.6 orders of magnitude, while differences between the 2010 Baseline and New Policy scenario remain within 0.2 orders of magnitude. The terrestrial eutrophication potential of NH₃ emitted in Norway shows the highest sensitivity to the emission year chosen. This implies that in the areas with significant nitrogen deposition from Norway, a relatively large number of ecosystems threatened due to terrestrial eutrophication in 1995 will become protected in 2010;
- In Europe, on average, the terrestrial eutrophication potential of NH₃ is 3.4-4.6 times higher than the terrestrial eutrophication potential of NO_x.

Table 4.5 Average acidification and terrestrial eutrophication potentials for West Europe, East Europe and total Europe (in Swiss SO₂- and NO_x-equivalents, respectively).

		A&B 1995	OA 1995	A&B 2010BL	OA 2010BL	A&B 2010NP	OA 2010NP
Acidification							
NH ₃	West Europe	1.3	4.8·10 ⁻¹	1.3	1.3·10 ⁻¹	1.3	1.2·10 ⁻¹
	East Europe	1.8	1.6·10 ⁻¹	1.9	4.2·10 ⁻²	1.9	3.7·10 ⁻²
	Total Europe	1.6	3.2·10 ⁻¹	1.6	8.2·10 ⁻²	1.6	8.0·10 ⁻²
NO _x	West Europe	4.1·10 ⁻¹	1.2·10 ⁻¹	4.0·10 ⁻¹	4.8·10 ⁻²	4.1·10 ⁻¹	4.8·10 ⁻²
	East Europe	7.0·10 ⁻¹	5.4·10 ⁻²	7.8·10 ⁻¹	1.5·10 ⁻²	7.6·10 ⁻¹	1.4·10 ⁻²
	Total Europe	5.0·10 ⁻¹	1.0·10 ⁻¹	5.7·10 ⁻¹	3.3·10 ⁻²	5.6·10 ⁻¹	3.3·10 ⁻²
SO ₂	West Europe	7.9·10 ⁻¹	3.3·10 ⁻¹	8.0·10 ⁻¹	1.3·10 ⁻¹	8.4·10 ⁻¹	1.3·10 ⁻¹
	East Europe	1.6	3.0·10 ⁻¹	2.0	1.1·10 ⁻¹	1.6	1.1·10 ⁻¹
	Total Europe	1.2	3.1·10 ⁻¹	1.5	1.2·10 ⁻¹	1.3	1.2·10 ⁻¹
Terrestrial eutrophication							
NH ₃	West Europe	3.7	2.9	3.8	2.4	3.8	2.4
	East Europe	5.0	2.0	5.3	2.2	5.2	2.0
	Total Europe	4.3	2.5	4.6	2.3	4.5	2.2
NO _x	West Europe	9.9·10 ⁻¹	6.2·10 ⁻¹	9.5·10 ⁻¹	4.6·10 ⁻¹	9.5·10 ⁻¹	4.5·10 ⁻¹
	East Europe	1.7	5.7·10 ⁻¹	1.8	5.3·10 ⁻¹	1.8	4.6·10 ⁻¹
	Total Europe	1.2	6.0·10 ⁻¹	1.3	4.9·10 ⁻¹	1.3	4.5·10 ⁻¹

See Table 4.1 for abbreviations

Acidifying and eutrophying normalisation figures for western Europe, eastern Europe and total Europe were also calculated (Table 4.6). Outcomes are given for different emission years and corresponding acidification and terrestrial eutrophication potentials are used in the calculations.

Table 4.6 West European, East European and total European normalisation levels for acidification (kg Swiss SO_x-equivalents) and terrestrial eutrophication (kg Swiss NO_x-equivalents).

Region	A&B 1995	OA 1995	A&B 2010BL	OA 2010BL	A&B 2010NP	OA 2010NP
Acidification						
Western Europe	1.97·10 ¹⁰	7.21·10 ⁹	1.05·10 ¹⁰	1.30·10 ⁹	1.03·10 ¹⁰	1.26·10 ⁹
Eastern Europe	3.02·10 ¹⁰	4.74·10 ⁹	2.50·10 ¹⁰	9.97·10 ⁸	1.98·10 ¹⁰	8.29·10 ⁸
Total Europe	4.99·10 ¹⁰	1.20·10 ¹⁰	3.55·10 ¹⁰	2.29·10 ⁹	3.01·10 ¹⁰	2.09·10 ⁹
Terrestrial eutrophication						
Western Europe	2.59·10 ¹⁰	1.81·10 ¹⁰	1.79·10 ¹⁰	1.02·10 ¹⁰	1.77·10 ¹⁰	1.00·10 ¹⁰
Eastern Europe	2.46·10 ¹⁰	9.36·10 ⁹	2.78·10 ¹⁰	9.95·10 ⁹	2.54·10 ¹⁰	8.40·10 ⁹
Total Europe	5.05·10 ¹⁰	2.74·10 ¹⁰	4.57·10 ¹⁰	2.02·10 ¹⁰	4.31·10 ¹⁰	1.84·10 ¹⁰

See Table 4.1 for abbreviations

Discussion

Comparison with other ranking procedures

The acidification potentials presented in this article are compared with acidification potentials calculated by Heijungs *et al.* (1992) and Potting *et al.* (1998). To increase the comparability of the potentials, some additional modifications are necessary: (1) region-specific potentials in Potting *et al.* (1998) are averaged over Europe; (2) the total system area (Europe) is taken as the reference region instead of Switzerland; (3) acidification potentials are recalculated by using SO₂ as a reference substance. As can be seen in Table 4.7, including fate, background depositions, and ecosystem sensitivity results in an acidification potential of NH₃ and NO_x respectively 1.5-2.7 and 1.7-2.4 times less important, if compared with SO₂, than proposed by Heijungs *et al.* (1992). The main reason for the above-mentioned difference is that, in general, the ecosystem critical loads for S are not as high as the critical loads for N. This difference in critical load is caused by immobilization and denitrification of nitrogen in the soil and net nitrogen uptake by plants (UBA 1996, 76-82).

Table 4.7 Recalculated acidification potentials (SO₂-equivalents), derived from Heijungs *et al.* (1992), Potting *et al.* (1998), and this report.

	Heijungs	Potting 1990	Potting 2010	A&B 1995	OA 1995	A&B 2010BL	OA 2010BL	A&B 2010NP	OA 2010NP
NH ₃	1.9	1.1	0.94	1.3	1.0	1.1	0.71	1.2	0.69
NO _x	0.70	0.36	0.23	0.41	0.33	0.38	0.29	0.43	0.29
SO ₂	1	1	1	1	1	1	1	1	1

See Table 4.1 for abbreviations

In addition, region-specific acidification potentials for the year 2010 as calculated by Potting *et al.* (1998) are compared with the region-specific acidification potentials obtained here. Region-specific acidification potentials for the year 2010 calculated by Potting *et al.* (1998) and for the 'above and below critical load' scenario and the 'only above critical load' 2010 baseline scenario are compared, respectively. As can be seen in Figure 4.2, the correlation between the acidification potentials given by Potting *et al.* (1998) and the analysis reported here is in most cases low ($r^2 < 0.5$). The largest relative differences are found in southern and eastern Europe. Although this may be partly caused by the fact that transfer matrices and emission scenarios are slightly different between the two studies, it is likely that the particular choice for an impact indicator definition and the corresponding model structure has a large influence on the outcomes of the region-specific acidification potentials. According to Potting (2000), the implication of using the change in unprotected ecosystem area is that ecosystems with depositions far above or far below their critical loads are not captured in the 'only around threshold' characterisation factors of Potting *et al.* (1998), which is in contrast with the impact definitions used in this paper.

 4.2a: NH_3 acidification potentials ($r^2 = 0.04$)

 4.2b: NH_3 acidification potentials ($r^2 = 0.48$)

 4.2c: NO_x acidification potentials ($r^2 = 0.01$)

 4.2d: NO_x acidification potentials ($r^2 = 0.41$)

 4.2e: SO_2 acidification potentials ($r^2 = 0.33$)

 4.2f: SO_2 acidification potentials ($r^2 = 0.67$)

Figures 4.2a-f Comparison of region-specific acidification potentials of NH_3 , NO_x and SO_2 from Potting *et al.* (1998) and this paper. Region-specific acidification potentials for the year 2010 (AP_{AEA} in ha.ton_1) from Potting *et al.* (1998) and for the 'above and below critical load' scenario ($\text{AP}_{\text{A\&B}}$ on SO_2 -eq.) and the 'only above critical load' scenario for 2010 baseline scenario emissions ($\text{AP}_{\text{OA-2010BL}}$ in SO_2 -eq.) are compared. For every comparison the fraction of the explained variance (Pearson correlation coefficient r^2) is calculated. Note that the acidification potential of SO_2 emission in the Kola/Karelia region is left out in the comparison. The potential derived from Potting *et al.* (1998) appeared to be an extreme outlier (29.0 ha.ton_1).

Uncertainty

An important limitation of RAINS-LCA is that it allows for flows across its system boundary. The consequence is that the fate of an emitted substance in Europe can not be taken fully into account. Most likely, this causes an underestimation of acidification and terrestrial eutrophication potentials of NO_x and for Russian regions, as NO_x has a relatively large transport potential and the Russian regions are relatively closely situated to the borders of the modelling domain (Huijbregts 1999). Inclusion of transfer matrices for NH_3 , NO_x and SO_2 within the Northern hemisphere (Galperin *et al.* 1995; Galperin and Soviev 1998) may improve the fate part of RAINS-LCA. However, this inclusion is only worthwhile if information is available for the calculation of corresponding ecosystem critical loads. Moreover, the current transfer coefficients in RAINS-LCA may be further improved, when 50-50 km transfer matrices, as based on Eulerian atmospheric transport modelling, become available. Advantages of the Eulerian model are that local dry deposition of NO_x and NH_3 can be taken into account integrally in the transport model calculations, so that the source-receptor matrices can be calculated more precisely, and that the spatial resolution of the transfer matrices will become closer to the spatial resolution of the ecosystem critical loads database.

Another important limitation of RAINS-LCA is that critical loads are used to construct the relationship between emissions and damages which goes far beyond the current critical load concept. A more suitable indicator may be based on the probability of species occurrence as a function of pH and nitrogen (N) availability (Kros *et al.*, 1995; Latour and Reiling, 1993; Latour *et al.*, 1994). Unfortunately, this information is currently only available for the Netherlands which makes it unsuitable for application in RAINS-LCA. Replacing the current approach by an indicator based on the probability of species occurrence is recommended if sufficient data become available on the appropriate scale.

Apart from the uncertainties in the current model structure, a considerable amount of uncertainty may be attached to the input data, needed in the calculation of emissions, receptor matrices, and critical loads (e.g., Alcamo and Bartnicki 1990; Barkman 1997; Hettelingh and Janssen 1993, 51-55). The combined effect of these input uncertainties on the uncertainty of acidification and terrestrial eutrophication potentials is, however, not known. This may be the subject of future research. With help of the uncertainty tests it may be possible to judge whether the regional differences between the potentials are significant in view of the uncertainties in the input data. This information may also be used to assess the significance of environmental product comparisons.

Application in LCA case studies

In principle, the use of the acidification and terrestrial eutrophication potentials in LCA case studies is relatively straightforward, although there may occur some complications and difficulties. First, according to their impact definition, acidification and terrestrial

eutrophication potentials may differ significantly. Huijbregts (1999c) showed that the correlation between the 'above and below critical load' potentials and 'only above critical load' potentials are low ($r^2 < 0.5$) for both acidification and terrestrial eutrophication, indicating that the impact definition can have a significant impact on the outcome of an LCA case study. As stressed by Udo de Haes *et al.* (1999), explicitly addressing value-driven choices is becoming more and more important in LCA. This highlights the importance of arguments as to whether a certain impact indicator may be preferred or not. As the ultimate goal of environmental policy is to minimize current and future environmental risks, one may argue that the use of one of the 'only above critical load' scenarios in the LCA impact assessment of acidifying and eutrophying air pollutants is preferable. In this case, the choice of one of the 'only above critical load' scenarios should primarily depend on the time horizon of the LCA case study, as differences between the 'only above critical load' outcomes of the two 2010 policy scenarios are negligible. From a precautionary point of view, however, the 'above and below critical load' scenario may be preferred, as every acidifying and eutrophying air pollutant is judged potentially harmful in this type of impact indicator.

Another difficulty may be that RAINS-LCA does not cover all LCA-relevant regions and pollutants. Only acidification and terrestrial eutrophication potentials for European regions are calculated. Other models, such as the RAINS-ASIA model (Foell *et al.* 1995), may be modified for the calculation of characterisation factors of regions outside Europe. Furthermore, acidification potentials for acidifying air pollutants other than NH_3 , NO_x , and SO_2 were not included in RAINS-LCA because transfer matrices for these pollutants are lacking on a European scale. Air pollutants, such as hydrogen chloride (HCl) and hydrogen fluoride (HF), may, however, be dominant in some life cycle inventories. Aquatic eutrophication potentials of emissions to air, soil and water, such as of N and P, are also lacking in RAINS-LCA. For this impact category, a solution may be to judge eutrophication of soils and surface water bodies as separate impact categories in LCA case studies. Eutrophication potentials presented in this paper may be used to assess the potential impact on terrestrial ecosystems.

Finally, a difficulty of the implementation of the region-specific acidification and terrestrial eutrophication potentials in LCAs may be that more spatial information is required than is currently available, in most cases. For the purpose of a spatially explicit life cycle impact assessment, emissions in life cycle inventories must be reported separately for the distinguished regions in Europe. If this spatial information is not available, average European acidification potentials may be used instead. One should, however, keep the following limitations in mind. Initially, emissions in many product life cycles partly take place outside Europe. The emissions taking place outside Europe cannot be characterized in a valid way with European averaged acidification and terrestrial eutrophication potentials. In addition, the averaged acidification and terrestrial eutrophication potentials for western Europe, eastern Europe and the whole of Europe assume that NH_3 , NO_x and SO_2 emissions coming from life cycle inventories have the same regional distribution as the total emissions of these substances in western Europe,

eastern Europe and the whole of Europe, respectively. This may, however, not be the case in reality. If it is expected that life cycle emissions of eutrophying and acidifying air pollutants are dominantly situated in a few (European) regions, region-specific acidification and terrestrial eutrophication potentials should be preferred in the life cycle impact assessment.

Conclusions

The spatially explicit model RAINS can be modified for LCA purposes. The adapted model, called RAINS-LCA, was used to calculate acidification and terrestrial eutrophication potentials of NH_3 and NO_x air emissions and acidification potentials of SO_2 air emissions for Europe and a number of European regions, taking fate, background depositions, and effects into account. Two different impact definitions were used in the calculations. The first impact definition takes into account the marginal change in the hazard index of all ecosystems in Europe, while the other impact definition focuses on ecosystem areas in Europe where the critical load is actually exceeded.

It was found that the inclusion of fate, background depositions, and ecosystem sensitivity result in a different ranking between substances. A simpler model overestimates the acidifying impact of emissions of N compounds by a factor of 2 relative to S compounds when compared to the outcomes of the current model. Furthermore, the results indicate that region-specific differences of terrestrial eutrophication and acidification potentials may be up to 1.5 and 3.5 orders of magnitude, respectively. They also show that 'only above critical load' terrestrial eutrophication and acidification potentials for the years 1995 and 2010 differ up to 0.6 and 1 order of magnitude, respectively. This implies that it is important to use region-specific and time-specific acidification and terrestrial eutrophication potentials, if it is expected that life cycle emissions of acidifying and eutrophying air pollutants are dominantly situated in a few (European) regions and/or within a specific year.

Further improvements in RAINS-LCA may be established by using the probability of species occurrence as a basis for the effect assessment. Furthermore, including a fate analysis within the Northern Hemisphere will increase the acidification and terrestrial eutrophication potentials of NO_x and for Russian regions to some extent. Calculation of acidification and terrestrial eutrophication potentials for additional regions other than in Europe may further improve the reliability of life cycle impact outcomes of product systems predominantly situated outside Europe. Finally, further research is needed to incorporate data uncertainty in the computation of acidification and terrestrial eutrophication potentials.

Notes

1. In the 'above and below critical loads' scenario, the marginal change in the hazard index after a marginal emission change of SO₂ in Switzerland (acidification) or after a marginal emission change of NO_x in Switzerland (terrestrial eutrophication) is 1.10(10⁻¹¹ and 1.35(10⁻¹¹ year.kg⁻¹, respectively.
2. Austria, Belgium, Denmark, Finland, France, Germany, Greece, Ireland, Italy, Luxembourg, the Netherlands, Norway, Portugal, Spain, Sweden, Switzerland, United Kingdom, the Baltic Sea, the North Sea, the Mediterranean Sea and the remaining N.E. Atlantic Ocean are considered to be part of Western Europe.
3. Albania, Belarus, Bosnia-Herzegovina, Bulgaria, Croatia, Czech Republic, Estonia, European part of Russia, Latvia, Lithuania, Hungary, Macedonia, Moldavia, Poland, Romania, Slovakia, Slovenia, Ukraine, and Yugoslavia are considered to be part of Eastern Europe.
4. The 0th, 1st, 2nd, 3rd, 4th, 5th, 6th, 7th, 8th, 9th, 10th, 15th, 20th, 25th, 30th, 35th, 40th, 45th, 50th, 55th, 60th, 65th, 70th, 75th, 80th, 85th, 90th, 95th and 100th percentile values of the cumulative critical load function per grid cell are available from the RAINS model.
5. Ammonia deposition causes a net release of protons in the soil by
(1) $\text{NH}_3 + \text{H}^+ \rightarrow \text{NH}_4^+$ and subsequently (2) $\text{NH}_4^+ + 2\text{O}_2 \rightarrow \text{NO}_3^- + 2\text{H}^+ + \text{H}_2\text{O}$
Note that the second reaction is a microbially mediated soil process.

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§ 4.2 Aquatic eutrophication

In life cycle impact assessment (LCIA), limited attention is generally given to a consistent inclusion of a fate analysis in the derivation of aquatic eutrophication potentials. This paper includes fate and potential effects in the calculation of aquatic eutrophication potentials of NH_3 and NO_x emitted to the air, N and P emitted to water, and N and P emitted to soil. These characterisation factors were calculated for the Netherlands, Europe and the world, respectively. Implementation in current LCIA practice is further facilitated by calculating normalisation scores for the Netherlands in 1997, Europe in 1995 and the world in 1990. Although the results presented may be a step forward, significant improvements are still needed in the assessment of pollutants causing aquatic eutrophication. In particular, the fate factors representing transport of NO_x and NH_3 air emissions via soils to the aquatic environment should be improved. In addition, differences in biological availability of nutrients and differences in the sensitivity of aquatic environments should be included in the calculation of effect factors for aquatic eutrophication.

Introduction

Up to now, the impact indicator for eutrophication is generally defined as the potential share of eutrophying substances in biomass formation of aquatic algae (see Heijungs *et al.*, 1992). The actual indicator in use is based on the average carbon:nitrogen: phosphorus (C:N:P) ratio, also called the Redfield ratio, as found by Redfield *et al.* (1963). A serious drawback of using this impact indicator in LCIA is that it does not represent eutrophying impacts on the terrestrial environment, and that fate, background depositions and ecosystem sensitivity are not included in the current characterisation factors. To improve this situation, Huijbregts *et al.* (2001) adapted the model RAINS (Alcamo *et al.*, 1990) to calculate terrestrial eutrophication potentials of ammonia (NH₃) and nitrogen oxide (NO_x) air emissions for Europe and a number of European regions, taking fate, background depositions and effects into account. For aquatic eutrophication, however, there are as yet no similar improvements (see Finnveden and Potting, 1999).

A first improvement in the current characterisation factors for aquatic eutrophication may be established by including fate factors in the characterisation of anthropogenic emissions to air and soil:

$$AEP_{s,i,e} = AFF_{s,i,e} \times AEF_s$$

where $AEP_{s,i,e}$ is the characterisation factor for aquatic eutrophication of compound s emitted in region i to compartment e (PO₄³⁻-eq.); $AFF_{s,i,e}$ is the fate factor representing the fraction of compound s emitted in region i to compartment e that is transported to the aquatic environment (-); and AEF_s is the effect factor representing potential biomass production of phytoplankton per mass unit of compound s relative to PO₄³⁻ (PO₄³⁻-eq.).

Huijbregts and Seppälä (2000) outlined a first step towards fate factors to be used in the calculation of aquatic eutrophication potentials of NH₃ and NO_x air emissions for Europe and a number of European regions. The results presented were, however, not directly suitable for obtaining aquatic eutrophication potentials for emissions to air, water and soils. This paper elaborates on the analysis of Huijbregts and Seppälä (2000) by including fate factors in the calculation of Dutch, European, and global characterisation factors for air and agricultural soil emissions causing aquatic eutrophication. To facilitate the use of these new characterisation factors in life cycle impact assessment (LCIA), normalisation scores for the Netherlands in 1997, Europe in 1995 and the world in 1990 are also presented.

Fate factors

Air emissions

Fate factors for NH_3 and NO_x directly emitted to air in region i ($\text{AFF}_{s,i,\text{air}}$) reflects two pathways (Huijbregts and Seppälä, 2000):

- (1) direct deposition in the aquatic environment ($\text{AFF}_{s,i,\text{air} \rightarrow \text{aqua}}$); and
- (2) run-off and leaching to the aquatic environment after deposition on the soil ($\text{AFF}_{s,i,\text{air} \rightarrow \text{soil} \rightarrow \text{aqua}}$).

Thus

$$\text{AFF}_{s,i,\text{air}} = \text{AFF}_{s,i,\text{air} \rightarrow \text{aqua}} + \text{AFF}_{s,i,\text{air} \rightarrow \text{soil} \rightarrow \text{aqua}}$$

where

$$\text{AFF}_{s,i,\text{air} \rightarrow \text{soil} \rightarrow \text{aqua}} = \sum_j \text{AFF}_{s,i,j,\text{air} \rightarrow \text{soil}} \times \text{AFF}_{s,j,\text{soil} \rightarrow \text{aqua}}$$

The $\text{AFF}_{s,i,j,\text{air} \rightarrow \text{soil}}$ is the fraction of pollutant s that is transported from region i to the soil compartment of region j via dry and wet deposition (-); and the $\text{AFF}_{s,j,\text{soil} \rightarrow \text{aqua}}$ represents the fraction of pollutant s that is transported from the soil in region j to the aquatic environment via leaching and run-off (-). Fate factors for phosphorous compounds directly emitted to air can also be calculated by these equations.

Soil emissions

Aquatic fate factors for nitrogen (N) and phosphorus (P) inputs in the soil of region i ($\text{AFF}_{s,i,\text{soil}}$), for instance, due to animal excretion and fertilisation, may reflect three main pathways:

- 1 run-off and leaching of (in)organic N and P from the soil to the aquatic environment ($\text{AFF}_{s,i,\text{soil} \rightarrow \text{aqua}}$);
- 2 deposition on the aquatic environment (after volatilisation (NH_3) or transport by wind driven particles (P) from the soil to the air ($\text{AFF}_{s,i,\text{soil} \rightarrow \text{air} \rightarrow \text{aqua}}$); and
- 3 run-off and leaching to the aquatic environment after volatilisation (NH_3) or transport by wind driven particles (P) from the soil to the air and subsequent deposition on the soil ($\text{AFF}_{s,i,\text{soil} \rightarrow \text{air} \rightarrow \text{soil} \rightarrow \text{aqua}}$).

Thus, fate factors of N and P emissions to the soil in region i transported to the aquatic environment can be calculated by

$$\text{AFF}_{s,i,\text{agrisoil}} = \text{AFF}_{s,i,\text{agrisoil} \rightarrow \text{aqua}} + \text{AFF}_{s,i,\text{agrisoil} \rightarrow \text{air} \rightarrow \text{aqua}} + \text{AFF}_{s,i,\text{agrisoil} \rightarrow \text{air} \rightarrow \text{soil} \rightarrow \text{aqua}}$$

where

$$AFF_{s,i,soil \rightarrow air \rightarrow aqua} = AFF_{s,i,soil \rightarrow air} \times AFF_{s,i,air \rightarrow aqua}$$

and

$$AFF_{s,i,soil \rightarrow air \rightarrow soil \rightarrow aqua} = AFF_{s,i,soil \rightarrow air} \times \sum_j AFF_{s,i,j,air \rightarrow soil} \times AFF_{s,j,soil \rightarrow aqua}$$

The $AFF_{s,i,soil \rightarrow air}$ represents the fraction of pollutant s that is transported from the soil of region i to the air via volatilisation or via transport by wind driven particles (-).

Characterisation factors

The equations listed above were used to calculate the fate factors for NH_3 and NO_x air emissions, and N and P agricultural soil emissions, respectively. However, due to the lack of available data, it was not possible to connect the $AFF_{s,i,j,air \rightarrow soil}$ and the $AFF_{s,j,soil \rightarrow aqua}$ for the receiving regions j . As a preliminary solution, it was decided to calculate the $AFF_{s,i,air \rightarrow soil \rightarrow aqua}$ using fate information only related to agricultural soils. It was assumed that

$$\sum_j AFF_{s,i,j,air \rightarrow soil} \times AFF_{s,j,soil \rightarrow aqua} \approx AFF_{s,i,air \rightarrow soil} \times AFF_{s,i,agrisoil \rightarrow aqua}$$

where

$$AFF_{s,i,air \rightarrow soil} = 1 - AFF_{s,i,air \rightarrow aqua}$$

Table 4.8 lists the partial fate factors and their average values for the Netherlands, Europe and the world. The $AFF_{air \rightarrow aqua}$ for NO_x and NH_3 global air emissions were approximated from a long-range transport model for the Northern hemisphere (Galperin *et al.*, 1995; Galperin and Sofiev, 1998), taking the ratio of the deposition in the marine environment and the total emission. Depositions in the marine environment of the Northern hemisphere and total emissions were taken directly from Galperin *et al.* (1995) and Galperin and Sofiev (1998). Deposition in the marine environment of the Southern hemisphere was estimated by multiplying the total deposition exported from the Northern hemisphere (Galperin *et al.*, 1995; Galperin and Sofiev, 1998) with the area fraction of the marine environment at the Southern hemisphere (Anonymous, 1997). The $AFF_{air \rightarrow aqua}$ for Dutch and European NH_3 and NO_x emissions were derived from country-specific fate information presented by Huijbregts and Seppälä (2000). Their

partial fate factors, however, did not include nitrogen deposition in the marine environment outside Europe. As a first approximation, the correction factors for deposition outside the modelling area used in the calculation of the global $\text{AFF}_{\text{NH}_3, \text{air} \rightarrow \text{aqua}}$ (0.03) and $\text{AFF}_{\text{NO}_x, \text{air} \rightarrow \text{aqua}}$ (0.06) were added to the partial fate factors $\text{AFF}_{\text{air} \rightarrow \text{aqua}}$ for NH_3 and NO_x emissions in the Netherlands and Europe. The $\text{AFF}_{\text{P, air} \rightarrow \text{aqua}}$ could not be determined due to lack of information.

The $\text{AFF}_{\text{N, agrisoil} \rightarrow \text{air}}$ for the Netherlands, Europe and the world was derived from region-specific nitrogen inputs to the agricultural soil via animal excretion and fertilizer use and corresponding volatilisation data (Van Harmelen *et al.*, 1999; Bouwman *et al.*, 1997). In all cases, the $\text{AFF}_{\text{P, agrisoil} \rightarrow \text{air}}$ was set to zero (Van Harmelen *et al.*, 1999). The Dutch and European $\text{AFF}_{\text{agrisoil} \rightarrow \text{aqua}}$ for N and P were based on the fate information of anthropogenic agricultural soil input for the Netherlands and Europe, respectively (Van Harmelen *et al.*, 1999; Beusen *et al.*, 1995). The global $\text{AFF}_{\text{agrisoil} \rightarrow \text{aqua}}$ for N was taken from Mosier *et al.* (1998), while the global $\text{AFF}_{\text{agrisoil} \rightarrow \text{aqua}}$ for P was set equal to the European value due to the lack of available data. For direct emissions to the aquatic compartment, the fate factors were set to 1. Effect factors, based on the Redfield ratio, were taken from Heijungs *et al.* (1992).

Table 4.8 Values for partial fate factors in the calculation of characterisation factors of emissions causing aquatic eutrophication.

Partial fate factors	Netherlands	Europe	World	Reference
$\text{AFF}_{\text{NH}_3, \text{air} \rightarrow \text{aqua}}$	0.29	0.19	0.17	a-d
$\text{AFF}_{\text{NO}_x, \text{air} \rightarrow \text{aqua}}$	0.34	0.27	0.32	a-d
$\text{AFF}_{\text{N, agrisoil} \rightarrow \text{aqua}}$	0.09	0.17	0.30	e-g
$\text{AFF}_{\text{P, agrisoil} \rightarrow \text{aqua}}$	0.04	0.03	0.03	e-g
$\text{AFF}_{\text{N, agrisoil} \rightarrow \text{air}}$	0.14	0.18	0.17	e, h
$\text{AFF}_{\text{P, agrisoil} \rightarrow \text{air}}$	0	0	0	e

AFF = Aquatic Fate Factor; ^a Galperin *et al.* (1995); ^b Galperin and Soviev (1998); ^c Anonymous (1997); ^d Huijbregts and Seppälä (2000); ^e Van Harmelen *et al.* (1999); ^f Beusen *et al.* (1995); ^g Mosier *et al.* (1998); ^h Bouwman *et al.* (1997).

Fate factors and effect factors were multiplied to obtain aquatic eutrophication potentials for NH_3 and NO_x air emissions, N and P soil emissions, and N and P water emissions (Equation 1). Table 4.9 shows the fate factors, effect factors and characterisation factors of emissions causing aquatic eutrophication.

Table 4.9 Fate factors, effect factors and characterisation factors for pollutants causing aquatic eutrophication.

Emissions	Factors	AFF Neth.	AFF Europe	AFF World	AEF	AEP Neth.	AEP Europe	AEP World
Air								
NH ₃		0.35	0.33	0.42	0.35	0.12	0.11	0.15
NO _x (as NO ₂)		0.40	0.39	0.52	0.13	0.05	0.05	0.07
Water								
N		1	1	1	0.42	0.42	0.42	0.42
P		1	1	1	3.06	3.06	3.06	3.06
Agricultural soil								
N		0.14	0.23	0.37	0.42	0.06	0.10	0.16
P		0.04	0.03	0.03	3.06	0.12	0.09	0.09

AFF = Aquatic Fate Factor; AEF = Aquatic Effect Factor; AEP = Aquatic Eutrophication Potential.

Normalisation scores

To facilitate the use of the aquatic eutrophication potentials (AEPs) in LCIA, normalisation scores for three reference situations were calculated. Normalisation is an optional step in the weighting between impact categories (ISO 1998). The procedure provides the decision maker with a measure of the relative contribution from a product system to the impact categories identified by dividing the potential impact per functional unit by the impact score of a reference situation. Total yearly emissions for a reference year in a reference region are normally used to calculate normalisation scores. ISO (1998) recommends to use several reference systems to show the consequence on the outcome of the LCIA phase. Here, normalisation scores were calculated for three reference situations: (1) the Dutch territory in 1997; (2) the European territory in 1995; and (3) the world in 1990. The reference years corresponding to the reference regions were chosen for practical reasons, as they are the most recent years available for all relevant emission data per reference region. For direct N and P emissions to water, however, no (recent) data was available for Europe. In this case, emissions from nine European countries were used to extrapolate to European emission totals. The extrapolation method is based on population numbers, as suggested by Beusen *et al.* (1995). Population numbers were taken from the World Resources Institute (1996).

In the calculation of normalisation scores, emissions of the Netherlands, Europe and the world were multiplied with the corresponding characterisation factors. Table 4.10 lists per reference situation the normalisation scores for aquatic eutrophication and the relative contribution of the emissions to air, water and agricultural soil to the total scores. Note that the characterisation factor of N emitted to the agricultural soil as used in the

calculation of normalisation scores deviates from the default characterisation factor of N emissions to the agricultural soil, as given in Table 4.9. To avoid double-counting, the AEP of N emissions to the agricultural soil was set at 0.04-0.13 $\text{PO}_4^{3-}\text{-eq.}$ instead of 0.06-0.16 $\text{PO}_4^{3-}\text{-eq.}$ in the calculation of the normalisation scores for the three reference situations. The reason is that volatilisation of N from the agricultural soil to the air was already included in the calculation of total NH_3 emissions to the air.

Table 4.10 Normalisation scores for aquatic eutrophication in the Netherlands (1997), Europe (1995) and the world (1990).

	Netherlands 1997 ^a	Europe 1995 ^{b-k}	World 1990 ^{i-o}
Air ($\text{kg.PO}_4^{3-}\text{-eq., \%}$)			
NH ₃	$2.32 \cdot 10^{07}$ (16.5)	$7.27 \cdot 10^{08}$ (10.2)	$7.66 \cdot 10^{09}$ (12.9)
NO _x (as NO ₂)	$2.36 \cdot 10^{07}$ (16.8)	$9.99 \cdot 10^{08}$ (14.0)	$6.97 \cdot 10^{09}$ (11.7)
Water ($\text{kg.PO}_4^{3-}\text{-eq., \%}$)			
N	$1.91 \cdot 10^{07}$ (13.6)	$1.09 \cdot 10^{09}$ (15.3)	$9.08 \cdot 10^{09}$ (15.3)
P	$2.23 \cdot 10^{07}$ (15.9)	$1.30 \cdot 10^{09}$ (18.2)	$9.70 \cdot 10^{09}$ (16.3)
Agricultural soil ($\text{kg.PO}_4^{3-}\text{-eq., \%}$)			
N	$3.62 \cdot 10^{07}$ (25.7)	$2.57 \cdot 10^{09}$ (35.9)	$2.28 \cdot 10^{10}$ (38.3)
P	$1.62 \cdot 10^{07}$ (11.5)	$4.61 \cdot 10^{08}$ (6.4)	$3.31 \cdot 10^{09}$ (5.5)
Total ($\text{kg.PO}_4^{3-}\text{-eq., \%}$)	$1.41 \cdot 10^{08}$ (100)	$7.15 \cdot 10^{09}$ (100)	$5.95 \cdot 10^{10}$ (100)

^a Van Harmelen *et al.* (1999); ^b Draaijers *et al.* (1997); ^c EMEP/MSC-W (1999); ^d EMEP/MSC-W (2000); ^e UBA (1998); ^f Stapleton *et al.* (2000); ^g World Resources Institute (1996); ^h European Communities (1999); ⁱ Eurostat (1995); ^j FAO (2000); ^k IPCC (1996); ^l Olivier *et al.* (1996); ^m Olivier *et al.* (1998); ⁿ Mosier *et al.* (1998); ^o Caraco (1995).

Discussion

The characterisation factors and normalisation data presented here may be regarded as a first attempt towards the inclusion of a full fate analysis in the LCIA of emissions causing aquatic eutrophication. However, several shortcomings should be solved in future research. First of all, the $\text{AFF}_{\text{air} \rightarrow \text{soil} \rightarrow \text{aqua}}$ of NO_x and NH₃ emissions should be calculated by taking into account region-specific deposition and subsequent leaching and run-off instead of using fate factors representative for agricultural soils only. Deposition patterns of NH₃ and NO_x air emissions on soils and corresponding data on transport of N to aquatic systems (Posch *et al.* 1999; Seitzinger and Kroeze 1998), may substantially improve the current calculation of the (region-specific) $\text{AFF}_{\text{air} \rightarrow \text{soil} \rightarrow \text{aqua}}$ for NO_x and NH₃ emissions. These models may also be used to calculate fate factors for direct N and P emissions to other soil types than agricultural soils. Secondly, spatial differentiation in fate

factors is only included to a minor extent. The results show that differences between the characterisation factors of the Netherlands, Europe and the world remain within a factor of 1.5 for air emissions and a factor of 3 for agricultural soil emissions. Fate factors for air and soil emissions may, however, vary substantially from region to region due to differences in geographical location towards the marine environment, and different conditions of climate, plant uptake, land use and soil types (Brentstrup *et al.* 2000; Grennfelt *et al.* 1994; Huijbregts and Seppälä 2000). If it is expected that life cycle emissions of eutrophying pollutants are dominantly situated in a few regions, the corresponding *region-specific* fate factors may be needed in LCIA. Region-specific information is currently available for the $AFF_{NH_3/NO_x,air \rightarrow aqua}$ of 44 European regions (Huijbregts and Seppälä 2000). In addition, the region-specific partial fate factors $AFF_{N,soil \rightarrow air}$ and $AFF_{N,soil \rightarrow aqua}$ may be derived from Brentstrup *et al.* (2000) or from Posch *et al.* (1999). It may also be useful to derive *activity-specific* fate factors for N and P emissions to the agricultural soil ($AFF_{s,agrisoil \rightarrow aqua}$ and $AFF_{N,agrisoil \rightarrow air}$). Particularly in LCAs of agricultural products or processes, activity-specific fate factors may substantially increase the reliability of the results. As shown by various authors (Bouwman *et al.* 1997; Brentstrup *et al.* 2000; Cederberg and Mattsson 2000; Matthews 1994), the application of different types of (in)organic fertilizers and farm management may result in different fate factors for emissions to the agricultural soil. Finally, there may be a need for the derivation of the fate factors for direct P emissions to the air. Using only the effect factor in the assessment of P air emissions will lead to a substantial overestimation of LCIA outcomes for product life cycles with large P emissions to the air.

The current use of effect factors solely based on the Redfield ratio also needs further improvement. The first problem to be tackled is that the total N and P released from various anthropogenic sources may have different capabilities to contribute to aquatic eutrophication, because the chemical form of nutrients may differ (e.g. Ekholm 1998). In addition, the differences in sensitivity of aquatic ecosystems towards eutrophication are not taken into account in the current calculations, implying that a unit release to the aquatic environment is judged equally important for all aquatic ecosystems. Finally, the concept of “limiting nutrient” (see Finnveden and Potting 1999) was disregarded. This means that all aquatic ecosystems are currently assumed to be N- as well P-limited, leading to a conservative LCIA outcome for aquatic eutrophication. As pointed out by Seppälä (1999), it is possible to include the biological availability of total nutrient loads and the spatial aspects of limiting nutrient in the determination of AEPs for eutrophying emissions in Finland. Further research is, however, needed to extend his analysis to other regions.

Conclusion

The characterisation factors presented here may be regarded as a significant step forward in the life cycle impact assessment of air and agricultural soil emissions causing aquatic

eutrophication. The inclusion of fate factors reduces the importance of N and P emissions to soil towards aquatic eutrophication with a factor of 2.5-7.5 and 25-35, respectively. Fate factors for NO_x and NH_3 emissions to air also decreases the aquatic eutrophication potentials of these emissions with a factor of 2-2.5 and 2-3, respectively. Implementation in current LCIA practice is further facilitated by presenting normalisation scores for the Netherlands in 1997, Europe in 1995 and the world in 1990. Nevertheless, important improvements are still needed in the calculation of both fate and effect factors for aquatic eutrophication. Priority should be given to improve the current fate factors for the transport of NO_x and NH_3 air emissions via soil to the aquatic environment and to include differences in the biological availability of nutrients and differences in the sensitivity of the aquatic environment in the effect factors for aquatic eutrophication.

Chapter 5

Case study

The evaluation of uncertainty is relatively new in environmental life cycle assessment (LCA). A comprehensive analysis of various types of uncertainty in LCA provides useful information to assess the reliability of decisions based on LCA and may guide future research towards reducing the most important sources of uncertainty. The environmental comparison of insulation thickness in buildings serves as a case study for the evaluation of uncertainty in LCA. Parameter uncertainty was assessed with help of Monte Carlo analysis. Normative choices were modelled with help of scenario analysis. The influence of choices concerning the allocation of environmental burdens in recycling processes, future waste scenarios, and the timing, geographical scale and definition of environmental impacts were taken into account. Model uncertainty due to the lack of spatial and temporal differentiation and due to the lack of suitable characterisation factors for sum emissions was assessed by comparing the outcomes of using different assumptions. The results indicate that parameter uncertainty was the most important source of uncertainty in the environmental comparison. The effect of insulation thickness on global warming was the only effect found to be significantly different between the insulation options studied, with the thickest insulation giving the lowest life cycle impact.

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Introduction

In the environmental life cycle assessment (LCA) of products it is not always easy to determine what is 'cleaner' or more in general environmentally better. The determination of environmental improvement may become particularly difficult when changes in complex products are at stake, that have a wide variety of significant environmental impacts associated with their life cycle and when data relevant to the environmental pressures generated during the life cycle of such products are uncertain. LCAs may give rise to incorrect decisions when uncertainty is not properly accounted for. Model outcomes can be uncertain for several reasons, which have implications for the way the uncertainty is dealt with (Morgan and Henoion, 1990). A general distinction can be made between parameter uncertainty, model uncertainty and uncertainty due to choices (Hertwich *et al.*, 2000; Huijbregts, 1998a). Parameter uncertainty is introduced by the empirical inaccuracy of input data. Model uncertainty is introduced by disregarding potentially relevant aspects within the present LCA structure. Uncertainty due to choices reflects that LCA outcomes inherently depends on (normative) choices in the modelling procedure. Although various types of uncertainty in LCA outcomes have been analysed in isolation (Heijungs, 1996; Weidema and Wesnaes, 1996; Steen, 1997; Chevalier and Le Tno, 1996; Maurice *et al.*, 2000) or in a simplified manner (Huijbregts, 1998b), a combination of above mentioned uncertainties in LCA case studies have never been assessed. A simultaneous assessment of the various sources of uncertainty is, however, needed to quantify the combined effect and the relative importance of the different types of uncertainty in LCA.

This paper addresses this important issue by analysing to what extent various sources of uncertainty may influence the environmental comparison of three insulation scenarios for a Dutch one-family dwelling. The comparison is considered relevant for environmental policy, as life cycle impacts of buildings are substantial and highly diverse (Reijnders and Van Roekel, 1999; Reijnders and Huijbregts, 2000), and a relatively large part of the environmental impact of buildings is associated with energy consumption in the use stage of a building's life cycle (Vringer and Blok, 2000). Insulation is important in reducing energy consumption in the use stage of a building, with increasing insulation leading to reductions in energy consumption. However, reduction of energy consumption during the occupation of buildings resulting from increased insulation thickness follows the law of diminishing energy savings. Furthermore, environmental impacts related to the life cycle of products providing for insulation tend to increase when the insulation effect increases, leading to the existence of environmentally optimal insulation in dwellings.

Parameter uncertainties were addressed by means of Monte Carlo analysis. The implications of normative choices are modelled with help of scenario analysis. Choices concerning allocation of environmental burdens in recycling processes, future waste scenarios, and the timing, geographical scale and definition of environmental impacts were modelled. Finally, the importance of model uncertainty due to the lack of spatial and temporal differentiation in the impact assessment of acidifying and eutrophying emissions

and model uncertainty due to the lack of suitable characterisation factors for sum emissions in the impact assessment of emissions causing toxicity and photochemical ozone formation were assessed by comparing outcomes of alternative model formulations. A resampling technique was used to automatize the assessment of model uncertainties.

Environmental life-cycle assessment

An LCA is generally divided in the goal and scope definition, the inventory analysis, the impact assessment and the interpretation (ISO, 1997a). In the goal and scope definition, the aim and the subject of an LCA study are determined and the basis of comparison, the so-called 'functional unit', is defined. The scope of this study concerns three insulation options. These were analysed on a building level with Expanded Polystyrene (EPS) as insulation material (Table 5.1). The first case reflects insulation thickness in wall, roof and floor commonly applied in Dutch building practice of new dwellings. The second case reflects insulation thickness considered as a practical maximum applied in current Dutch building practice, while the third case reflects insulation thickness which may be applied in future Dutch building practice. The functional unit applied is *'the provision of heat comfort during the life time of the reference Dutch one-family dwelling'*.

Table 5.1 Insulation thicknesses in the building components wall, flat roof, sloping roof and ground floor for three insulation options

Case	Wall	Flat roof	Sloping roof	Ground floor
EPS1	95 mm	150 mm	150 mm	150 mm
EPS2	185 mm	200 mm	200 mm	200 mm
EPS3	185 mm	400 mm	400 mm	400 mm

The dimensions of the dwelling and the determination method of the energy performance for heat provision are given by NNI (1994, 1995). If different insulation options are to be compared, not only the amount of insulation materials, applied to the one-family building, will differ, but there will also be changes in the amount of other materials used. For instance, increasing the wall insulation thickness from 95 mm to 185 mm is only possible when, instead of using sandlime bricks for the inner wall, a wooden inner wall with insulation material inside is applied. These changes were also taken into account in the environmental comparison (Table 5.2). In the inventory analysis, for each of the three insulation options data were gathered for all the relevant processes involved in the life cycle (NNI, 1994, 1995, 1997; Adan, 1994; Huffmeijer, 1995; Ceuterick, 1993; Weibel and Stritz, 1995; Kaskens *et al.*, 1992; Richter *et al.*, 1995; Habersatter and Fecker, 1998; DHV-AIB, 1995, Boustead, 1993-1997; Frischknecht *et al.*, 1996; Mak *et*

al., 1996). Matrix computation was used to obtain the inventory table (Heijungs, 1994; Hendrickson *et al.*, 1998). The outcome of the inventory analysis is a list of all extractions of resources and emissions of substances caused by the functional unit for every insulation option considered.

Table 5.2 Typical amounts of materials and energy used per function unit for the three insulation options

Input	Unit	EPS1	EPS2	EPS3
Natural gas	m ³	44000	39000	34000
Expanded Polystyrene	kg	330	470	840
Sandlime brick	kg	6200		
Portland cement	kg	1250	25	75
Gypsum plaster	kg	150		
Rock wool	kg		10	10
Gypsum cardboard	kg		450	450
Polyethylene foil	kg		20	20
Timber wood	kg		500	900
Stainless steel	kg		100	100
Clay brick	kg		50	150
Particle board	kg		10	600
Concrete	kg		75	200
Polyurethane glue	kg		1	25

The impact assessment aims to improve the understanding the environmental importance of the inventory result (Udo de Haes *et al.*, 1999). Releases of pollutants and the extractions of resources of a product system are aggregated using a number of environmental impact categories, such as global warming, stratospheric ozone depletion and human toxicity.

$$S_{j,k} = \sum_r \sum_i \sum_x Q_{j,x,i,r} \times M_{x,i,r,k}$$

where $S_{j,k}$ is the impact score for impact category j per functional unit of product system k (e.g. kg(CO₂-equivalents for global warming); $Q_{j,x,i}$ is the characterisation factor for impact category j of substance x emitted to compartment i in region r (e.g. CO₂-equivalents for global warming); and $M_{x,i,r,k}$ is the emission of substance x to compartment i in region r per functional unit of product system k (kg). Characterisation factors, defined as the change in impact per unit amount of additional 'release' (or extraction) (Heijungs *et al.*, 1992), represent the relative importance of the stressor to an impact category. Well-known characterisation factors are human toxicity potentials (Hertwich *et al.*, 1998;

Huijbregts *et al.*, 2000a), global warming potentials (Albritton *et al.*, 1995, 1996), and ozone depletion potentials (Solomon *et al.*, 1995). Potential impacts of emissions causing climate change (Albritton *et al.*, 1995, 1996; Solomon *et al.*, 1995), tropospheric photochemical ozone formation (Derwent *et al.*, 1996, 1998; Hayman and Derwent, 1997; Jenkin and Hayman, 1999), toxic impacts on humans and ecosystems (Huijbregts *et al.*, 2000a, 2001a), acidification and eutrophication (Huijbregts *et al.*, 2000c; Huijbregts and Seppälä, 2001) were assessed in the comparison. The final phase in an LCA study is the interpretation of the results from the previous three steps, to draw conclusions and to formulate recommendations for decision makers.

Uncertainty analysis

Parameter uncertainty

Estimates of parameter uncertainty were represented by an uncertainty factor k which is defined such that 95% of the values of a stochastic variable (X) are within a factor k from the median $M(X)$ of a lognormal distribution (Slob, 1994). In case of lack of empirical data, a triangular uncertainty distribution was defined, based on expert judgement, in which the uncertainty factor k is defined such that 100% of the values of a stochastic variable (X) are

Table 5.3 Parameter uncertainty estimates of the functional unit, technology coefficients and emission coefficients.

	Distribution (k)	References
Functional unit		
average indoor and outdoor temperature	L (1.3)	a, b
resources	L (1.5)	a-e
loss fractions	T (2)	p
Technology coefficients		
central, non-substitutable resources	L (2)	f, g
less central and substitutable resources	L (10)	f, g
waste handling fractions	T (2)	p
Emission coefficients		
CO ₂ air emissions	L (1.05)	h
SO ₂ air emissions	L (2)	f, g
Air emissions other than CO ₂ and SO ₂	L (10)	f, g
Water emissions	L (100)	f, g
Soil emissions	L (100)	f, g
L = lognormal distribution, between brackets the uncertainty factor k^L , defined as the ratio of the median and 97.5 th percentile; T = triangular distribution, between brackets the uncertainty factor k^T , defined as the ratio of the modus and the maximum value; p = personal judgement. ^a Lomas and Eppel (1992); ^b Pettersen (1994); ^c Adan (1994); ^d Huffmeijer (1995); ^e Ceuterick (1993); ^f Maurice <i>et al.</i> (2000); ^g Finnveden and Lindfors (1998); ^h Olivier (1998).		

within a factor k from the modus $M'(X)$ of a triangular distribution. Table 5.3 shows the uncertainty in parameters used in the derivation of the functional unit, the technology matrix, and the environmental intervention matrix. Table 5.4 gives an overview of the uncertainty in characterisation factors due to parameter uncertainties in the characterisation models. Note, however, that the uncertainty factor representing the variance in the human toxicity potentials reflects not only parameter uncertainty but also inherent variation between humans, such as differences in food intake (Huijbregts *et al.*, 2000b).

Table 5.4 Parameter uncertainty estimates of characterisation factors.

Characterisation factor	Distribution (k)	References
Global Warming Potential ^a	L (1.4, 2.5)	h-j
Stratospheric Ozone Depletion Potential	L (1.5)	k-n
Photochemical Ozone Creation Potential ^b	L (1.2-2.1)	o-r
Acidification Potential ^c	L (2.2)	s-u
Terrestrial Eutrophication Potential ^d	L (2.2)	s-u
Aquatic Eutrophication Potential	L (1.8)	v, w
Terrestrial Ecotoxicity Potential ^{e, f}	L (500, 1000)	x
Fresh water Aquatic and Sediment Ecotoxicity Potential ^{e, f}	L (50, 100)	x
Marine Aquatic and Sediment Ecotoxicity Potential ^{e, f}	L (50, 200)	x
Human Toxicity Potential ^{f, g}	L (50)	x

L = lognormal distribution, between brackets the uncertainty factor(s) k^L , defined as the ratio of the 50th and 97.5th percentile of the uncertainty distribution: ^a The the uncertainty factor k^L of the GWP of substances with a net positive radiative forcing (e.g. CH₄) is 1.4, while the uncertainty factor k^L of the GWP of substances with a net negative radiative forcing (e.g. CFC-11) is 2.5; ^b the uncertainty factor k^L for the POCP depends on the substance-specific rate coefficient k_{OH} (Jenkin and Hayman, 1999). If $k_{OH} < 4.0 \cdot 10^{-13} \text{ cm}^3 \cdot \text{molecules}^{-1} \cdot \text{s}^{-1}$, $k^L = 2.1$; if $k_{OH} > 4.0 \cdot 10^{-11} \text{ cm}^3 \cdot \text{molecules}^{-1} \cdot \text{s}^{-1}$, $k^L = 1.2$; and if $4.0 \cdot 10^{-13} < k_{OH} < 4.0 \cdot 10^{-11} \text{ cm}^3 \cdot \text{molecules}^{-1} \cdot \text{s}^{-1}$, $k^L = -0.2 \cdot \ln(k_{OH}) - 3.5$; ^c the correlation coefficient between acidification potentials of NH₃, NO_x and SO₂ emitted in the same region is set at 0.9 (Seppälä, 1999); ^d the correlation coefficient between terrestrial eutrophication potentials of NH₃ and NO_x emitted in the same region is set at 0.9 (Seppälä, 1999); ^e The lowest uncertainty factor k^L is connected to the ecotoxicity potentials of substances directly emitted to the air or directly emitted to the compartment in which the impact occurs, while the highest uncertainty factor k^L is connected to the other ecotoxicity potentials; ^f the correlation coefficient between toxicity potentials of a substance emitted to air, fresh water and/or industrial soil is set at 0.9 (Huijbregts *et al.*, 2000b); ^g the variance in the human toxicity potentials is not only caused by parameter uncertainties but also by human variability (Huijbregts *et al.*, 2000b); ^h Albritton *et al.* (1995); ⁱ Albritton *et al.* (1996); ^j Janssen and Fransen (1997); ^k Solomon *et al.* (1995); ^l Daniel *et al.* (1995); ^m Daniel *et al.* (1999); ⁿ Selmy *et al.* (1997); ^o Jenkin and Hayman (1999); ^p Atkinson (1988); ^q SRC (1993); ^r SRC (2000); ^s Alcamo and Bartnicki (1990); ^t Barkman (1997); ^u Seppälä (1999); ^v Beusen *et al.* (1995); ^w Redfield *et al.* (1963); ^x Huijbregts *et al.* (2000b).

The uncertainty propagation of parameter uncertainties was performed by means of Monte Carlo analysis with Latin Hypercube sampling (LHS) in Crystal Ball™ 4.0e (Decisioneering, 1998). Each LHS experiment consisted of 10.000 iterations which generally produces a representative picture of the complete uncertainty distribution of the model outcome (Morgan and Henoion, 1990). As the environmental comparison is concerned with relative differences, the interdependency between the product systems under

consideration should be taken into account (Huijbregts, 1998b). Therefore, data inputs equal for the insulation combinations under study, such as characterisation factors and environmental interventions caused by the same economic activities, were varied simultaneously in the Monte Carlo analysis. This was done by computing the quotients of the product systems for their potential contribution to the impact categories and the scenarios involved. The environmental profiles of the product systems compared were considered to be significantly different, if 95% of the iterations lays above or beneath 1.

Crystal Ball™ 4.0e is also equipped with a tool that calculates the uncertainty importance of each parameter. It calculates the Spearman rank correlation coefficient between each input parameter and each impact category outcome. If a parameter and a certain outcome have a high correlation coefficient, this implies that the uncertainty in this parameter has a relatively large impact on the uncertainty in the impact score. In the current assessment, the relative contribution of each uncertain parameter to the uncertainty of impact scores is approximated by the square value of the rank correlation coefficient r normalised to 100%.

Uncertainty due to choices

When performing LCAs, normative choices are unavoidable. In the inventory analysis uncertainty due to the choice for a specific open-loop recycling allocation method and the choice for a future waste scenario were combined. The 'cut-off method' and the 'avoided-impacts method' were used to allocate the environmental burdens associated with the recycling of the products. These methods reflect two extreme visions on how to allocate environmental burdens in open-loop recycling processes (Kortman *et al.*, 1996). The cut-off method allocates the environmental interventions caused by the waste recycling process to the receiving product system, while the avoided-impacts method allocates the environmental interventions caused by the waste recycling process to the product system under study, but also credits the product system by subtracting the avoided environmental interventions from the original inventory table. In addition, a pessimistic and optimistic future waste recycling scenario were defined for the three insulation options under study. Finally, two 'extreme' combinations were constructed and the effect of the two combinations on the LCA outcomes were calculated by means of scenario analysis (Huijbregts, 1998a). The cut-off method combined with the pessimistic future waste recycling scenario and the avoided-impacts method combined with the optimistic future waste recycling scenario were the two extreme combinations. Uncertainty due to choices in the impact assessment of emissions causing global warming, toxic impacts, acidification and terrestrial eutrophication was also assessed. Firstly, the choice for a certain time horizon was considered. Results were obtained for global warming using characterisation factors for the time horizons 20, 100 and 500 years (Albritton *et al.*, 1995, 1996), while for toxicity the results for an infinite time horizon was also included (Huijbregts *et al.*, 2000a, c). Another potentially important

choice is the decision whether or not to include potential toxic impacts exported from the emitting region (Hertwich *et al.*, 1998), as exposure that occurs outside the selected area may fully dominate the potential impacts, obscuring those in the emitting region (Huijbregts *et al.*, 2001a). Results for the impact assessment of the toxicity categories were calculated by including and excluding potential toxic impacts outside the scale of emission. Finally, the choice of including or excluding 'below threshold' impact changes for acidification and terrestrial eutrophication was assessed. Two scenarios were used in the calculation of impact scores for acidification and terrestrial eutrophication: (1) the marginal impact change in all ecosystems considered and (2) the marginal impact change in ecosystems where the no-effect level is actually exceeded (Huijbregts *et al.*, 2000c).

Model uncertainty

In LCA, spatially and temporally variation in emissions and characterisation factors is generally disregarded. In this study, uncertainty due to the lack of spatial variability was assessed for terrestrial eutrophication and acidification. Region-specific characterisation factors of 44 European regions were available for NO_x, NH₃ and SO₂ air emissions (Huijbregts *et al.*, 2000c). The gain of having region-specific knowledge was analysed by separately tabulating NO_x, NH₃ and SO₂ air emissions in the Netherlands and comparing the uncertainty in the model outcomes using Dutch characterisation factors with the outcomes in the model outcomes assuming that no region-specific information was available. For the unit processes lacking spatial information, in every LHS iteration substance-specific characterisation factors of one region were randomly drawn with replacement from the characterisation factors of the 44 regions available. This bootstrap procedure was applied for every unit process independently.

Acidification potentials and terrestrial eutrophication potentials, based on the marginal impact change in ecosystems where the no-effect level is actually exceeded, depend not only on the emitting region, but also on the emission year chosen (Huijbregts *et al.*, 2000c). To take this temporal dependency into account, current air emissions, related to the construction of the building, and future emissions, occurring during the occupation and destruction of the building, were separately tabulated in the inventory analysis and multiplied with their corresponding characterisation factors. The importance of having this information was assessed by comparing the temporally explicit model outcomes with model outcomes calculated by randomly drawing with replacement characterisation factors related to the current and future situation.

Another model uncertainty in LCA is the lack of suitable characterisation factors for sum emissions. To assess the importance of this lack of information in our case study, photochemical ozone creation potentials (POCP) of individual volatile organic substances belonging to (subgroups of) non methane volatile organic carbon (NMVOC) emissions were identified (Derwent *et al.*, 1996). Again, in every LHS iteration one value was separately drawn with replacement from the set of POCPs for all the unit processes

reporting NMVOC emissions. In the impact assessment of sum emissions of metals to air and fresh water, the set of toxicity potentials of 19 metals from Huijbregts *et al.* (Huijbregts *et al.*, 2000a, 2001a) was used for this purpose.

Results

For every comparison, frequency plots were produced, representing the uncertainty distributions of the ratio of the impact scores. Table 5.5 lists some statistical characteristics of the uncertainty distributions taking account of all the spatial and temporal information available. In all cases, the building with the thickest insulation shows the smallest contribution of the building sector to global warming. All other comparisons did not show significantly different outcomes. Combined uncertainty, defined as the ratio of the highest 95th and lowest 5th percentile of the uncertainty distributions involved, is the lowest for the comparison of the contribution to global warming (up to a factor 1.5). The comparison of the impact categories stratospheric ozone depletion, photochemical ozone creation, acidification, terrestrial eutrophication and aquatic eutrophication show uncertainties between a factor 1.5 and 3. Uncertainty in the comparison of the toxicity impact categories is generally the largest (up to a factor 10).

Scenario differences in the inventory analysis and the impact assessment, defined as the ratio of the lowest and highest median value of the scenarios involved, are for all impact categories within a factor 1.5. Model uncertainty, defined as the scenario-specific ratio of the 95th and 5th percentile excluding parameter uncertainty in the calculations, also remain within a factor 1.5. The lack of spatial information in the inventory analysis, except for Dutch emissions, introduces uncertainty in the outcomes for acidification and terrestrial eutrophication up to a factor 1.5. If, the region-specific information available for the Netherlands was disregarded, uncertainty increases up to a factor 1.1 for both acidification and terrestrial eutrophication. Disregarding temporally explicit information increased the uncertainty in the model outcomes up to a factor 1.1 and 1.5 for terrestrial eutrophication and acidification. Model uncertainties due to lack of specific NMVOC or heavy metal emissions can be up to a factor 1.5. Parameter uncertainties, defined as the scenario-specific ratio of the 95th and 5th percentile excluding model uncertainty in the calculations, result in uncertainties between a factor 2 to 10 in the comparison of toxicity scores. For global warming, the lowest influence of parameter uncertainties is found (a factor 1.1 to 1.2). For the other impact categories, parameter uncertainties cause between a factor 1.5 and 2.5 variation in the environmental comparison.

The uncertainty importance analysis, used to assess which parameters have a relatively large impact on the uncertainty in the comparison, revealed that parameter uncertainties in the energy simulation model of the occupation phase, such as indoor temperature, ventilation losses and insulation properties of EPS are important in the comparison of contributions to global warming (> 60%). For stratospheric ozone depletion, the dominant cause of parameter uncertainty is uncertainty in Halon 1301 emissions due to

oil extraction and conversion (> 50%). Parameter uncertainty in the comparison of tropospheric ozone formation was predominantly caused by uncertainties in pentane emissions during blowing of EPS (up to 30%), NMVOC emissions due to natural gas exploration (up to 15%), and again energy use calculations for the use phase of the building (up to 20%). Uncertainty in NO_x emissions due to combustion of natural gas during the occupation phase of the building (up to 35%), NO_x emissions caused by cement production (up to 25%), and energy use during the occupation of the building (up to 30%) are found important for aquatic eutrophication, terrestrial eutrophication and acidification. Uncertainty in characterisation factors of Dutch emissions may also contribute to the uncertainty in the comparison of acidifying and terrestrially eutrophying impacts (up to 15%).

Uncertainty in the comparison of ecotoxicological impacts is predominantly caused by uncertain estimates of the amount of heavy metal emissions (e.g. Co, Ni and V) related to natural gas exploration (together up to 10%), energy use during the occupation of the building (up to 10%), and ecotoxicity potentials of heavy metals (together up to 30%). If the avoided impact allocation method is used, uncertainty in the amount of steam produced during EPS production is also found important for the fresh water ecotoxicity outcomes (up to 10%). Finally, important parameter uncertainties in the comparison of the human toxicity profiles were uncertain estimates of Polycyclic Aromatic Hydrocarbon (PAH) air emissions caused by natural gas combustion during the occupation of the building (up to 10%) and human toxicity potentials (HTP) of PAH, As, Cr and Se emissions to air (together up to 20%).

Discussion

For all impact categories, except global warming, uncertainties were too large to indicate which insulation option should be preferred from an environmental point of view. To improve this situation most effectively, reducing uncertainties introducing the largest spread in the model outcomes should have priority. In none of the comparisons normative choices, the lack of spatial and temporal differentiation, and the lack of suitable characterisation factors for sum emissions appeared to be a more important source of uncertainty than parameter uncertainties. Although uncertainty in the absolute outcomes of the product systems involved can be high, the influence of these types of uncertainty on *relative differences* between the product systems, which is the focus in an environmental comparison, almost completely level out between the product systems involved. Parameter uncertainty appeared to be the most important source of uncertainty for all the impact categories involved. In particular, parameters applied in the energy simulation model, material use for building construction, emission coefficients for the production of EPS, oil and natural gas exploration, and natural gas combustion were found important. Furthermore, uncertainty in Dutch acidification and terrestrial

Table 5.5 Results of the environmental comparison. The median comparison indicators and corresponding 90% confidence intervals (in parentheses) are listed. Comparison indicators significantly different from 1 ($p < 0.05$) are indicated with an asterisk. TH = Time horizon; CL = Critical load; GS = Geographical scale; C-O = cut-off open loop recycling combined with the pessimistic future waste recycling scenario; AI = avoided-impacts open loop recycling combined with the optimistic future waste recycling scenario.

Impact category	EPS1/ EPS2		EPS2/EPS3		EPS1/EPS3	
	C-O	AI	C-O	AI	C-O	AI
Global warming						
- TH = 20 years	1.13 (1.08-1.22)*	1.14 (1.09-1.24)*	1.11 (1.05-1.19)*	1.14 (1.08-1.22)*	1.26 (1.15-1.44)*	1.30 (1.18-1.51)*
- TH = 100 years	1.13 (1.08-1.22)*	1.15 (1.09-1.24)*	1.11 (1.05-1.19)*	1.14 (1.08-1.22)*	1.26 (1.15-1.44)*	1.30 (1.18-1.52)*
- TH = 500 years	1.14 (1.08-1.22)*	1.15 (1.09-1.24)*	1.11 (1.05-1.19)*	1.14 (1.08-1.22)*	1.27 (1.15-1.45)*	1.31 (1.18-1.53)*
Stratospheric ozone depletion						
	1.00 (0.77-1.12)	0.97 (0.76-1.17)	0.84 (0.63-1.04)	0.73 (0.59-1.02)	0.85 (0.49-1.15)	0.70 (0.46-1.16)
Photochemical ozone formation						
	0.91 (0.65-1.16)	0.94 (0.67-1.19)	0.78 (0.55-1.06)	0.79 (0.56-1.07)	0.73 (0.44-1.11)	0.70 (0.43-1.07)
Acidification						
- CL = above & below	1.03 (0.74-1.29)	1.14 (0.84-1.65)	0.81 (0.62-1.02)	0.92 (0.65-1.18)	0.85 (0.49-1.18)	1.08 (0.56-1.72)
- CL = only above	0.98 (0.72-1.30)	1.05 (0.77-1.47)	0.74 (0.60-1.01)	0.79 (0.61-1.05)	0.73 (0.45-1.10)	0.85 (0.49-1.34)
Terrestrial eutrophication						
- CL = above & below	1.09 (0.85-1.45)	1.17 (0.94-1.76)	0.91 (0.65-1.09)	1.00 (0.67-1.24)	1.03 (0.59-1.32)	1.20 (0.70-1.92)
- CL = only above	1.09 (0.85-1.43)	1.16 (0.95-1.65)	0.93 (0.68-1.10)	1.01 (0.70-1.23)	1.03 (0.61-1.34)	1.19 (0.72-1.81)
Aquatic eutrophication						
	1.09 (0.85-1.46)	1.17 (0.96-1.78)	0.99 (0.66-1.08)	0.96 (0.68-1.12)	1.01 (0.60-1.34)	1.16 (0.72-1.63)
Fresh water aquatic ecotoxicity						
- TH = 20 years; GS = continental	1.33 (0.87-3.04)	1.39 (0.96-2.91)	0.77 (0.58-1.06)	0.72 (0.56-1.05)	1.14 (0.56-2.14)	1.11 (0.60-2.01)
- TH = 100 years; GS = continental	1.32 (0.86-3.08)	1.39 (0.95-2.88)	0.77 (0.58-1.05)	0.71 (0.56-1.05)	1.12 (0.56-2.14)	1.10 (0.59-2.00)
- TH = 500 years; GS = continental	1.28 (0.83-2.87)	1.34 (0.92-2.77)	0.76 (0.58-1.04)	0.71 (0.56-1.03)	1.08 (0.53-2.02)	1.06 (0.57-1.89)
- TH = infinite; GS = continental	1.23 (0.80-2.70)	1.28 (0.87-2.65)	0.75 (0.58-1.03)	0.71 (0.57-1.02)	1.03 (0.50-1.91)	1.02 (0.53-1.83)
Fresh water sediment ecotoxicity						
- TH = 20 years; GS = continental	1.33 (0.87-3.05)	1.39 (0.95-2.88)	0.78 (0.59-1.06)	0.72 (0.57-1.06)	1.15 (0.58-2.14)	1.11 (0.60-1.99)
- TH = 100 years; GS = continental	1.30 (0.86-2.90)	1.36 (0.94-2.79)	0.77 (0.59-1.05)	0.72 (0.57-1.05)	1.12 (0.57-2.05)	1.10 (0.59-1.95)
- TH = 500 years; GS = continental	1.27 (0.83-2.85)	1.33 (0.91-2.76)	0.76 (0.59-1.04)	0.72 (0.57-1.04)	1.08 (0.54-2.02)	1.06 (0.57-1.87)
- TH = infinite; GS = continental	1.23 (0.80-2.66)	1.28 (0.87-2.59)	0.75 (0.59-1.03)	0.71 (0.58-1.03)	1.03 (0.52-1.90)	1.02 (0.55-1.81)
Marine aquatic ecotoxicity						
- TH = 20 years; GS = continental + global	1.02 (0.56-2.14)	1.09 (0.67-2.18)	0.72 (0.59-1.02)	0.71 (0.58-1.02)	0.78 (0.37-1.55)	0.83 (0.42-1.52)
- TH = 100 years; GS = continental + global	1.06 (0.63-2.36)	1.13 (0.70-2.37)	0.72 (0.59-1.01)	0.70 (0.58-1.01)	0.81 (0.40-1.68)	0.85 (0.44-1.67)
- TH = 500 years; GS = continental + global	1.07 (0.64-2.38)	1.13 (0.70-2.41)	0.72 (0.59-1.01)	0.70 (0.58-1.01)	0.82 (0.41-1.69)	0.85 (0.44-1.65)
- TH = infinite; GS = continental + global	1.15 (0.75-2.64)	1.20 (0.81-2.58)	0.72 (0.58-1.02)	0.69 (0.57-1.02)	0.92 (0.46-1.84)	0.92 (0.49-1.76)
- TH = infinite; GS = continental	1.13 (0.74-2.52)	1.19 (0.80-2.47)	0.73 (0.58-1.02)	0.70 (0.57-1.02)	0.90 (0.45-1.77)	0.92 (0.49-1.71)
Marine sediment ecotoxicity						
- TH = 20 years; GS = continental + global	1.03 (0.59-2.17)	1.09 (0.68-2.15)	0.73 (0.59-1.03)	0.72 (0.58-1.03)	0.80 (0.39-1.57)	0.85 (0.43-1.55)
- TH = 100 years; GS = continental + global	1.04 (0.62-2.24)	1.11 (0.69-2.28)	0.73 (0.59-1.01)	0.71 (0.58-1.02)	0.81 (0.41-1.63)	0.85 (0.44-1.59)
- TH = 500 years; GS = continental + global	1.05 (0.61-2.30)	1.11 (0.68-2.28)	0.73 (0.59-1.01)	0.70 (0.58-1.01)	0.80 (0.40-1.62)	0.84 (0.43-1.59)
- TH = infinite; GS = continental + global	1.12 (0.74-2.54)	1.18 (0.78-2.48)	0.72 (0.58-1.02)	0.69 (0.57-1.01)	0.89 (0.44-1.77)	0.90 (0.48-1.70)
- TH = infinite; GS = continental	1.12 (0.74-2.46)	1.17 (0.79-2.40)	0.72 (0.58-1.02)	0.70 (0.58-1.02)	0.89 (0.45-1.70)	0.91 (0.48-1.66)
Terrestrial ecotoxicity						
- TH = 20 years; GS = continental + global	0.74 (0.22-1.12)	0.78 (0.25-1.16)	0.72 (0.57-1.04)	0.75 (0.58-1.08)	0.51 (0.14-1.16)	0.57 (0.16-1.23)
- TH = 100 years; GS = continental + global	0.72 (0.20-1.11)	0.76 (0.22-1.15)	0.70 (0.57-1.01)	0.73 (0.57-1.04)	0.49 (0.12-1.10)	0.53 (0.14-1.18)
- TH = 500 years; GS = continental + global	0.71 (0.19-1.09)	0.74 (0.21-1.12)	0.69 (0.57-1.01)	0.72 (0.57-1.02)	0.47 (0.12-1.07)	0.51 (0.13-1.14)
- TH = infinite; GS = continental + global	0.85 (0.44-1.15)	0.87 (0.43-1.16)	0.78 (0.58-1.08)	0.81 (0.59-1.10)	0.62 (0.33-1.21)	0.66 (0.33-1.24)
- TH = infinite; GS = continental	0.84 (0.46-1.15)	0.86 (0.45-1.17)	0.77 (0.58-1.07)	0.80 (0.59-1.09)	0.62 (0.34-1.30)	0.65 (0.34-1.24)
Human toxicity						
- TH = 20 years; GS = continental + global	0.97 (0.54-1.15)	0.96 (0.45-1.16)	0.88 (0.58-1.12)	0.91 (0.61-1.13)	0.83 (0.36-1.26)	0.85 (0.33-1.29)
- TH = 100 years; GS = continental + global	0.95 (0.50-1.15)	0.95 (0.42-1.16)	0.86 (0.59-1.11)	0.90 (0.60-1.13)	0.80 (0.33-1.25)	0.83 (0.30-1.28)
- TH = 500 years; GS = continental + global	0.93 (0.37-1.14)	0.93 (0.34-1.15)	0.84 (0.56-1.11)	0.88 (0.58-1.12)	0.76 (0.24-1.24)	0.78 (0.23-1.27)
- TH = infinite; GS = continental + global	1.03 (0.68-1.40)	1.04 (0.61-1.46)	0.85 (0.59-1.10)	0.86 (0.60-1.11)	0.88 (0.44-1.31)	0.90 (0.42-1.33)
- TH = infinite; GS = continental	0.99 (0.61-1.18)	0.99 (0.52-1.19)	0.87 (0.60-1.12)	0.90 (0.62-1.13)	0.84 (0.41-1.27)	0.86 (0.37-1.30)

eutrophication potentials, and uncertainty in toxicity potentials of heavy metals and carcinogenic PAHs significantly contribute to the uncertainty in the model comparison of toxic impacts on humans and ecosystems. The spread in human toxicity potentials resulting from human variability was of minor importance in this case study. The reason is that variation in human toxicity potentials (HTPs) of air emissions, important contributors to the uncertainty in the comparison, is dominantly caused by parameter uncertainty (Huijbregts *et al.*, 2000b).

Apparently, the relevancy of our case study outcomes would most effectively benefit from reducing parameter uncertainties in the various LCA steps. A detailed description of uncertainty ranges of environmental interventions per unit process in databases and other data sources is, however, generally lacking, complicating the feasibility of reducing uncertainties in the inventory analysis. A first step in this respect is the development of a common database format, in which uncertainty ranges for life cycle inventory data should be listed (Weidema, 1999). Reducing parameter uncertainties in the impact assessment of toxic substances mainly require additional information of substance-specific input parameters that describe transport mechanisms, substance degradation, and no-effect concentrations (Huijbregts *et al.*, 2000b), while uncertainty in no-effect concentrations appeared to be the most important source of uncertainty in the calculation of acidification and terrestrial eutrophication potentials (Alcamo and Bartnicki, 1990; Barkman, 1997).

It should be stressed that the uncertainty analysis did not cover all possible sources of uncertainty and that the results are only representative for this particular case study. Firstly, model uncertainties related to the calculation of energy demand during the occupation of the building were not assessed. For instance, the NNI model (14, 15) applies a simplified heat balance in its calculations, and it does not account for a possible increase in cooling demand due to increased insulation thickness. Secondly, the importance of the lack of spatial differentiation for other impact categories than acidification and terrestrial eutrophication was not assessed due to lack of region-specific characterisation factors. This may, however, be an important factor in the assessment of (metal) toxicity (Huijbregts *et al.*, 2001a), aquatic eutrophication (Huijbregts and Seppälä, 2001) and photochemical ozone formation (Andersson-Sköld and Holmberg, 2000). Furthermore, the models used in the calculation of characterisation factors may suffer from significant uncertainties in their model structure (Hertwich *et al.*, 2000; Huijbregts *et al.*, 2000c; Ragas *et al.*, 1999). In the context of our study, it was not feasible to assess the impact of these model uncertainties in our uncertainty analysis. In addition, not all potentially relevant impact categories and associated uncertainties were taken into account in the environmental comparison, such as radiation (Frischknecht *et al.*, 2000), land use (Köllner, 2000) and abiotic depletion (Guinée and Heijungs, 1995). The weighting step between impact categories was also excluded in the environmental comparison, excluding the uncertainty in normalisation data and weighting factors, but also preventing a final assessment of the relevancy of the relative differences found. A further analysis of these uncertainties is certainly required in LCA context. The influence

of the goal and scope definition on the importance of the different types of uncertainty should also be addressed in future research. If, for instance, different types of insulation materials, such as expanded polystyrene and polyurethane, are to be compared instead of different insulation thickness options of the same insulation material, the importance of the different types of uncertainty may change.

Despite the fact that it was only possible to analyse part of the uncertainties relevant for LCA, our evaluation showed for the first time the influence of various types of uncertainty in the various LCA steps. The product systems compared did not significantly differ from each other, except for global warming. It appeared that the uncertainty in *relative differences* between product systems was mainly influenced by parameter uncertainties and less by normative choices and model uncertainties taken into account.

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Chapter 6

Concluding remarks

This thesis mainly deals with the evaluation of uncertainty and variability in the life cycle impact assessment of toxic, acidifying and eutrophying emissions. This section puts the various types of uncertainty and variability into perspective and gives recommendations for further research.

Toxicity potentials

In this thesis, toxicity potentials combine the results of a multi-media fate and exposure models with simple effect parameters for humans and ecosystems. As shown in Section 3.1, different models may produce different outcomes. Differences of several orders of magnitude were found between the newly calculated toxicity potentials and those previously calculated by Guinée *et al.* (1996). In addition to the improved model structure and substance-specific input parameters, three new impact categories (marine aquatic environment, marine sediment environment, fresh water sediment environment) were included in the calculations. Although this may lead to a more detailed impact assessment, the additional impact categories may also decrease the practicability of LCA case studies. Thus, the question arises whether these additional impact categories contain any additional value of information. Figure 6.1 shows the comparison between the toxicity potentials of the different ecotoxicological impact categories. Ecotoxicity potentials regarding the sediment and aquatic marine and freshwater environment appeared to be highly correlated (R^2 of the logarithms is 0.98), while the correlation between the other ecotoxicity potentials is rather low (R^2 of the logarithms < 0.40).

Figure 6.1 Comparison of ecotoxicity potentials. SETP = marine and fresh water sediment ecotoxicity potentials; AETP = marine and fresh water aquatic ecotoxicity potentials; METP = marine aquatic and sediment ecotoxicity potentials; FETP = fresh water aquatic and sediment ecotoxicity potentials; TETP = terrestrial ecotoxicity potentials; FAETP = fresh water aquatic ecotoxicity potentials; MAETP = marine aquatic ecotoxicity potentials

The high correlation between ecotoxicity potentials of the sediment and aquatic environment implies that it may be sufficient to reduce the five ecotoxicological impact categories identified into: (1) terrestrial environment, (2) marine aquatic and sediment environment, and (3) fresh water aquatic and sediment environment. Ecotoxicity potentials of the combined impact categories may, for instance, be calculated by taking the averages of the aquatic and sediment toxicity potentials. Figure 6.2 shows the comparison between ecotoxicity potentials for the terrestrial, marine and fresh water environment and the human toxicity potentials (R^2 of the logarithms < 0.20). The low correlations found show the importance of a separate assessment of human toxicity and ecotoxicity in LCA.

Figure 6.2 Comparison of Human Toxicity Potentials (HTP) and various ecotoxicity potentials (FETP, METP, TETP)

Reducing the number of initial emission compartments may also increase the practicability of LCA case studies. However, comparing the toxicity potentials of the five initial emission compartments considered, no good correlations are found, except for ecotoxicity potentials of emissions to industrial soil and agricultural soil (Figure 6.3). For emissions of the same substance to industrial soil and agricultural soil, ecotoxicity potentials are within 1 order of magnitude, while human toxicity potentials differ up to 4.2 orders of magnitude. This can be clarified by the fact that particularly

Figure 6.3 Comparison of ecotoxicity potentials (ETPs) and human toxicity potentials (HTPs) for the five initial emission compartments industrial soil, agricultural soil, fresh water, seawater and air.

human exposure routes differ after emissions to agricultural soil compared with emissions to industrial soil. Thus, except for the assessment of ecotoxicological impacts after emissions to industrial and agricultural soil, differentiating between initial emission compartments is considered important for all the toxicological impact categories identified.

Comparing the range of toxicity potentials with the variation due to parameter uncertainty and human variability, it appeared that the differentiating power of the toxicity potentials is larger than the parameter uncertainty and human variability

involved. The 20 orders of magnitude range in toxicity potentials per impact category is caused by differences in the properties of the substances and the initial emission compartments considered. Section 3.2 showed that the variance in toxicity potentials due to parameter uncertainty and human variability, expressed by the ratio of the 97.5%-ile and the 2.5%-ile, ranges from about 1.5 to 6 orders of magnitude.

Parameter uncertainty may, however, substantially influence the toxicity outcomes of LCA case studies (Section 5). Decreasing uncertainties in parameters that describe transport mechanisms, substance degradation, and no-effect concentrations will further increase the differentiating power of the calculations (Section 3.2). Addressing human variability may also be important in the assessment of human toxicity due to emissions to water and soil. As the variation in human exposure parameters is irreducible, the choice concerning which part of the human population should be taken as a basis for the relative comparison of toxic substances, may be an important one. The current scoring system is designed to protect the average person, but other choices, such as protecting highly exposed individuals, may also be defensible (Hertwich *et al.*, 1999; Huijbregts, 1999).

The variance in toxicity potentials resulting from normative choices in the modelling procedure can also be significant (Section 3.3). Time horizon dependent differences up to 6.5 orders of magnitude were found for metal toxicity potentials. Furthermore, exclusion of potential impacts on the global scale changed the toxicity potentials of metals and volatile persistent halogenated organics up to 2.3 orders of magnitude. Although the differences found can be large, these normative choices do not always significantly alter the results of the LCA case studies (Chapter 5).

Acidification and eutrophication

The spatially explicit model RAINS-LCA was developed to include fate, background depositions and ecosystem sensitivity information in the calculation of acidification and terrestrial eutrophication potentials of ammonia (NH_3) and nitrogen oxide (NO_x) air emissions and acidification potentials for sulfur dioxide (SO_2) air emissions. Differences in acidification and terrestrial eutrophication potentials, caused by site-dependent and substance-dependent differences in fate and effects, are 2.8-3.6 and 2.0-2.2 orders of magnitude, respectively. The variance in terrestrial eutrophication potentials and acidification potentials due to parameter uncertainty, expressed by the ratio of the 97.5%-ile and the 2.5%-ile, is about a factor 5 (Section 5). Comparing the range of acidification and terrestrial eutrophication potentials with the variation due to parameter uncertainty, it appeared that the differentiating power is larger than the uncertainty involved. These results imply that it may be important to use region-specific acidification and terrestrial eutrophication potentials in LCA case studies. Regional specification in environmental comparisons may be particularly important, if the emitting regions of the dominant acidifying and eutrophying emissions differ between the product systems involved. If the dominant acidifying and eutrophying emissions occur in a few regions,

regional specification may also be important in product optimisation studies, as regional differences may have an influence on the optimisation strategies.

Normative choices were also assessed in the calculation of acidification and terrestrial eutrophication potentials. Two impact definitions were explored: (1) the marginal change in the hazard index of all ecosystems in Europe; (2) the marginal change in the hazard index of ecosystems in Europe where the critical load is actually exceeded. Correlations (R^2 of the logarithms) between terrestrial eutrophication potentials and acidification potentials of the two impact definitions are respectively below 0.8 and 0.7 (Figure 6.4). If the dominant acidifying and eutrophying emissions occur in a few regions or the emitting regions differ between the product systems involved, the impact definitions may result in different orders of preference. In other cases, the choice of the impact definition may not be very influential (Chapter 5).

Figure 6.4 Comparison of the 'Above and Below' scenario (A&B), the 'Only Above' scenario for 1995 (OA1995), and the 2010 Baseline economic forecast 'Only Above' scenario (OA2010BL) for terrestrial eutrophication (TEP) and acidification (AP), respectively.

Figure 6.5 shows that 'only above critical load' terrestrial eutrophication and acidification potentials for the years 1995 and 2010 differ up to a factor 4 and 10 with average differences of a factor 1.5 and 3, respectively. Figure 6.5 also indicates that differences between the two 2010 forecast scenarios are within a factor 3 for both terrestrial

eutrophication and acidification potentials. Differences in acidification and terrestrial eutrophication potentials related to the year of emission and forecast scenario chosen may be considered less important compared to region-specific differences in characterisation factors of acidifying and terrestrially eutrophying pollutants.

Figure 6.5 Comparison of the 'Only Above' scenario for 1995 (OA1995), 2010 Baseline scenario (OA2010BL) and 2010 New Policy scenario (OA2010NP) for terrestrial eutrophication (TEP) and acidification (AP), respectively.

The focus in the calculation of aquatic eutrophication potentials was on the inclusion of fate factors. In contrast to terrestrial eutrophication and acidification, spatial differentiation was considered to limited extent due to lack of site-specific fate and effect data. As a result, model uncertainty of the aquatic eutrophication potentials may still be substantial. However, completely disregarding fate of emissions causing aquatic eutrophication, as is the case in currently defined best practice (Guinée, 2000), will introduce even larger model uncertainty. Including fate in the characterisation factors of NO_x and NH_3 air emissions results in a decrease of respectively a factor 2-2.5 and 2-3. In addition, characterisations factors for N and P emissions to soil, decrease with a factor 2.5-7.5 and 25-35, respectively.

Further research

Although a substantial effort has been spent in the improvement of current life cycle impact assessment methods and the development of procedures to deal with uncertainty and variability in LCAs, still much work remains to be done. The following topics related to the subjects covered in this thesis can be recommended for further research:

- 1 the development of publicly available databases with up-to-date inventory data including uncertainty estimates at the process level;
- 2 the collection of more (reliable) chemical data, particularly persistence and effect data, as for many chemicals such data are lacking;
- 3 the improvement of the current model structure of USES-LCA by including a groundwater compartment, a more detailed seawater compartment, and a fate and effect analysis of transformation products in the calculation of toxicity potentials. Other models may be used as a basis for these improvements (e.g. the models described by McKone, 1993; Verbruggen *et al.*, 1997; Fenner *et al.*, 2000);
- 4 the introduction of spatially explicit models for the calculation of metal toxicity potentials to account for currently lacking site-dependent processes in USES-LCA, such as reversible adsorption of heavy metals to soils, the slow conversion of reversibly adsorbed heavy metals into forms irreversibly adsorbed to the soil matrix, and the uptake of metals by organisms;
- 5 the replacement of the simple compartment aggregation procedure on the basis of volumes for marine aquatic ecotoxicity and on the basis of mass' for marine sediment and terrestrial ecotoxicity by a more suitable aggregation procedure perhaps based on other compartment characteristics, such as species density;
- 6 the inclusion of impacts on higher predators (e.g. birds, mammals) in the life cycle impact assessment of toxic substances;
- 7 the inclusion of a further weighting step in the calculation of human toxicity potentials for (non)-carcinogenic substances, as the type of impact that firstly occurs is used in the calculations irrespective of its severity. The further weighting step may, for instance, be based on the concept of Disability Adjusted Life Years (DALYs), as described in detail by Hofstetter (1998);
- 8 the extension of the fate and effects analysis of acidification and terrestrial eutrophication from the European scale to the global scale. Adaption of existing global fate and effect models, for instance, the global nitrogen and sulfur model of UNEP/RIVM (1999), may be useful in this respect.
- 9 the improvement of fate factors for transport of NO_x and NH₃ air emissions via soils to the aquatic environment. Existing global and regional fate models may be adapted for this purpose (Seitzinger and Kroeze, 1998; Beusen *et al.*, 1995; Posch *et al.*, 1999);
- 10 the inclusion of differences in biological availability of nutrients and differences in the sensitivity of the aquatic environment in the effect factors for aquatic eutrophication;
- 11 the extension of the current analysis for toxicity, acidification and eutrophication by reflecting 'damage to ecosystem quality'. Probability of species occurrence may be a useful operational endpoint in this respect. (Goedkoop and Spriensma, 1999; Huijbregts *et al.*, 2001b).

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Summary

As described in **Chapter 1**, Environmental life cycle assessment (LCA) is a tool for the assessment of the environmental impact of product systems. Although the framework itself is well-established, its usefulness is still limited due to the fact that uncertainty and variability is often neglected. The aim of this thesis is to contribute to a quantitative evaluation of uncertainty and variability in environmental life-cycle assessment. It also intends to improve the characterisation factors used for the evaluation of toxic, acidifying and eutrophying emissions.

Chapter 2 provides a framework to classify types of uncertainty and variability in LCAs. Uncertainty is divided in parameter uncertainty, model uncertainty, and uncertainty due to choices, while variability covers spatial variability, temporal variability, and variability between objects and sources. A tool to deal with parameter uncertainty and variability between objects and sources in both the inventory and the impact assessment is probabilistic simulation. Uncertainty due to choices can be dealt with in a scenario analysis. The feasibility of dealing with temporal and spatial variability is limited, implying model uncertainty in LCAs. Other model uncertainties can be reduced partly by more sophisticated modelling, such as the use of multi media models in the characterisation phase. The comparison of two exemplary types of roof gutters shows how the effect of combined parameter uncertainties in the inventory and in the characterisation factors for global warming and acidification may be evaluated by means of Monte Carlo analysis. To illustrate the influence of choices, the effect on the comparison is shown of two different allocation procedures in open-loop recycling and three time horizons for global warming potentials.

Chapter 3 outlines an improved model to calculate toxicity potentials: the global nested multi-media fate, exposure and effects model USES-LCA. It is based on the Uniform System for the Evaluation of Substances 2.0 (USES 2.0). USES-LCA was used to calculate for 181 substances toxicity potentials for the six impact categories fresh water aquatic ecotoxicity, marine aquatic ecotoxicity, fresh water sediment ecotoxicity, marine sediment ecotoxicity, terrestrial ecotoxicity and human toxicity, after initial emission to the compartments air, fresh water, seawater, industrial soil and agricultural soil, respectively. Differences of several orders of magnitude were found between the new toxicity potentials and previously calculated ones. For three substances, the variance in toxicity potentials resulting from input parameter uncertainties and human variability was quantified. For Atrazine, 2,3,7,8-TCDD and Lead, variation, expressed by the ratio of the 97.5%-ile and the 2.5%-ile, ranges from about 1.5 to 6 orders of magnitude. The major part of this variation originates from a limited set of substance-specific input parameters, i.e. parameters that describe transport mechanisms, substance degradation, indirect exposure routes and no-effect concentrations. Furthermore, the variance in toxicity potentials resulting from choices in the modelling procedure was quantified by means of scenario analysis. A first scenario analysis showed to what extent potential

impacts in the relatively short term are obscured by the inclusion of impacts on the very long term. Toxicity potentials representing potential impacts over time horizons of 20, 100 and 500 years were compared with toxicity potentials representing potential impacts over an infinite time horizon. Time horizon dependent differences up to 6.5 orders of magnitude were found for metal toxicity potentials, while for toxicity potentials of organic substances under study, differences remain within 0.5 orders of magnitude. The second scenario analysis addressed to what extent potential impacts on the continental scale are obscured by the inclusion of impacts on the global scale. Exclusion of potential impacts on the global scale changed the toxicity potentials of metals and volatile persistent halogenated organics up to 2.3 orders of magnitude.

Chapter 4 outlines the spatially explicit model RAINS-LCA which was developed for the calculation of acidification and terrestrial eutrophication potentials of ammonia (NH_3) and nitrogen oxide (NO_x) air emissions of and acidification potentials for sulfur dioxide (SO_2) air emissions for Europe and a number of European regions, taking fate, background depositions and effects into account. Two impact definitions are explored in the calculations: (1) the marginal change in the hazard index of all ecosystems in Europe; (2) the marginal change in the hazard index of ecosystems in Europe where the critical load is actually exceeded. The inclusion of fate, background depositions and ecosystem sensitivity results in a different ranking of substances compared to simpler model outcomes. In the context of acidification, emissions of nitrogen compounds are regarded about a factor 2 less important relative to sulfur compounds. Furthermore, using RAINS-LCA as opposed to simpler models, it was found that region-specific differences in terrestrial eutrophication and acidification potentials range up to 1.5 and 3.5 orders of magnitude, respectively. By means of scenario analysis, it was also shown that 'only above critical load' terrestrial eutrophication and acidification potentials for the years 1995 and 2010 differ up to 0.6 and 1 order of magnitude, respectively. Chapter 4 also extended the calculation of aquatic eutrophication potentials with fate factors for NH_3 and NO_x emitted to the air, and N and P emitted to soil. The inclusion of fate factors reduces the importance of N and P emissions to soil towards aquatic eutrophication with a factor 2.5-7.5 and 25-35, respectively. Fate factors for NO_x and NH_3 emissions to air also decreases the aquatic eutrophication potentials of these emissions with respectively a factor 2-2.5 and 2-3.

Chapter 5 evaluates three different types of uncertainty in the environmental comparison of insulation thickness in buildings. Parameter uncertainties in the functional unit, the inventory analysis, and the impact assessment were assessed with help of Monte Carlo analysis. The influence of choices concerning the allocation of environmental burdens in recycling processes, future waste scenarios, and the timing, geographical scale and definition of environmental impacts were addressed by means of scenario analysis. Model uncertainty due to the lack of spatial and temporal differentiation and due to the lack of suitable characterisation factors for sum emissions was assessed by comparing the outcomes of using different model assumptions. The results indicate that parameter uncertainty was the most important source of uncertainty

in the environmental comparison. The effect of insulation thickness on global warming was the only effect found to be significantly different between the insulation options studied, with the thickest insulation giving the lowest life cycle impact.

Chapter 6 puts the various types of uncertainty and variability into perspective and gives recommendations for further research. The following general conclusions were drawn:

- 1 The impacts on aquatic and sediment ecosystems can be clustered for the marine and fresh water environment without significant loss of information;
- 2 Except for the assessment of ecotoxicological impacts after emissions to industrial and agricultural soil, differentiating between initial emission compartments is considered important for all the toxicological impact categories identified;
- 3 Relative differences between toxic impacts of product systems may depend on the time horizon and the geographical scale considered, if metals and/or volatile persistent halogenated organics dominantly contribute to the toxic impact of product systems;
- 4 If dominant acidifying and eutrophying emissions occur in a few regions or the emitting regions differ between the product systems involved, the choice of the impact definition and regional specification may influence LCA outcomes;
- 5 Differences in acidification and terrestrial eutrophication potentials related to the year of emission and forecast scenario chosen may be considered less important compared to region-specific differences in characterisation factors of acidifying and terrestrially eutrophying pollutants;
- 6 Comparing the range of toxicity, acidification and terrestrial eutrophication potentials with the variation due to parameter uncertainty and/or human variability, it appeared that the differentiating power of these potentials substantially exceeds this variation;
- 7 The inclusion of fate factors decreases the aquatic eutrophication potentials of NO_x and NH_3 emissions to air and N and P emissions to soil substantially compared to the expected parameter uncertainty involved.

Finally, recommendations for further research were given. These include the development of publicly available databases with up-to-date inventory data and corresponding uncertainty estimates, and ways to further improve the fate and effects analysis of emissions causing toxicity, acidification and eutrophication.

Samenvatting

De milieugerichte levenscyclusanalyse (LCA) is een instrument dat de milieu-effecten van producten analyseert (**Hoofdstuk 1**). De gehele product-levenscyclus van de onttrekking van grondstoffen, de productie van benodigde materialen, de assemblage van het product, het gebruik van het product, en de afvalverwerking van het product wordt hierbij in kaart gebracht. Hoewel het instrument een transparante structuur kent, is de daadwerkelijke toepassing en de interpretatie van behaalde resultaten meer problematisch. Een belangrijke reden is dat de onzekerheden in de uitkomsten van LCA-studies nog niet of nauwelijks in kaart zijn gebracht. Onzekerheid kan worden veroorzaakt door gebrek aan kennis over de processen of normatieve keuzes die van belang zijn in de toepassing van LCA's. Verder kunnen inherente verschillen in gevoeligheid van mensen en ecosystemen, variabiliteit genoemd, de uitkomst van een LCA-studie beïnvloeden. Het doel van dit proefschrift is om bronnen van onzekerheid en variabiliteit in LCA zichtbaar te maken. Tevens worden weegfactoren voor toxische, verzurende en vermestende stoffen, die thans worden gebruikt bij de toepassing van LCA's, verbeterd.

Hoofdstuk 2 beschrijft een schema voor de classificatie van onzekerheid en variabiliteit in LCA. Onzekerheid is onderverdeeld in parameter-onzekerheid, onzekerheid als gevolg van normatieve keuzes en model onzekerheid. Ruimtelijke variatie, variatie over de tijd en variatie tussen bronnen en objecten zijn vormen van variabiliteit. Monte Carlo analyse is een techniek om de effecten van parameter onzekerheid en variatie tussen bronnen en objecten op modeluitkomsten in kaart te brengen. Er wordt een kansverdeling toegekend aan iedere input-parameter van het model. Deze kansverdeling geeft de onzekerheid of variabiliteit weer van de betreffende parameter. Vervolgens wordt uit iedere kansverdeling willekeurig een getal getrokken, waarna de model-uitkomsten worden berekend. Dit wordt meerdere malen herhaald. Uiteindelijk levert deze wijze van berekenen een beeld op van de spreiding in het milieuprofiel van een produkt.

Het effect van normatieve keuzes op modeluitkomsten kan in beeld worden gebracht via het analyseren van diverse scenario's. Het rekening houden met variatie in tijd en ruimte is moeilijk haalbaar, aangezien emissies naar het milieu in de meeste gevallen worden opgeteld voor LCA, los van tijd en ruimte. Dit impliceert modelonzekerheid. Geavanceerdere modellen en gedetailleerdere datasets kunnen nodig zijn om modelonzekerheden te reduceren. Vervolgens laat een simpel voorbeeld zien hoe het effect van parameter-onzekerheid en normatieve keuzes op LCA-uitkomsten in de praktijk kan worden berekend.

Hoofdstuk 3 beschrijft het model USES-LCA waarmee weegfactoren voor toxische stoffen zijn berekend. Per stof zijn weegfactoren zijn berekend voor uitstoot naar lucht, zoet water, zout water, landbouwbodem en industriële bodem. Dit is apart gedaan voor mogelijke gezondheidseffecten op mensen en ecosystemen, waarbij ecosystemen verder zijn onderverdeeld in bodem, zoet oppervlaktewater, zout oppervlaktewater, zoet water

sediment en zout water sediment. De berekeningen zijn uitgevoerd voor 181 stoffen. Met deze weegfactoren is het mogelijk om een kwantitatieve uitspraak te doen over de relatieve belangrijkheid van emissies. Bijvoorbeeld de uitstoot van 1 kg dioxine naar de lucht wordt ongeveer 95000 keer schadelijker geacht voor de menselijke gezondheid dan de uitstoot van 1 kg cadmium naar landbouwbodem. De onzekerheid in dergelijke uitspraken kan echter aanzienlijk zijn.

Om een idee te krijgen over de mate van onzekerheid is voor drie stoffen het effect van parameter-onzekerheid, zoals onzekerheid over de afbraaksnelheid van een stof, en verschillen in menselijke eigenschappen, zoals spreiding in lichaamsgewicht, op de weegfactoren van deze stoffen onderzocht. Het blijkt dat de onzekerheid varieert van een factor 30 tot 1.000.000. Deze onzekerheidsfactor is berekend door de waarde waarbij een kans van 97,5% bestaat dat deze groter is dan de werkelijke waarde (de 97,5^{de} percentielwaarde) te delen door de waarde waarbij een kans van 2,5% bestaat dat deze groter is dan de werkelijke waarde (de 2,5^{de} percentielwaarde). Met name de onzekerheid in afbraaksnelheden en de onzekerheid aangaande effecten op mensen en ecosystemen blijken een grote invloed te hebben op de onzekerheid in de weegfactoren van toxische stoffen.

Daarnaast is het effect van normatieve keuzes op de weegfactoren van de 181 toxische stoffen zichtbaar gemaakt. Ten eerste zijn weegfactoren die de mogelijke effecten weerspiegelen over een termijn van 20, 100 en 500 jaar vergeleken met weegfactoren voor een oneindige tijdshorizon. Verschillen tussen de uitkomsten voor de verschillende termijnen kunnen oplopen tot een factor 3.000.000 voor metalen, terwijl voor organische stoffen de verschillen tussen de termijnen verhoudingsgewijs gering zijn (maximaal een factor 3). Daarnaast leidt het niet-meenemen van effecten op de mondiale schaal tot een verlaging van de weegfactoren voor metalen en vluchtige persistente gehalogeneerde koolwaterstoffen met maximaal een factor 200.

Hoofdstuk 4 beschrijft het model RAINS-LCA waarmee weegfactoren voor de verzurende en/of bodemvermestende emissies van stikstofoxiden, zwaveldioxide en ammoniak naar de lucht zijn berekend. Doordat het model gedetailleerde regiospecifieke informatie bevat over het gedrag en effecten van deze stoffen in het milieu, bleek het mogelijk om voor 44 Europese regio's stofspectifieke weegfactoren te berekenen. Twee verschillende definities van effect zijn doorgerekend: (1) de verandering in mogelijke effecten voor alle ecosystemen in Europa en (2) de verandering in mogelijke effecten voor ecosystemen waar de kritische effect-grens reeds is overschreden. Bij de tweede wijze van berekening zijn depositie-gegevens gebruikt voor het jaar 1995 en twee economische scenario's voor het jaar 2010. De resultaten laten zien dat in vergelijking tot een simpeler verzuringsmodel het gedetailleerde model RAINS-LCA gemiddeld lagere weegfactoren voor stikstofoxiden en ammoniak berekent (factor 2). Daarnaast blijkt dat regiospecifieke verschillen tussen de weegfactoren kunnen oplopen tot een factor 30 voor vermesting van de bodem en een factor 3000 voor verzuring. Verschillen tussen de weegfactoren voor 1995 en 2010 blijven binnen een factor 10.

Voor de berekening van weegfactoren voor vermesting van wateren is het relevant de

fracties van luchtmissies van stikstofoxiden en ammoniak en bodememissies van stikstof en fosfaat te weten die uiteindelijk in het water terecht komen. Het rekening houden met deze fracties leidt respectievelijk tot een factor 2-2,5 en 2-3 verlaging van de weegfactoren voor stikstofoxiden en ammoniak luchtmissies en een factor 2,5-7,5 en 25-35 verlaging van de weegfactoren voor stikstof en fosfaat bodem emissies.

Hoofdstuk 5 evalueert de effecten van parameter-onzekerheid, normatieve onzekerheid en model-onzekerheid op de uitkomsten van een vergelijkende LCA voor de toepassing van verschillende diktes isolatiematerialen in woningen. Parameter onzekerheden in materiaalstromen, emissies en weegfactoren zijn meegenomen in de berekening. Daarnaast is de invloed van uiteenlopende toerekeningsmogelijkheden van milieueffecten bij recycling van materialen in andere productsystemen en diverse toekomstige afvalverwerkingsscenario's in kaart gebracht. De invloed van de keuze voor een specifieke tijdhorizon, geografische schaal en effect definitie is ook zichtbaar gemaakt in de vergelijkende LCA. De mate van model-onzekerheid als gevolg van gebrek aan ruimtelijke en temporele differentiatie en het gebrek aan weegfactoren voor som-emissies, zoals 'metalen', is getoetst door de uitkomsten uitgaande van verschillende modelaannames met elkaar te vergelijken. De resultaten laten zien dat onzekerheden in input-parameters de grootste bron van onzekerheid vormen in deze vergelijkende LCA. Daarnaast bleek dat slechts de uitkomsten voor broeikas effect significant van elkaar verschillen, waarbij de dikste isolatie te prefereren is.

Hoofdstuk 6 plaatst de verschillende typen onzekerheid en variabiliteit in perspectief en geeft aanbevelingen voor toekomstig onderzoek. Op basis van deze analyse zijn de volgende conclusies getrokken:

- voor het zoet water en zout water milieu kunnen de effecten van toxische stoffen op oppervlaktewater en sediment-ecosystemen worden geclusterd zonder groot verlies aan informatie;
- behalve voor de evaluatie van effecten op ecosystemen door uitstoot naar industriële of landbouwbodem, is kennis van het specifiek compartiment waarnaar de uitstoot van een toxische stof plaatsvindt relevant in LCA;
- relatieve verschillen tussen productscores voor toxiciteit kunnen afhankelijk zijn van de gekozen tijd- en ruimteschaal, indien metalen en/of vluchtige persistente gehalogeneerde koolwaterstoffen in het geding zijn;
- de keuze van de effect-definitie en regionale differentiatie kunnen van invloed zijn op LCA-uitkomsten voor verzuring en vermist van de bodem, als de dominante uitstoot is gesitueerd in een beperkt aantal regio's, of als de regio's waar de uitstoot plaatsvindt, sterk van product tot product verschillen;
- temporele verschillen en verschillen in economische scenario's zijn minder groot dan de gevonden regionale verschillen in weegfactoren voor verzuring en vermist van de bodem;
- het onderscheidend vermogen van de weegfactoren voor toxiciteit, verzuring en vermist is groter dan de invloed van parameter onzekerheid en/of de invloed van inherente verschillen in menselijke eigenschappen op de weegfactoren.

Tenslotte zijn aanbevelingen geformuleerd voor verder onderzoek. Een belangrijke aanbeveling is de ontwikkeling van een openbare database met kwalitatief goede informatie inclusief schattingen van onzekerheidsverdelingen. Daarnaast zijn verscheidene mogelijkheden genoemd om de weegfactoren voor toxische, verzurende en vermestende stoffen verder te verbeteren.

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Curriculum Vitae

Mark Huijbregts werd op 26 september 1972 geboren in Oranjestad te Aruba. In 1976 verhuisde hij samen met zijn ouders en zus naar Hapert waar hij de basisschool heeft gevolgd. In 1990 behaalde hij het VWO diploma aan het Pius X College te Bladel. In hetzelfde jaar startte hij met de studie Biomedische Gezondheidswetenschappen aan de Medische Faculteit van de Katholieke Universiteit Nijmegen (KUN). In 1993 besloot hij om zich ook in 'natuur en milieu' te verdiepen via de studie Biologie en bovenbouwstudie Natuurwetenschappelijke Milieukunde aan de Faculteit der Natuurwetenschappen van de KUN. In het kader van deze studies deed hij ondermeer onderzoek naar het rekening houden met landschaps-, natuur-, en cultuurhistorische waarden bij dijkversterkingen, de toxiciteit van polychloorbifenylen in vroege ontwikkelingsstadia van de karper, en de afstemming van milieukwaliteitsnormen en gezondheidsnormen voor de mens. In 1996 resulteerde dit in een doctoraal diploma Biomedische Gezondheidswetenschappen en een *cum laude* doctoraal diploma Natuurwetenschappelijke Milieukunde. Aansluitend begon hij met steun van de Nederlandse Organisatie voor Wetenschappelijk Onderzoek zijn promotie-onderzoek aan de Universiteit van Amsterdam bij de Interfacultaire Vakgroep Milieukunde. Dit proefschrift is een weergave van de resultaten van zijn promotie-onderzoek. Sinds oktober 2000 is hij als postdoc-onderzoeker verbonden aan de afdeling Milieukunde van de KUN.