LCA impact assessment of toxic releases

Generic modelling of fate, exposure and effect for ecosystems and human beings with data for about 100 chemicals

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Summary	Equivalency factors have been developed for human toxic and ecotoxic chemicals for use in environmental life cycle assessment (LCA). Some 100 factors have been calculated using the *Uniform System for the Evaluation of Substances* (USES 1.0) as developed by RIVM. With USES 1.0 fate and exposure data have been included in the determination of equivalency factors. Some of these factors consequently differ widely from formerly published equivalency factors.

Contents

Foreword

Since the publication of the government's first National Environmental Policy Plan, an integrated approach to environmental problems has been at the core of environmental policy in the Netherlands. It is not only in the field of product policy that the "cradle-to-grave" principle serves as the basic point of departure; in many other areas, too, it has become customary to include all the phases of the life cycle and all environmental compartments in the assessment process. In practice, the tool of environmental life cycle analysis (LCA) is frequently used to carry out such an assessment. In the Netherlands the 1992 LCA manual – developed by CML in collaboration with TNO and Bureau B&G – has become a standard work for use in this field. This is not to say that the method is now "complete" on all points: a number of elements are still under development.

This report presents a new LCA approach for toxic substances. The LCA manual gives a relative yardstick for the potential toxic effect of a substance, with no allowance being made for its diffusion, degradation and persistence. Precisely these factors may be of major influence on the degree of (eco)toxicity. As part of its work on substance policy, RIVM has developed a computer model called *Uniform System for the Evaluation of Substances* (USES) to assess, as realistically as possible, the degree to which the no-effect level is transgressed in practice. This model does make allowance for diffusion, degradation and persistence. By combining the expertise of RIVM with that of CML, it has proved possible to apply the USES system to derive toxicity potentials for the LCA manual. The main benefit of this project is not only that substance assessment has for the first time been linked to the LCA method, but that it also shows LCA users how they themselves can establish the LCA classification factor for (eco)toxicity for "unknown" substances, it being virtually impossible to run the model in advance for all existing substances. This shortcoming is satisfactorily resolved by the computation method presented in this report.

This year work is to be started on updating the 1992 manual, thereby incorporating all new developments – national and international – in the field of LCA methodology, including the method of establishing the potential toxicity presented in this report. To ensure that this manual is based not only on theory, a think tank with a large number of LCA users is to be set up, to steer the process of updating the manual. The new manual is scheduled for publication in early 1997.

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Preface

In this project equivalency factors for toxic releases for use in environmental life cycle assessment (LCA) have been calculated. To this end, the *Uniform System for the Evaluation of Substances* (USES 1.0), a model developed by RIVM for the risk assessment (RA) of chemicals, has been applied with a newly developed LCA "country file".

Appendix A contains a list of equivalency factors for 94 chemicals for making an impact assessment for the impact categories of human toxicity, aquatic ecotoxicity and terrestrial ecotoxicity. If other substances with potential toxic impacts are involved in an LCA, or if the reader wishes to repeat the calculations carried out in this project, the USES 1.0 model, the LCA country file and the substance data files are needed. The model version USES 1.0 can be purchased from the Distribution Centre of the Ministry of VROM.[1] The LCA country file, the data on the substances for which equivalency factors have been calculated and a manual explaining how to calculate LCA equivalency factors with USES 1.0 can be obtained on request from CML.[2]

The USES 1.0 model is currently being further harmonized with the EU guidance document on risk assessment of substances. For LCA the revisions of the model with respect to parameter input are of particular importance, since in this way the system can readily be adapted for use in LCA. This revised version, called *European Union System for the Evaluation of Substances* (EUSES), will probably be available at the end of 1996. The system EUSES can be purchased from the *European Chemicals Bureau* (ECB) in Ispra, Italy.[3] Those who are not yet in possession of the USES 1.0 program are advised to wait for the new release. As far as can be foreseen at the time of publication of this report, the aforementioned manual on how to calculate LCA equivalency factors with USES 1.0 will also be applicable to EUSES.

The course of the project has been guided by a steering committee consisting of H.L.J.M. Wijnen (VROM-DGM-IBPC), G.L. Duvoort (RIVM-LAE) and P.T.J. Van der Zandt (VROM-DGM-SVS). The authors wish to express their gratitude for their useful efforts and inputs.

We extent our special thanks to Lucie Vollebregt (University of Amsterdam) for her previous work on the inclusion of fate and exposure aspects in the LCA impact assessment of toxic releases, which has served as a very important basis for the present report. We also thank Anneke Wegener Sleeswijk for her contribution to chapters 3 and 5.

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[1] The USES 1.0 manual and diskette (Distribution No. 11144/150) can be obtained for about Dfl. 150 from: Ministry of Housing, Spatial Planning and Environment, Department of Information and International Relations, P.O. Box 20951, 2500 EZ The Hague, The Netherlands.

[2] The diskette and a brief manual can be obtained for expenses from: CML, attn. Mrs. E. Philips, P.O. Box 9518, 2300 RA Leiden, The Netherlands.

[3] European Chemicals Bureau, CEC Joint Research Centre, 21020 Ispra (Varese), Italy.

Samenvatting

Doelstelling van het project *Toxicity in LCA*, dat is uitgevoerd in een samenwerking van CML en RIVM in opdracht van het Ministerie van Volkshuisvesting, Ruimtelijke Ordening en Milieubeheer (VROM), was om equivalentiefactoren voor humaan-toxische en ecotoxische stoffen op te stellen voor gebruik in levenscyclusanalyses van produkten (LCA), gebruik makend van de concepten MOS (*margin of safety*; toegepast op humane toxiciteit) en PEC/PNEC (*predicted environmental concentration/predicted no-effect concentration*; toegepast op aquatische en terrestrische ecotoxiciteit) zoals door het RIVM in het model en programma *Uniform System for the Evaluation of Substances* (USES 1.0) ontwikkeld. In deze studie is USES 1.0 toegepast als basis voor de berekening van equivalentiefactoren. Het programma is zelf niet aangepast, maar er is een speciale *country file* ontwikkeld met LCA-specifieke parameters voor een aantal invoergegevens (bv. volumina van milieucompartmenten, windsnelheid, etc. voor een *unit world*).

Voor 94 stoffen zijn equivalentiefactoren berekend; een lijst met equivalentiefactoren is in dit rapport opgenomen als appendix. Voor de meeste van deze stoffen waren chemische en toxicologische gegevens reeds in het kader van USES 1.0 verzameld; daarnaast zijn enkele stoffen, zoals zware metalen, SO_2 en NO_2 opgenomen vanwege hun belang in de gemiddelde LCA. Hoewel USES 1.0 niet voor die stoffen ontwikkeld is, kan het er met enige aanpassingen voor gebruikt worden.

Door USES 1.0 te gebruiken voor de berekening van de equivalentiefactoren zijn, naast gegevens met betrekking tot de toxiciteit, gegevens met betrekking tot het lot van stoffen en de blootstelling daaraan verwerkt. Het gaat hierbij om persistentie, (bio)afbreekbaarheid, intercompartimentaal transport en, voor humane toxiciteit, gegevens over blootstellingsroutes zoals het ademvolume en de consumptie van drinkwater, vis, vlees, zuivelprodukten en groenten. Deze gegevens zijn alle in het USES 1.0 model verwerkt.

De verschillen tussen de "oude" equivalentiefactoren, die alleen op toxiciteitsgegevens waren gebaseerd, en de "nieuwe" equivalentiefactoren, waarbij ook gegevens over het lot van en de blootstelling aan stoffen meespelen, blijken significant te zijn. Zoals te verwachten was, zijn de equivalentiefactoren van persistente stoffen zoals metalen en dioxines aanzienlijk hoger dan eerder.

Deze nieuwe list met LCA equivalentiefactoren voor toxische stoffen sluit niet het werk af. In dit rapport is slechts voor 94 toxische stoffen een equivalentiefactor berekend. Deze voorlopige lijst dient uitgebreid te worden met andere potentieel toxische stoffen. Dit impliceert de noodzaak om stofgegevens te verzamelen om de berekeningen met USES 1.0 uit te voeren. In principe kan de lezer dit zelf doen: het USES 1.0 model is verkrijgbaar bij VROM, en de LCA *country file* en de gegevensbestanden voor de stoffen die nu doorgerekend zijn is verkrijgbaar bij het CML.[1] Het ontbreken van een openbaar gegevensbestand maakt echter dat de beschikbaarheid van gegevens een belangrijk aandachtspunt blijft bij de verdere ontwikkeling van equivalentiefactoren voor LCA op basis van USES 1.0.

Verder is een aantal onderzoeksvragen geïdentificeerd voor de verdere ontwikkeling van equivalentiefactoren voor LCA op basis van USES 1.0. Hieronder is de ontwikkeling van het USES 1.0 model zelf, de keuze van de toxiciteitsparameter, de keuze van de effectcategorieën en het opnemen van ruimtelijk gedifferentieerde informatie in de equivalentiefactoren. Veel van deze onderwerpen hebben momenteel de aandacht van risico-analysespecialisten. In dit rapport wordt geadviseerd om in de LCA-wereld de resultaten van die discussies te volgen, om ze op hun bruikbaarheid te beoordelen en waar bruikbaar na te volgen.

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[1] In de *preface* staan de adressen van VROM en CML vermeld.

Summary

The aim of the project *Toxicity in LCA*, which has been carried out in close collaboration between CML and RIVM and was commissioned by the Dutch Ministry of Housing, Spatial Planning and the Environment (VROM), was to develop equivalency factors for human toxic and ecotoxic chemicals for use in life cycle assessment of products (LCA), following the MOS (margin of safety; applied for human toxicity) and PEC/PNEC (predicted environmental concentration/predicted no-effect concentration; applied for aquatic and terrestrial ecotoxicity) concepts as developed by RIVM in the model and program *Uniform System for the Evaluation of Substances* (USES 1.0). The version USES 1.0 was used as the basis for calculating the equivalency factors in this study. The program itself has not been adapted, but a special country file has been developed containing LCA-specific values for a number of input parameters (e.g. volumes of environmental compartments, wind speed, etc. for a unit world).

Equivalency factors have been calculated for 94 chemicals; a list of equivalency factors is included in this report as an appendix. For most of these substances data on chemical and toxicological properties had already been gathered within the framework of USES 1.0 work; some additional substances, such as heavy metals, SO_2 and NO_2, have also been included because of their importance in a typical LCA. Although not originally developed for this purpose, with some adaptations USES 1.0 can also be applied to these chemicals.

By calculating LCA equivalency factors with USES 1.0, fate and exposure data of chemicals have been included in addition to toxicity data. The fate and exposure data included in this way are on persistency, (bio)degradation and intermedia transport and, for human toxicity, data on exposure routes such as respiration volume and consumption of drinking water, fish, meat, dairy products and vegetables. These parameters and data are all part of the USES 1.0 model.

The differences between the "old" equivalency factors, based only on toxicity data, and the "new" equivalency factors, which also include fate and exposure data, appear to be significant. As expected, the equivalency factors of persistent chemicals such as metals and dioxins all have a much higher value than before.

With this new list of LCA equivalency factors for toxic releases, the job is not finished. In this report equivalency factors have been calculated for only 94 toxic chemicals. This preliminary list should be extended to other potentially toxic chemicals, implying a need to gather the chemical data necessary to perform calculations with USES 1.0. In principle, the reader can do this additional work himself: the USES 1.0 model is available at VROM, and the LCA country file and the data files of the substances now calculated are available at CML.[1] However, since there is still no public database containing the required substance data, data availability will remain an

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[1] See the preface for the addresses of VROM and CML.

important point of attention in the development of LCA equivalency factors using USES 1.0.

A number of research topics have also been identified for further improving the LCA equivalency factors based on USES 1.0, including improvements of USES 1.0 itself, choice of the toxicity parameter, definition of impact categories for toxicity, and the inclusion of spatial information in equivalency factors. Most of these topics are currently being addressed by RA experts in ongoing discussions. In this report, it is advised that the results of these discussions are followed by LCA researchers, assessed as to their usefulness for LCA, and if apparently useful, included in updated equivalency factors.

Chapter 1

INTRODUCTION

1.1 MOTIVES AND AIMS OF THE PROJECT

In this section the motives and aims of the project are reviewed. To this end, below we give a definition of LCA and of the characterization step within LCA, a brief historical overview of methods used to date for the assessment of toxic releases in LCA and the aims of the present project.

Definition and main structure of LCA

Environmental life cycle assessment (LCA) is a tool for assessing the environmental impacts of a product, or more precisely, of a system required for a particular unit of function (product system or function system).

The Dutch *Policy Document on Products and Environment* [1] confirms that LCA is an important assessment tool for product-oriented environmental policy. LCA is a decision-support tool with the following characteristics:

- it covers the entire life cycle (from resource extraction to waste processing);
- it includes all relevant environmental impacts that can be attributed to a product (from resource depletion to smell);
- it supports a decision by supplying information; the eventual decision is based on a weighting that includes additional aspects such as costs, technical/economical feasibility, environmental impacts which cannot be attributed to a product, and social consequences.

LCA provides a systematic framework which helps to identify, quantify, interpret and evaluate the environmental impacts of a product, function or service in an orderly way. It is a diagnostic tool which [2]:

- can be used to compare existing products or services with each other or with a standard;
- may indicate promising areas for improving existing products;
- may aid in the design of new products.

Since 1990 there has been substantial growth in the number of LCA studies. Several comprehensive methodological projects have been undertaken and an initial version of a *Code of Practice* has been drafted by an international committee of LCA experts [3]. One of the main elements of this *Code of Practice* is a methodological framework comprising four components: goal definition and scoping, inventory analysis, impact assessment and improvement assessment.

- Goal definition and scoping define the subject of study and the functional unit to be investigated.
- In the inventory analysis all extractions of resources and emissions of hazardous substances attributable to the product system(s) studied are listed in an inventory table.

- In the impact assessment it is first determined which impact categories (environmental problem types) are to be considered and which extractions and emissions contribute to which of these impact categories. In the *Code of Practice* this step is called classification. In a following step, the characterization, the "analysis/quantification, and where possible, aggregation of the impacts within the given impact categories" takes place [3]. To permit better interpretation, it has been proposed to carry out normalization of the impact scores [3,4,5,6]. To this end, the impact scores of a particular product (system) are divided by the total extent of the relevant impact for a certain area (e.g. the world) and a certain period of time (e.g. one year). The final step of impact assessment is the valuation, in which the relative importance of each of the impact categories is assessed.
- Valuation results may be used as a basis for choosing among product alternatives, or for the purposes of product improvement.

The last component of the *Code of Practice* framework is the improvement assessment, in which the options for improving the product system(s) under study are identified. For a more comprehensive discussion of the principles and elaboration of the individual steps, we refer to [4,7,8, 9,10,11,12].

The great interest in LCA, and the large number of principles, methods and nomenclature used throughout the world has put LCA on the agenda of the International Organization for Standardization (ISO). The current proposals for framework and terminology differ somewhat from those presented above.[1] Because ISO is still developing its draft documents, we have chosen to use the terms most widely recognized at present: those of SETAC's *Code of Practice*.

Characterization within LCA

Three Dutch institutes, CML, TNO-IMET and B&G, have written a guideline book with an accompanying scientific background document [4] as part of the *National Reuse of Waste Research Programme* (NOH). These documents have been used as reference documents in the Netherlands and throughout the world. One of the elements of LCA that has received extensive attention since the finalization of the NOH project is characterization (or, as it was called in [4]: classification) [13,14,15,16,17].

The results of the inventory analysis, the inventory table, is a long list of quantified environmental interventions (emissions of substances and extractions of resources), usually aggregated over the entire life cycle. Such a list may, for instance, include the following emissions: 12 kg CO_2 to air, 5 kg SO_2 to air, 0.5 mg mercury to soil, 2 mg benzene to water, etc. In an LCA such a list may comprise some 50 to 250 items. The interventions in an inventory table are highly aggregated, since the cradle and grave of a product may be years and thousands of kilometres apart. The intervention "emission of 5 kg SO_2 to air" may, for example, consist of 1 kg in Pakistan in 1970, 0.1 kg in the Netherlands in 1995, 3.0 kg in Brazil in 2010 and 0.9 kg on the

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[1] Some important proposed changes are (i) the addition of a definition step before the classification, (ii) the removal of the improvement assessment, and (iii) the inclusion of an interpretation phase which includes, *inter alia*, sensitivity analyses.

"world market" (with no further geographic specification) in 1996. Dutch product-oriented environmental policy is based on the premise that harmful impacts may not be shifted to either other countries or other generations. An LCA generally has a functional unit of a product as its subject, e.g. the consumption of a bag of potato crisps. All interventions ("emission of 3 mg mercury to water") associated with this product (function) are determined as a mass (kg) only, disregarding the time base of the emission[1]; emission fluxes (kg/hr) are not considered in LCA.

Interpretation of this list is problematical and assessments of the relative hazard of CO_2 compared with SO_2 are often necessary since products hardly ever have exactly the same items on this list. This is the purpose of the impact assessment component of an LCA. In the classification step, emissions and resources are marked with respect to the impact categories (environmental themes) to which they may contribute. In the characterization step, their contribution to impact categories is quantified. In this step, emissions contributing to the same impact category are aggregated based on knowledge from environmental models and chemical and physical properties (fate and toxicity). For example, emissions of CO_2, CH_4 and (H)CFCs are weighted and aggregated to one overall score for global warming by means of the GWPs established by the IPCC [18].

To avoid use of a large number of environmental models in each LCA for undertaking characterization, the concept of equivalency factors has been developed. Equivalency factors are numbers indicating the contribution of one unit of an emission (or an extraction) to a particular impact category. By multiplying the magnitude of the emission by its equivalency factor and aggregating the results per impact category, a total score for that particular impact category is obtained:

$$\textit{impact score}_{cat} = \sum_{subs} \textit{equivalency factor}_{cat,subs} \times \textit{emission}_{subs} \tag{1.1}$$

The equivalency factor is defined for each type of emission (or resource) and for each impact category (resource depletion, global warming, acidification, etc). Equivalency factors, although not necessarily in relation to LCA, have been suggested for the following impact categories: global warming (GWP: [18]), ozone depletion (ODP: [19]), photochemical ozone creation (POCP: [20]), acidification (AP: [4,21]), and nutrification (NP: [4]). However, how to develop appropriate equivalency factors for toxic releases has always remained a controversial topic in LCA impact assessment/characterization discussions.

In this context, it is important to stress that not the actual impacts, but the "constructed" impacts, i.e. the potential contribution to the actually occurring impacts, is calculated. In this sense the impact assessment in LCA is different than that in EIA or RA: the impacts are constructed impacts which cannot be empirically validated (see §1.2 for a more extensive discussion of this important issue).

Brief historical overview of toxicity methods

Prior to the NOH project that produced the Dutch Guidelines and Backgrounds documents [4],

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[1] This mass loading is sometimes termed a pulse.

emissions contributing to the impact category "airborne toxicity" were weighted by means of MAC-values[1] [22,23]: a chemical with a MAC-value of 1 mg/m^3 is considered to be ten times as toxic as a chemical with a MAC-value of 10 mg/m^3, and is consequently weighted ten times heavier. By dividing the magnitude of the emission by its MAC-value, a result expressed in m^3 is obtained:

$$impact\ score_{\text{airborne toxicity}} = \sum_{subs} \frac{1}{MAC_{subs}} \times emission_{subs,air} \tag{1.2}$$

The resulting number is referred to as the "critical volume": the air volume (in cubic metres) needed to dilute the emission to such an extent that the MAC-value is just not exceeded. The overall score for airborne toxicity can be determined by calculating the critical volume for all toxic airborne emissions of the life cycle and by aggregating these to one number for the total critical volume. Dozens of emissions may be interpreted and aggregated in this way into one number.

Aquatic toxicity is assessed in a similar way by calculating critical volumes for waterborne emissions by applying drinking water (OVD) standards. The score has the unit litre (water).

Although these indicators for airborne and waterborne toxicity work, are simple and attractive, a number of strong objections have been raised against the use of MAC-values and OVD-values:

- they are a compromise between toxicological and economic/technical considerations[2];
- MAC-values are thresholds for the shop floor and based on limited exposure (5 days a week, 8 hours a day) of a particular population (healthy people between 18 and 65 years of age);
- they are based on the harmfulness of chemicals to humans, without taking into account the harmfulness of the same chemicals to flora, fauna and/or ecosystems;
- the assessment method does not include degradation processes and transport processes to other environmental compartments.

The reader is referred to [24] for an overview and discussion of different methods for assessing toxic impacts in LCA.

A historical review may also be drafted in another way (cf. [25,26]). An assessment of toxic impacts could be based on one or more of the following elements[3], starting with the magnitude of the emission (classified in certain categories):

- the inherent toxicity (hazard) or, alternatively formulated, the sensitivity of target species to the chemical released;

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[1] MAC means maximum accepted concentration; MAC-values are defined for a limited number of pollutants in the atmosphere. So-called MIC-values have also sometimes been used. These are not only based on toxicity, but also take into account the contributions the chemical considered might make to other impact categories (acidification, global warming, etc.).

[2] Recall that MAC means maximum accepted concentration, not maximum acceptable concentration.

[3] It should be emphasized that these elements do not represent steps of a procedure, but dimensions along which different types of information may be added for a more sophisticated assessment.

- the fate of the chemical released in the environment and/or the pathways of exposure of target species;
- the actual background concentration levels of the chemical released and, if relevant, of other chemicals.

Finally, all these elements may be added in more or less spatial detail, e.g. concerning chimney height, temperature or dilution volume. A general formula for a toxicity score for category *cat* is now:

$$impact\ score_{cat} = \sum_{subs}\sum_{comp} B_{cat,subs} \times T_{cat,subs} \times F_{cat,subs,comp} \times emission_{subs,comp} \qquad (1.3)$$

where $T_{cat,subs}$ denotes the inherent toxicity of chemical *subs* for target category *cat*, $F_{cat,subs,comp}$ is a factor that expresses to what extent a chemical *subs* emitted to compartment *comp* reaches members of target category *cat* (so it measures fate and/or exposure), and $B_{cat,subs}$ indicates the influence of background concentrations of substance *subs* on target category *cat*.

The number and nature of categories and compartments distinguished determines the level of spatial detail. For instance, a distinction between air, water, and soil is not very sophisticated, while a distinction between, say, the Baltic sea and other seas, or indoor air and outdoor air, or clay soil with a particular vegetation and other soils, is much more sophisticated.

Equation (1.3) is a general one, since a structure is outlined, with no indication of its precise elaboration. However, this equation can be used to illustrate the historical development of assessment methods for toxic emissions in LCA; see Table 1.1 for a discussion of [4,8,22,27, 28,29,30,31,32,33,34,35,36].

Table 1.1: Categorization of a number of available methods for assessment of toxic releases in LCA. Legend: *B* denotes dependency on background concentrations, *T* the quality of how inherent toxicity is taken into account, and *F* the quality of how fate/exposure are taken into account; + = included in method, +/− = partly included in method, and − = not included in method.

method	*comp*	*cat*	$B_{cat,chem}$	$T_{cat,chem}$	$F_{cat,chem,comp}$	spatial diff.
Anonymous, 1984 [22]	air, water	air, water	−	+/−	−	−
Anonymous, 1992 [8]	air, water	human, aquatic ecosystem, terrestrial ecosystem	−	+	+/− (only some fate data)	−
Assies, 1994 [27]	air, water, soil	human, aquatic ecosystem, terrestrial ecosystem	+	+	+	−
Gebler, 1992 [28]	air, water, soil	ecosystem	−	+	+	−
Guinée & Heijungs, 1993 [29]	air, water, soil	human, aquatic ecosystem, terrestrial ecosystem	−	+	+	−
Hauschild *et al.*,1993 [30]	air, water, soil	aquatic ecosystem, terrestrial ecosystem	−	+	+/− (only some fate data)	+/−
Heijungs *et al.*, 1992 [4]	air, water, soil	human, aquatic ecosystem, terrestrial ecosystem	−	+	+/− (only a few exposure data)	−
Herrchen, 1993 [31]	air, water, soil	ecotoxicity	−	+	+	−
Hunt *et al.*, 1974 [32]	air, water	air, water	−	−	−	−
Jolliet, 1994 [33]	air, water	human, aquatic ecosystem, terrestrial ecosystem	−	+	+	−
Mekel *et al.*, 1990 [34]	air, water	air, water	−	+/−	−	−
Tellus Institute, 1992 [35]	air	human	−	+	−	−
Vollebregt, 1993 [36]	air, water, soil	human, aquatic ecosystem, terrestrial ecosystem	−	+	+	−

In the preliminary method of the NOH Guide [4] the core of the critical volumes method – dividing the magnitude of the emission by a threshold value and aggregating the results – remains unchanged. However, MAC-values are no longer used. Instead, "purely" toxicological threshold values are applied that are based on continuous exposure. As a result there is now no distinction between airborne and waterborne toxicity, but rather between human toxicity, aquatic ecotoxicity and terrestrial ecotoxicity. The score for human toxicity covers emissions to air, water and soil. The human toxicity assessment is made by applying so-called ADI-values and TDI-values; the aquatic and terrestrial ecotoxicity assessments are made by applying ecosystem NOECs extrapolated from species toxicity data according to the so-called EPA extrapolation method [37]. With these revisions three of the four objections have been eliminated:

- the threshold values are determined on purely toxicological grounds, with no allowance for any economic considerations[1];
- the threshold values are based on continuous exposure of the whole population or whole ecosystem;
- impacts on human beings and ecosystems are both assessed, but separately.

One very important objection remained in this preliminary method:

- the assessment method does not include degradation processes and transport processes to other environmental compartments.

The incentive for undertaking the project *Toxicity in LCA* was the need to eliminate this final objection.

The long-term model for toxicity assessment in LCA should include as appropriately as possible the fate of chemicals and their pathways of exposure in the environment. The fate is determined by aspects related to the residence time of a chemical in a compartment: degradation, intermedia transport by e.g. evaporation and deposition, immobilization, etc.

Simultaneously with the NOH project, a project was carried out that aimed to apply the PEC/PNEC concept to LCA impact assessment [36]. The origins of the PEC/PNEC concept lie in the risk assessment (RA) of chemicals. Based on assumptions with respect to the emission rate of a chemical, the predicted environmental concentration (PEC) of the chemical in air, water, soil, sediment, etc. is calculated. These concentrations can be related to threshold values such as the predicted no-effect concentration (PNEC). The PEC/PNEC ratio is taken to be a measure or indicator of the risk: a value of 1 or more may indicate a need for policy measures, a value between 0 and 1 not. In calculating the PEC, environmental processes such as degradation and transport are modelled. While the PEC/PNEC concept may somehow be of use in LCA, two questions must first be dealt with:

- Is it possible to calculate a PEC-like quantity[2] in LCA?
- Is it possible to weigh this PEC relative to the PNEC in order to aggregate toxic emissions

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[1] Ecosystem threshold values are still influenced by non-toxicological considerations to a minor extent, however, as they are based on a 95% species protection level. This 95% remains a normative number. Besides this 95% criterion, threshold values of some substances appear to be influenced by flavour decline of fish, for example, which is a non-toxicological consideration. These values have been adapted accordingly.

[2] Vollebregt [36] introduces the term PREC, the *product-related environmental concentration.*

to a limited number of scores for toxicity?

In the report on this project [36; our translation of the original Dutch], the following is stated: "The module developed is not yet useful for application in LCA, because of its sensitivity to the parameter degradation. It is thus recommended to consider whether the Mackay-level III multimedia model as proposed by CML satisfactorily solves these shortcomings." (p.70)

The method referred to is that described by Guinée & Heijungs [4,29]. As mentioned above, the proposal of Guinée & Heijungs requires further elaboration. This is exactly what this project aims to do.

Aims of the project

In the course of the aforementioned NOH project that yielded the guidelines and background document, it already became clear that these documents could not solve all the problems involved in the impact assessment of toxic releases, let alone provide a list of such equivalency factors. In the guidelines pragmatic solutions were suggested, and in the background document a number of reasons were specified why these solutions have no definitive status. The project *Toxicity in LCA* aims to replace one of these pragmatic solutions by a better-based method, as outlined in the previous paragraph.

More specifically, the aim of this project was to develop, in close collaboration between CML and RIVM, equivalency factors for human toxic and ecotoxic chemicals for use in LCA employing the PEC/PNEC concept as applied in USES 1.0 [38,39,40]. The USES 1.0 system is the basis for calculating these equivalency factors. The program itself has not been adapted, but a special "country file" has been developed containing specific input parameters in order to fulfil the conditions of LCA. Equivalency factors have been calculated for 94 chemicals, including organic chemicals for which chemical property data had already been gathered within the framework of USES 1.0 work, some ten metals and a few inorganic compounds (SO_2, NO_x, NH_3). For these chemicals a new list of LCA equivalency factors is included in this report.

USES 1.0, the substance data file and the LCA country file can all be obtained on request (see preface). The European update of USES 1.0, which is currently being developed, will also be available in due course (again, see preface).

It is important to stress that, although application of USES 1.0 to calculate equivalency factors may be complicated for LCA practitioners, the equivalency factors themselves are easy to apply, in the same way as it is easy to apply the currently available equivalency factors (like GWPs) in this area.

Summarizing, the objectives of the project *Toxicity in LCA* are:

- to examine USES 1.0 and the PEC/PNEC concept adopted in it and locate the parameters which have to be dealt with in order to permit equivalency factors to be calculated using USES 1.0;
- to generate an "LCA country file" containing input parameters in order to render USES 1.0

suitable for LCA purposes;

- to feed USES 1.0 with data on at least a number of priority chemicals, and generate – analogous to the GWPs – a list of equivalency factors for the interpretation and aggregation of toxic emissions in LCA.

1.2 LCA IN RELATION TO OTHER TOOLS

LCA is a decision support tool, not a decision-making tool [12]. LCAs generate information that can be used in decision-making by governments, businesses and consumers. To further define the scope and range of LCA, it is useful to compare this tool with other environmental decision support tools such as Substance Flow Analysis (SFA) [cf. 41] (also known as material balances), Technology Assessment (TA), Environmental Impact Assessment (EIA), Risk Assessment (RA) and Environmental Audit (EA). As discussed by Udo de Haes & Huppes [42] and Heijungs *et al.* [43], all these tools have different prime economic objects of analysis. LCA analyses the environmental impacts of a product through its entire life cycle; SFA analyses the flows and accumulations of one substance (or substance group) in the economy (considering all phases, *viz.* extraction, production, consumption and disposal) and the environment within a defined region and period (generally one year); TA assesses the environmental, social, economic and other relevant aspects of future technologies; EIA analyses the environmental impacts of investments and plans envisaged for specific locations; RA analyses the adverse impacts of technical plant; a distinction can be made between RA in a strict sense and RA in a broader sense; the former analyses very small probabilities of extremely adverse effects due to one plant in a specific location, while the latter considers risks to be any adverse effects of a plant occurring with a certain probability; EA, finally, deals mainly with the environmental performance of individual business units or firms [42].

The different scopes of the various tools also have important implications for the methodology, especially when used for impact assessment. This is due to the different time and space characteristics of the various tools. For example, RA in a broader sense allows statements to be made on toxicity in terms of actual risks, e.g. concentrations exceeding a particular threshold value, because RA focuses on processes at one specific site. With LCA, however, only potential impacts can be assessed, one reason being that the time dimension is not taken into account in process emission data. This problematical issue can be illustrated by an example; see the text frame (which has been taken from [44]). Because of these differences, the tools mentioned each have a specific role to fulfil and to a large extent yield complementary information.

Despite differences in the object of the various tools for environmental decision support, there is great potential for transferring concepts, models and data from one tool to another [45]. The project reported on here is an illustration of this: a model that has been developed for the tool of RA, and the data acquired to run it, are now used to further develop the tool of LCA.

1.3 STRUCTURE OF THE REPORT

This report is structured as follows. Chapter 2 is devoted to an exposition of USES 1.0, and addresses some points on which the design of USES 1.0 is not, or not sufficiently, suitable for the

It is impossible to base statements on toxicity in LCA on concentrations below the standard, be it MAC, NOEC or ADI. This is a difficult point, which will be worked out below in some more detail.

Assume that two methods of shaving are compared: the functional unit is one shaving activity, method A is with a razor blade and method B involves an electric razor. The life cycle of method A includes the production of shaving-soap. Assume this takes place in a small factory. The life cycle of method B includes the production of PVC, which will be assumed to take place in a large plant. A result of the analysis might be that method A including the production of shaving-soap needed for one shaving is environmentally worse than method B including the production of PVC needed for one shaving.

However, due to the large production volume of the PVC plant, the PVC process *in its actual extent* is worse than the shaving-soap process *in its actual extent*. This aspect cannot be considered by LCA. LCA emission data are obtained by dividing yearly emission amounts by the yearly production amounts. The operating *time* of the process is then divided out and the result is a number of emission loadings per amount of product produced. In LCA the volume of a specific process has thus become irrelevant. The process in its actual extent is only relevant for Environmental Impact Assessment (EIA) and Risk Assessment (RA). This makes that with an LCA, statements in terms of actual risks cannot be made. Even if you would like to do so, just forget it.

We hope to have demonstrated above that it is fundamentally impossible to perform an actual risk analysis within the framework of LCA. But what do these results represent? The results of a life cycle impact assessment do not represent *actual* risks but *potential* risks. No one will die of the emissions for one shaving. But all tiny contributions of all activities make together the environmental problem.

LCA is not concerned with the degree to which a NOEC is actually *exceeded*, but with the degree to which it is potentially *filled up*. We still believe that the NOEC can be used as a suitable measure for the strength of a toxic substance in LCA. The exact form of the dose-response curve is essential for an *actual risk assessment*. Of course, the actual impacts are important as well. Actual assessments, such as RA and EIA, may thus never be superseded by LCA.

(Taken from [44].)

purpose of LCA. This leads to identification of five main problems to be addressed, a task that is undertaken in the five successive chapters, 3 to 7. Chapter 8 describes the procedure according to which new equivalency factors have been and are to be calculated. Chapter 9 is devoted to some concluding remarks. The practical result of the project, the new equivalency factors for 94 chemicals, is presented in Appendix A.

Chapter 2

USES 1.0 MODEL IN LIFE CYCLE IMPACT ASSESSMENT OF TOXIC RELEASES

2.1 SHORT DESCRIPTION OF USES 1.0

The acronym USES stands for *Uniform System for the Evaluation of Substances*. USES 1.0 is a tool that can be used for rapid, quantitative assessment of the hazards and risks of (organic) substances to man and the environment. In USES 1.0 various methods for the assessment of substances are integrated and harmonized into one assessment scheme. This section provides a short description of the system. For a full description, the reader is referred to [38].

USES 1.0 is designed to serve as a system attuned to current chemical management policies and provides a "state-of-the-art" in chemical hazard and risk assessment. As far as possible the assessments are performed within the scope of international directives, regulations and recommendations, such as those set by the European Union and the OECD Chemical Programme.

The present version of USES 1.0 was developed in close consultation with research institutes, industry, experts from the Dutch Ministry of Housing, Spatial Planning and Environment, the Dutch Ministry of Welfare, Public Health and Cultural Affairs and the National Institute of Public Health and Environmental Protection. USES 1.0 is currently being improved and adapted in cooperation with European Union member states and the European chemical industry, with the aim of developing a European version of USES: EUSES.

Main structure

The system USES 1.0 consists of several main modules. The function of each module will be described below during discussion of the main structure of USES 1.0, comprising exposure assessment, effect assessment and risk characterization of chemical substances. USES 1.0 consists of the following modules:

- data entry module;
- emission module;
- distribution module;
- intake module;
- effect module;
- evaluation module;
- data output module.

RISK CHARACTERIZATION

The main principle in USES 1.0 is comparison of the results of an effect assessment (dose-response assessment) and an exposure assessment (Figure 2.1). This comparison, termed risk characterization, takes place in the evaluation module of USES 1.0. This comparison is performed by calculating the risk characterization ratios per substance; a ratio between the estimated exposure concentration and a suitable effect or no-effect parameter. This risk characterization ratio, also known as the PEC/PNEC ratio[1] (predicted environmental concentration/predicted no-effect concentration), is an indicator of the incidence and severity of adverse effects. If possible, this risk characterization is further quantified by means of uncertainty analysis to yield a risk estimate. This risk estimate is a quantitative estimate of the probability of clearly described effects occurring, incorporating uncertainty analysis.

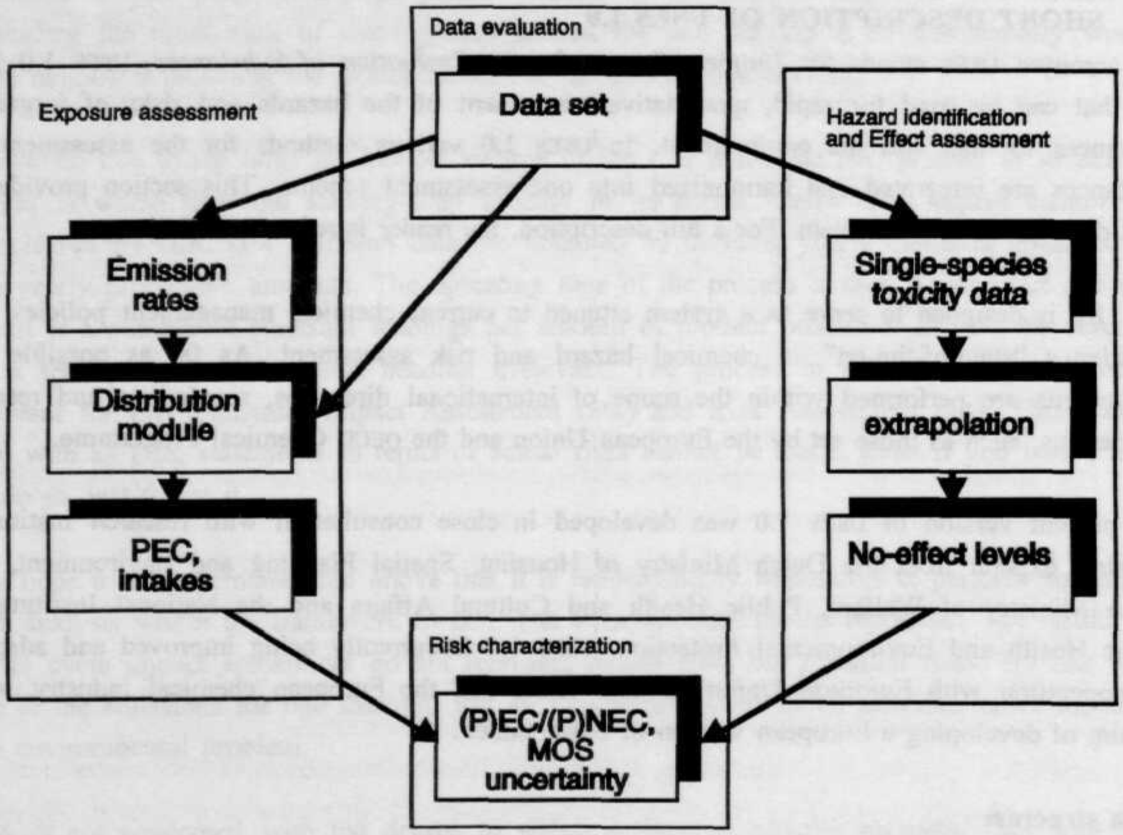

Figure 2.1: Main structure of USES 1.0 (Source: [38]).

EXPOSURE ASSESSMENT

Doses and environmental concentrations are predicted in a three-step procedure:

- estimation of the emission;
- estimation of the distribution;
- estimation of the intake of a substance.

The releases to environmental compartments are predicted on the basis of the volume produced or imported and the usage pattern of the chemical concerned. These calculations take place in

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[1] For human toxicity not the PEC/PNEC, but the margin of safety (MOS) is calculated. This is defined as ADI/"PDI": the acceptable daily intake divided by the predicted daily intake.

the emission module of USES 1.0, in which emission factors for various life cycle stages are chosen from a database, giving due consideration to the properties, applications and functions of the substance.

Next, environmental concentrations are calculated using models that take into account the transport and fate of the substance. The distribution module of USES 1.0 contains all the models necessary to estimate the distribution of a substance in the environment at the appropriate scale, i.e. personal, local or regional scale. Endpoints are concentrations in various environmental compartments, *viz.* air, surface water, groundwater, sediment and soil.

Finally, based on estimated environmental concentrations and/or concentrations in products, the intake module of USES 1.0 calculates the dose reaching top predators (worm- and fish-eating mammals and birds) and man, using bioconcentration factors and intake models.

EFFECT ASSESSMENT

The effect assessment in USES 1.0 is based on various protection targets: populations and ecosystems to be protected:

- human populations:
  - directly exposed;
  - indirectly exposed through the environment (e.g. through consumption of crops and meat);
- Ecosystems and populations:
  - micro-organisms in sewage treatment plants;
  - aquatic ecosystems;
  - soil ecosystems;
  - top predators, indirectly exposed through the environment (fish- and worm-eating birds and mammals).

Effect assessment entails a dose-response assessment of human toxicological and ecotoxicological data. In the effect module of USES 1.0 the no-effect levels for the relevant time scales, acute or long term, are determined for the various protection targets. In ecotoxicological effect assessment, predicted no-effect concentrations (PNECs) are derived from experimental toxicity data on single species using extrapolation factors to calculate PNEC-values for ecosystems. In human toxicological effects assessment a no-observed-adverse-effect level (NOAEL) is derived from the available data, which, if necessary, can be extrapolated to a no-effect level for humans (NEL_{man}).

Dimensions of the system

The dimensions in USES 1.0 are determined largely by the spatial scale, the time scale and the "realism scale".

SPATIAL SCALE

For the effect assessment standard environmental conditions are used. Because of geographical variations in conditions, USES 1.0 allows the user to choose between various default files containing different environmental conditions, the so-called country files. Exposures and concentrations can be calculated on 3 spatial scales: the personal scale (users are considered to be exposed directly), the local scale and the regional scale. At the regional scale diffuse, continuous emissions to a standard environment are considered. Steady-state partitioning between compartments is assumed. The targets exposed are non-specific.

TIME SCALE

For the effect assessment a distinction can be made between continuous and discontinuous emissions, the latter being assumed to lead to short-term, peak exposures or long-term average exposure concentrations, depending upon the frequency and duration of the emissions and the life span of the organisms considered. In the toxicity assessment a distinction can also be made between short-term (acute) and long-term (chronic) toxicity effects. On a regional scale diffuse emissions are regarded as continuous, leading to steady-state environmental concentrations, which can be considered to be estimates of long-term average exposure levels. The exposure levels can be compared to no-effect levels derived from long-term toxicity data.

REALISM SCALE

The values for nearly all parameters vary over a wide range owing to uncertainties resulting from limited scientific understanding and variability due to diversity in time and space. USES 1.0 is designed to estimate "realistic worst case" hazard levels, meaning that, whereas the chosen standard exposure scenario in itself represents an unfavourable, but still reasonable, situation, approximately mean, median or realistic parameters are used whenever possible. For a reliable risk assessment an uncertainty analysis is included. In the present version of USES 1.0 the uncertainty analysis is limited to the risk assessment of aquatic organisms and micro-organisms in sewage treatment plants on a local scale. In the uncertainty analysis, variables are characterized by a median value and an uncertainty factor, quantifying uncertainties due to limited scientific understanding and spatial variations. Temporal variations have not been included, except for those in emission estimation. The overall result of the uncertainty analysis is a probability density function for the risk characterization ratio.

Description of the emission module of USES 1.0

The emission module is not relevant for the purpose of LCA, since LCA produces its own emission numbers during inventory analysis. For this reason the emission module of USES 1.0 will not be further described in this report.

Description of the distribution module of uses 1.0: the regional model

In USES 1.0 exposure estimates can be made on a regional or local scale. Calculations on a local scale are carried out by means of dedicated local models for various stages in the life cycle of a substance. The regional computations are performed using a multimedia fate model. For LCA only the regional model is relevant, since it is not feasible to assess local effects for each process in the overall process tree studied in LCA (see also Chapter 5). This description of USES 1.0 therefore focuses on the regional distribution model.

The regional computations are performed using a multimedia fate model of the so called Mackay type, named Simplebox [46]. Simplebox solves a set of systematically written mass-balance equations. Each equation describes the mass balance of the chemical in one compartment. The solution of the set of equations represents the steady-state concentration in each compartment.

The version of Simplebox in USES 1.0 describes eight compartments: air, water, suspended particles, aquatic organisms, sediment, natural soil, agricultural soil and industrial soil. The concentration in shallow groundwater on the regional scale is set equal to the concentration in the pore water of the agricultural soil. Leaching from the top layers to the deeper groundwater is considered to be an outflow from the system. The processes handled in Simplebox are emissions, degradation and advective and diffusive mass transport (Figure 2.2). Formation of decay products (metabolites) is not considered in the present model.

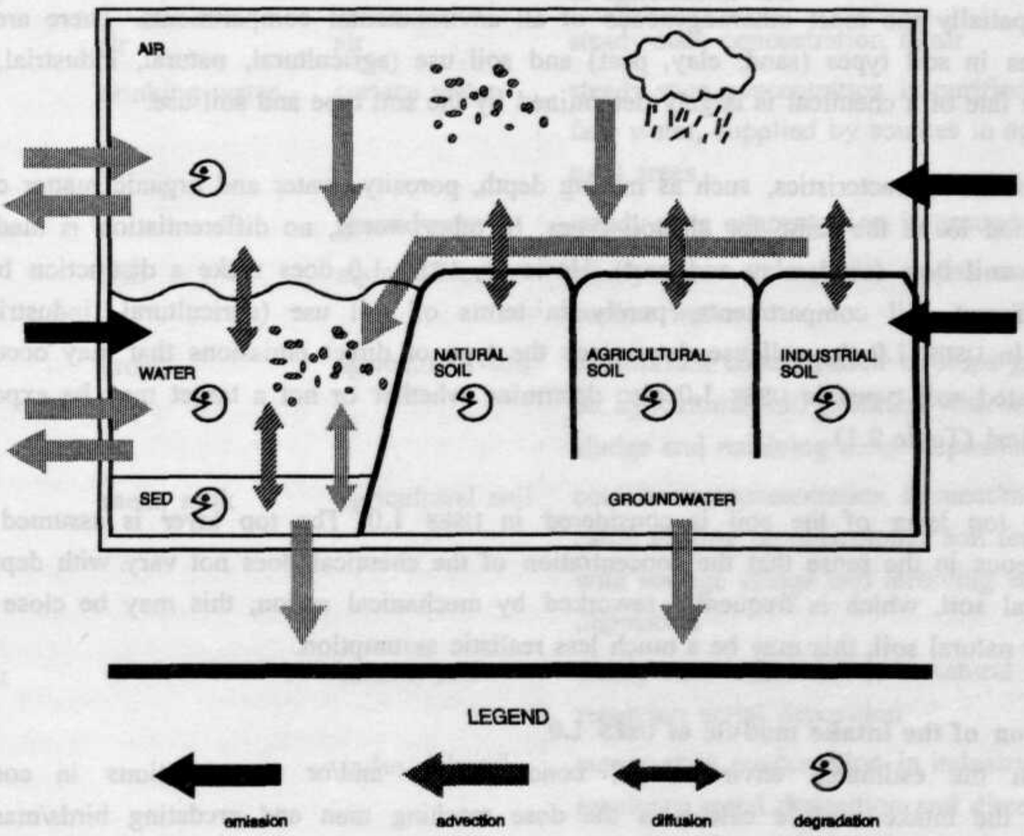

Figure 2.2: Compartments and processes described in the regional distribution model Simplebox (Source: [38]).

Air and water are continuously flushing in and out of the system. This leads to "import" and "export" mass flows of the chemical to and from the system. The air and water compartments are considered to be well-mixed. The refreshment rate is characterized by the atmospheric residence time and a single, typical hydraulic residence time.

Suspended matter is also imported and exported through water flows. Suspended matter may also be produced in the system itself, by growth of small aquatic organisms (bacteria, algae). There is a continuous exchange of particles (and thus chemicals) between the water and the sediment through sedimentation and resuspension.

Biota refers to living organisms in water, from bacteria to fish. This compartment is usually small and therefore plays an insignificant role with regard to the overall fate of the chemicals.

Only the top 3-centimetre layer of the sediment is considered in this system; this layer is viewed as well-mixed, freshly deposited material, commonly found in sedimentation areas. The older sediments that have been buried under this top layer are not considered as part of the system; substances that reach these sediments can thus be regarded as immobilized.

Soil is spatially the most inhomogeneous of all environmental compartments. There are many differences in soil types (sand, clay, peat) and soil use (agricultural, natural, industrial, urban etc.). The fate of a chemical is largely determined by the soil type and soil use.

At present the characteristics, such as mixing depth, porosity, water and organic matter content, are assumed to be the same for all soil types. In other words, no differentiation is made with regard to soil type (sand, clay and peat). However, USES 1.0 does make a distinction between three different soil compartments, purely in terms of soil use (agricultural, industrial and natural). In USES 1.0 the soil use determines the type of direct emissions that may occur. The differentiated soil types in USES 1.0 also determine whether or not a target may be exposed to the chemical (Table 2.1).

Only the top layer of the soil is considered in USES 1.0. The top layer is assumed to be homogeneous in the sense that the concentration of the chemical does not vary with depth. For agricultural soil, which is frequently reworked by mechanical action, this may be close to the truth. For natural soil, this may be a much less realistic assumption.

Description of the intake module of USES 1.0

Based on the estimated environmental concentrations and/or concentrations in consumer products, the intake module calculates the dose reaching man and predating birds/mammals. Figure 2.3 shows the indirect exposure route of man and predators to chemical releases. Exposure is calculated using the environmental concentrations estimated in the distribution module.

EXPOSURE OF HUMANS THROUGH THE ENVIRONMENT

The total daily intake of a substance by human beings is based on the concentration of the compound in drinking water, air, fish, crops, cattle meat and milk. Default values for the physical features of humans and their consumption pattern are described in the country file (e.g. average human body weight is 70 kg, daily intake of dairy products is 0.378 kg wet weight per day).

Table 2.1: **Protection targets and exposure scenarios in USES 1.0.**

target	medium of exposure	compartment	exposure assumption (regional model)
aquatic ecosystems	surface water	surface water	steady-state surface water concentration
terrestrial ecosystems	agricultural soil	agricultural soil	steady-state concentration in agricultural soil
fish-eating predators	fish	aquatic biota	equilibrium concentration in fish caught in surface water
worm-eating predators	worms	agricultural soil	equilibrium concentration in worms caught in agricultural soil
man	air	air	steady-state concentration in air
	drinking water	surface water	steady-state concentration in purified surface water, supplied by sources in agricultural areas
		groundwater	steady-state concentration in groundwater
	fish	aquatic biota	steady-state concentration in fish caught in surface water
	crops	agricultural soil	equilibrium concentration in crops grown on agricultural soil fertilized with sewage sludge and receiving aerial deposition
	meat, milk	agricultural soil	equilibrium concentration in meat/milk of cattle grazing on agricultural soil fertilized with sewage sludge and receiving aerial deposition
no target	—	natural soil	steady-state concentation in natural soil receiving aerial deposition
	—	industrial soil	steady-state concentation in industrial soil receiving aerial deposition and direct emissions from industry

Drinking water is assumed to be produced from contaminated surface water purified in a treatment plant or from groundwater. It is assumed that there is no removal of xenobiotics during groundwater abstraction. Owing to many uncertainties in removal efficiencies, the drinking water purification is modeled quite conservatively.

The concentration in fish is calculated from the surface water concentration by means of a bioconcentration factor, assuming equilibrium between water and fish. Concentrations in crops and grass are calculated using bioconcentration or biotransfer factors. Crops and grass are exposed to soil and air concentrations. The concentration in cattle and milk depends on the

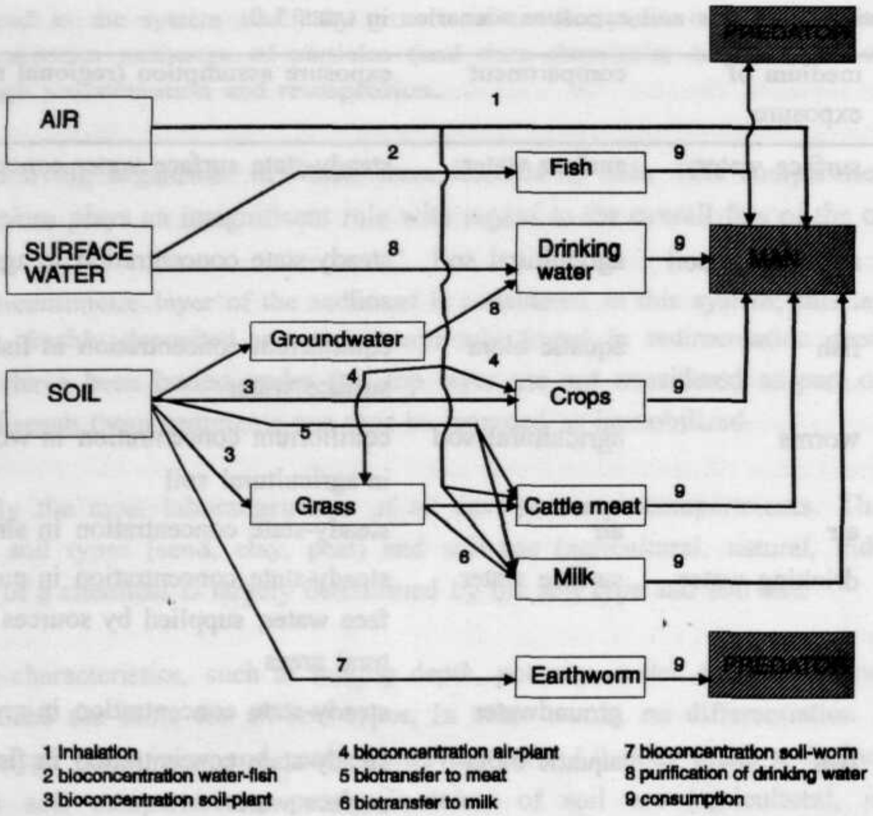

Figure 2.3: Schematic representation of the exposure of man and predators via the environment.

concentration in soil, grass and air (note: no crops or animal fodder).

In the regional assessment (relevant for LCA) the input for the intake module consists of steady-state concentrations in air, water, agricultural soil and groundwater. These concentrations are averages for the entire system; this means that the ultimate human exposure scenario for regional distribution is also averaged. The regional assessment can be seen as an indication of the potential hazard to the average inhabitant of the system due to continuous, diffuse emission.

CONSUMER EXPOSURE

The USES 1.0 model has a module which estimates the direct exposure to substances during the consumption of a product containing the substance. In the present LCA method this direct human exposure during consumption is not accounted for.[1] Consequently, no description of this module in USES 1.0 is given here.

EXPOSURE OF BIRDS AND MAMMALS THROUGH THE ENVIRONMENT

To give an indication of the potential for a substance bioaccumulating through food chains, three exemplary food chains are regarded in USES 1.0:

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[1] Incorporation of direct exposure presents a new challenge to developers of LCA methodology, unless it is decided that it should not form a part of LCA. Similar discussions could be held for an LCA of tobacco, for example.

- birds and/or mammals with a diet consisting entirely of fish in polluted surface water, or a ditch adjacent to soil of application (in the case of pesticides);
- birds and/or mammals with a diet consisting entirely of worms in polluted agricultural land or soil of application (in the case of pesticides);
- in the case of pesticides: birds and mammals exposed through diet (including crops/insects, fish/worms and direct ingestion of treated seeds or granules) or drinking water (surface water or spray drift from crops).

Concentrations in earthworms and fish are calculated using bioconcentration factors for soil-to-worm and water-to-fish. These concentrations in earthworms and fish are assumed to be the exposure concentrations for worm- and fish-eating top predators (birds and mammals).

Description of the effect module of USES 1.0

In this module no-effect levels for relevant time scales are determined for several groups at risk: humans, aquatic organisms, terrestrial organisms, sewage treatment plant (STP) micro-organisms and top predators. This calculation is performed using evaluated results of single-species tests with experimental animals or human toxicity data.

NO-EFFECT LEVELS FOR ECOSYSTEMS

The maximum permissible level is defined as the concentration of a compound at which (theoretically) 95% of the species in an ecosystem are protected. The negligible level is taken to be 1% of the maximum permissible concentration or, in the case of natural compounds, as the concentration measured in relatively unpolluted areas. The levels are not based upon scientific arguments but are the result of continuous interaction between policy-makers and scientists in the Netherlands.

In this report the assessment factors for the extrapolation of single-species tests to ecosystem level proposed by the EU [47] are applied and have been implemented in the country file:

- 1000 is applied to the lowest $L(E)C_{50}$ of base-set toxicity data (fish, daphnia and algae);
- 100 is applied if one NOEC from long-term toxicity data is available;
- 50 is applied to the lowest NOEC of long-term toxicity data for two species in two taxonomic groups;
- 10 is applied to the lowest NOEC of long-term toxicity data for fish, daphnia and algae;
- if field data exist, they must be reviewed on a case-by-case basis.

For more details regarding these factors the reader is referred to USES 1.0 [38].

The following data are generally available for deriving no-effect levels:

- acute toxicity to single species, expressed as a concentration (LC_{50} or EC_{50}, in mg/l);
- chronic or subchronic toxicity to single species, expressed as a concentration (NOEC, in mg/l);
- acute and/or (sub)chronic toxicity to mammals, expressed as a concentration (inhalation: LC_{50}, in mg/l) or a dose (oral: LD_{50} or NOAEL, in mg/kg).

NO-EFFECT LEVELS FOR PREDATORS

Toxicity values for predators are not usually available, and it is therefore necessary to carry out an extrapolation. The lowest no-effect concentration in the diet (NOECs) of birds and mammals is preferably taken. If no NOEC is available, a NOAEL can be translated to a NOEC using the consumption rate of the species from which the toxicity data were derived. The resulting NOEC is assigned an extrapolation factor of 10, in accordance with Slooff [48]. If an LC_{50} for birds is given, this value is assigned a factor 1000, after which it is compared to the extrapolated NOEC. The lowest value is used.

In current LCAs toxicity is focused on human toxicity and ecotoxicity. In the case of ecotoxicity a distinction is made between toxicity to the terrestrial and aquatic ecosystem. At present only species at the beginning of the food chain are considered in deriving the ecotoxicity. The species *higher up in the food chain, such as predators, are not (yet) considered.*

NO-EFFECT LEVELS FOR MAN

The risk to man is generally evaluated by comparing the result of the exposure assessment with a no-effect level for man. In USES 1.0, the general approach is to compare the estimated exposure directly with the NOAEL from toxicity studies. For LCA calculations an uncertainty factor has been used for the extrapolation of the NOAEL (or LOAEL) to the chronic and subchronic NEL_{man} for non-genotoxic substances [38, Table 10, p. 57].

2.2 ISSUES TO BE ADDRESSED APPLYING USES 1.0 IN LCA

USES 1.0 is a system for the assessment of toxic chemicals that employs the PEC/PNEC concept for ecotoxicity and the MOS concept for human toxicity. The essence of the system is to compare a predicted concentration or intake with a toxicity standard. Thus, for ecotoxicity, a predicted environmental concentration (PEC) of a chemical is estimated using an emission module and a distribution module, and this PEC compared with a predicted no-effect concentration (PNEC) determined with a toxicity module. For human toxicity, the MOS is calculated by dividing the acceptable daily intake of a chemical (ADI) by the predicted daily intake ("PDI") as determined by the emission, distribution and intake modules.

The USES 1.0 model can be very useful in the context of LCA. Applying USES 1.0 has a number of major advantages:

- USES 1.0 includes so much scientific knowledge that it would be inefficient to neglect this and repeat this work all over again.
- The qualities of USES 1.0 are supported by the majority of the government and business community in the Netherlands and will also be supported by the EU in the future.
- Application of USES 1.0 in LCA could result in further harmonization of the basic points of departure of substance- and product-oriented environmental policy.
- Several hazards are not yet considered in USES 1.0, but may be incorporated in the near future. Examples include global warming, ozone depletion, acidification and eutrophication. All these hazards are considered as separate categories in the assessment of products in LCA. With a view to harmonizing the predicted hazards it is highly recom-

mended to predict the hazards according to one comprehensive procedure/method. In this project, however, attention is focused on the toxicity assessment of USES 1.0.[1]

Although USES 1.0 covers all aspects of importance for assessing toxic releases, and could therefore be very useful for LCA characterization of toxic emissions, USES 1.0 is not useful for LCA without some changes. In this project the program itself has not been adapted, but a special "country file" developed containing specific input parameters in order to fulfil the conditions of LCA.

In summary, USES 1.0 is unsuitable on the following points (in parentheses, the chapters of this report in which the issues are discussed further):

- USES 1.0 is not entirely suitable for the assessment of inorganic chemicals and ions, while in LCA product assessment should be based on inorganic and organic substances (Chapter 3).
- USES 1.0 includes an emission module to estimate emission magnitudes, while LCA preferably imports the calculated emissions directly from the inventory (Chapter 3).
- USES 1.0 also includes – besides environmental processes – a number of economic processes, such as sewage treatment, drinking water purification and pesticide application, while in LCA these economic processes are dealt with differently (Chapter 3).
- USES 1.0 is based on the environmental conditions in the Netherlands and Western Europe, while LCA is concerned with environments all around the world (Chapters 3 and 5).
- USES 1.0 models impacts in a region, such as the Netherlands, i.e. the concentration of substances in the environment of the Netherlands is calculated due to emissions inside and outside the Netherlands, while an LCA preferably assesses the impacts of an emission at any given place (Chapters 3 and 5).
- USES 1.0 models the steady-state concentration in several environmental compartments due to (pseudo)continuous emission fluxes, while in LCA the impacts of just one product are analysed (Chapter 4).
- USES 1.0 is intended primarily to prioritize above-or-near-threshold situations, whereas the European mainstream approach to LCA takes emissions into account regardless of whether thresholds are exceeded (Chapter 6).
- USES 1.0 calculates a risk indicator per substance, while LCA aims to aggregate substances with similar impacts to one overall score, to facilitate decision-making by reducing the volume of information (Chapter 7).

2.3 THE PROBLEM OF AGGREGATION IN RELATION TO THE OBJECTIVE OF LCA

Inventory analysis plays a key role in the life cycle assessment procedure. In this step, an overview is made of all the extractions of resources and all the emissions of pollutants during the entire life cycle of the product alternative(s). In general, the processes which constitute the

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[1] At present, a Unilever-financed PhD-project is being executed at CML with the aim of harmonization of fate and exposure models for the different impact categories.

life cycle take place at different locations and at different times. Moreover, all these processes release different substances in different amounts. The outcome is an enormous amount of information: different substances are emitted in different amounts at different locations and at different times; see Figure 2.4.

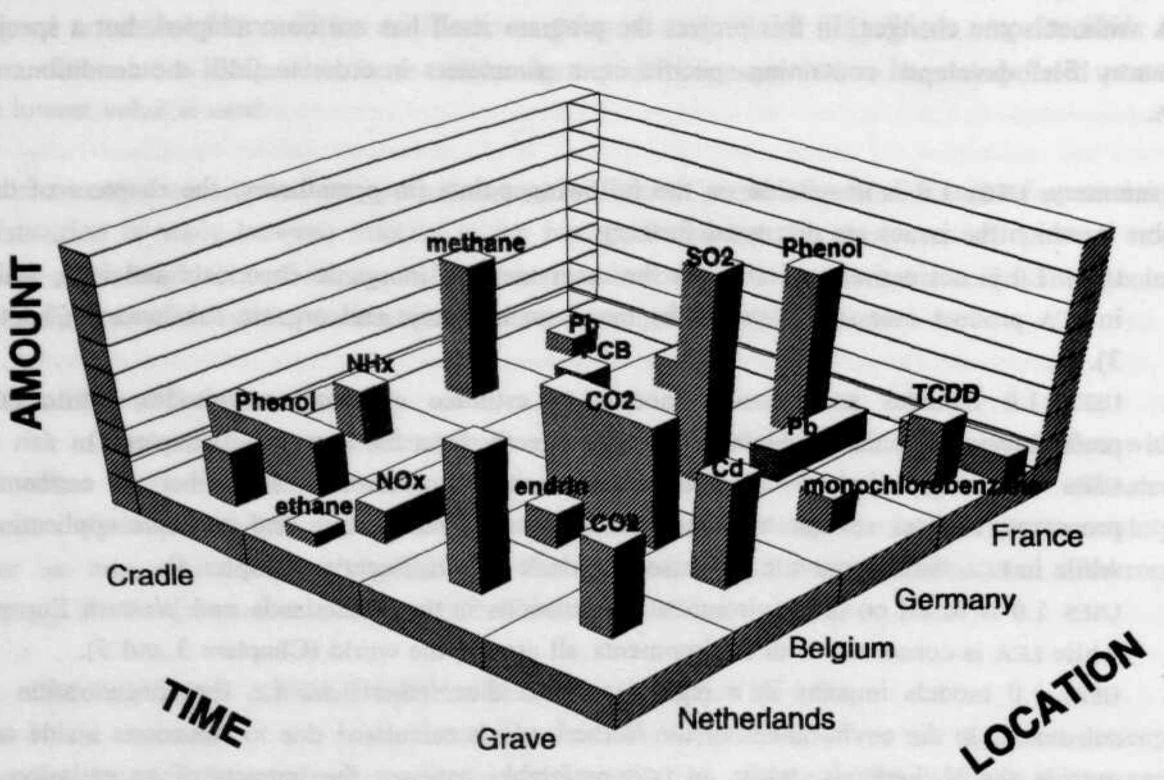

Figure 2.4: Illustration of the complexity of the information involved in LCA: emissions of different amounts of different substances at different locations at different times must be considered.

Some form of aggregation is essential if the aim is to arrive at a concise form of decision support. Usually, this aggregation is performed in two stages:

- Emissions of the same substance are aggregated in the inventory analysis. This means (i) that emissions now and emissions next year are added, (ii) that emissions here and emissions abroad are added, (iii) that emissions of large amounts and emissions of small amounts are added, and (iv) that emissions that take place as a peak and emissions that are dispersed over time are added. The general idea behind this approach is that this applies to emissions of all substances, and it is believed that differences in the impacts of substances are due to differences in the intrinsic properties of the substances and the total amounts released, rather than to differences in emission patterns (fluxes). This is obviously a simplification.

- Emissions of different substances are aggregated in the impact assessment. This means that emissions of different chemicals (e.g. heavy metals and organic solvents) are to be weighted according to their potential for causing certain environmental problems. The general idea behind this approach is that each substance can be characterized by two parameters, one for fate and exposure and one for toxicity (or more generally: environmental impact).

This report concentrates on the second type of aggregation. However, some reflections on the justification of the first type of aggregation are essential for understanding the types of choices that have to be made in the second type of aggregation.

In a typical life cycle assessment a few hundred processes may be involved. All these processes have a variety of characteristics with respect to location and time:

- The processes emit substances at different places. This may lead to differences in fate (due to e.g. differences in climate or soil type), to differences in exposure (due to e.g. the proximity of populated areas), to differences in toxicity (due to e.g. the presence of sensitive ecosystems), etc. Moreover, some processes (such as plastics factories) have a fixed location, while other processes (such as car transportation) move through various regions. Another difficulty is that some processes cannot be localized: for instance, oil that is bought on the world market is produced throughout the world.
- The processes emit substances at different times. Moreover, some processes (such as bottle production) take place instantaneously, while other processes (such as using a car) release their pollutants over a very long period of time. Finally, one process may have discontinuous emissions (like a car), while another may have continuous emissions (like 24-hour production plants).

Given this variety of emission patterns, it is not only fundamentally but also practically impossible to make an estimate of the actual toxic impacts that will become manifest as a result of the product's life cycle. Actual impacts at specific times and places are the domain of risk assessment; by its nature, life cycle assessment cannot deal with this issue. The objective of RA is to indicate the occurrence of toxic impacts or their probability of occurrence. As such, situations in which concentrations are below some reference value are regarded as safe. In contrast, the objective of LCA is to clarify the relationship between a product life cycle and its potential for contributing to toxic impacts. This means that LCA does not make statements with respect to safety, non-safety or any other absolute measure. Neither does it take these questions of safety or non-safety into account.

Instead, LCA focuses on the amount of a substance that is released, implying that a prediction of safe or unsafe concentrations is impossible. LCA, as envisaged in this report, is thus not applied to predict impacts but to include generic environmental knowledge about the fate, exposure and toxicity of chemicals in evaluating product alternatives with respect to their environmental aspects. This evaluation is based on the principle of pollution prevention, or "less is better": a smaller emission is always better in terms of avoiding potentially hazardous concentrations of a chemical [49].[1]

The above considerations have strong implications, both for the methodology of LCA and for its role relative to other procedures.

- The amount of a substance released during a life cycle is the main basis for further impact assessment. This implies that emissions of the same substance at different locations, at different times and in different amounts can be aggregated. This aggregated emission of a certain substance will often be the result of the inventory analysis, and serves as a basis for subsequent impact assessment.
- LCA does not replace RA; rather, the procedures are complementary. RA can be said to be based on the principle of risk aversion, while LCA has its roots in the principle of pollution prevention.

Chapter 4 is partly devoted to the aggregation of emissions of different amounts of the same substance, and to the aggregation of emissions at different times of the same substance. A related topic of Chapter 4 is the fact that USES 1.0 is a model for risk assessment that is based on an input of steady-state emission fluxes (in kg/hr or a derived unit) and concentrations, while the output of the inventory analysis is a list of emission loadings (in kg or a derived unit). Chapter 5 contains a discussion on the aggregation of emissions of the same substance at different locations. Chapter 7 focuses on the problem of aggregating emissions of different substances.

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[1] Since the scope of LCA extends beyond emissions (depletion of natural resources is also considered), the full wording is here "pollution prevention and resource conservation principle". According to [49], this principle "recognises that any emission created is regarded as waste and is to be seen as a potential opportunity to conserve resources".

Chapter 3

MODEL ADAPTATIONS FOR USE IN LCA

3.1 DESCRIPTION OF THE PROBLEM

Current LCA practice is mass-oriented. The method focuses on the amount of chemical released, disregarding place and time of the event(s). While this is useful and meaningful for effects other than toxicity, assessment of toxic effects calls for a concentration-oriented approach. The reason is that the effects of short-term exposure to a high concentration of a chemical are generally markedly different from the effects of long-term exposure to a low concentration, even if the exposure amounts (as evaluated form the product of release flux and duration) are equal. The RA methodology therefore focuses on concentrations and takes emission fluxes as an input. As a result of the different orientation of RA, the approach adopted in USES 1.0 differs from LCA practice on a number of points. This chapter describes the adaptations made to the standard USES 1.0 computations that were necessary to make the USES 1.0 approach applicable for LCA purposes.

Current LCAs disregard time, duration and place of release, and view the environment as a closed system. The regional and continental approach of USES 1.0 – allowing import from and export to elsewhere – is incompatible with this procedure. A further incompatibility is that in the USES 1.0 approach chemicals can "escape" from the system by the processes of leaching from soil to groundwater and burial of sediment. These incompatibilities can be solved by making some adjustments to the standard settings of USES 1.0. Changes of this sort can only be made by means of the so-called "country-file editor". A special "LCA country file" has been edited to suit the purpose of LCA. Furthermore, the sea should be added as an additional compartment (including the associated distribution parameters). Finally, including the compartment groundwater in the way described in the current USES 1.0 [38; p.160] implies that the mass balance is no longer correct. Groundwater should preferably be included as a full compartment in the system of mathematical equations of USES 1.0.

In current LCAs no distinction is generally made, mainly for practical but also for fundamental reasons, between emissions and impacts in the Netherlands and those in foreign countries (cf. §2.3). An emission and an impact may occur anywhere. This implies that it is desirable not to model the Dutch or West European environment, but some average world. It is to be anticipated that international use and acceptance of the approach developed in this project will be enhanced if the modelled "unit world" is of a more general nature, or, even better, covers a number of generic regions (see also Chapter 5).

In USES 1.0 emission fluxes are estimated on the basis of the production volume and use of the chemical. In an LCA the magnitudes of the emissions are calculated in the inventory analysis and do not have to be estimated using the emission module of USES 1.0. For the present purpose of calculating equivalency factors, standard emission fluxes are set in USES 1.0. Equivalency factors are computed for the "constructed situation" of releases of standard amounts per unit time to the different environmental compartments.

Part of the modelling in USES 1.0 is concerned with economic processes, such as wastewater treatment, pesticide application and drinking water purification. In an LCA wastewater treatment is considered to be an economic process, which means that the inventory table is already adjusted for any sewage treatment plant (STP). This part of USES 1.0 should thus be switched off.[1] Also, the application of pesticides (and other substances) in the agricultural sector is considered to be an economic process and should therefore be dealt with in the inventory analysis. The application of these substances should not be part of the emission or distribution module of USES 1.0. For the process of drinking water purification an exception is proposed. Unlike the above-mentioned processes, incorporation of this process does not follow logically from the function of the product. Consequently, this process could easily be forgotten in the inventory analysis. Given the impact of drinking water purification on human exposure to substances, this is highly undesirable. If the purification model of USES 1.0 is used, the removal of substances from the drinking water should lead to an increase of the concentration in the sludge. Also, the fate of the sludge should be modelled. In USES 1.0 this is not yet the case.

Assessment of the (eco)toxicological impacts of chemicals in USES 1.0 focuses on organic chemicals. For LCA purposes, inorganic chemicals (such as heavy metals) need to be addressed as well. For the purpose of computing equivalency factors for inorganic chemicals, empirical partition coefficients and bioconcentration factors are entered into USES 1.0, instead of using the estimation procedure on the basis of physico-chemical properties. As an exception, for all inorganic metals except mercury, estimation is based mainly on partition coefficients and BCFs. For other inorganic chemicals physico-chemical properties are used to arrive at an estimate.

3.2 CURRENT SITUATION: THE COUNTRY FILE

This section describes the parameter settings that make USES 1.0 simulate an "LCA world", how calculations for inorganic chemicals can be performed with USES 1.0 and several other system settings. For a more detailed description of the procedure to be followed when making calculations with USES 1.0 and of the parameters taken for particular substances, the reader is referred to the country file and the data files (see Preface). It must be conceded that the procedure employing the LCA country file does not solve all the problems raised in the previous section. For instance, the incorporation of the sea as a fully modelled compartment was beyond the scope of the present study.

Configuring USES 1.0 by means of the country file

The standard regional/continental scale computation of USES 1.0 is not suitable as a starting point for computing equivalency factors for LCA. By means of the country-file editor, a special "LCA environment" has been created for this purpose. By loading the LCA country file into USES 1.0, a

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[1] Of course, it is perfectly feasible to use the modelled STP in the inventory calculations; see §9.1.

number of changes are made to default settings that cannot otherwise be made. Basically, the regional scale has been modified to mimic a continental system resembling Western Europe, but with extremely long residence times of air and water (little refreshment). To this end the following changes have been made to the standard regional scale in USES 1.0:

- System area: the area of the regional scale has been set to $3.56 \cdot 10^6$ km^2 (area of continental Western Europe).
- Fractions of water and soil: the area fraction of water has been set to 3%; the area fraction of natural soil has been set to 60%; the area fraction of agricultural soil has been set to 27%, and the area fraction of industrial soil has been set to 10% (typical values for Western Europe).[1]
- Infiltration/leaching: the parameter "fraction of rainwater that infiltrates into soil" has been set to the value 0.25 (typical value for continental Western Europe).
- Residence times of air and water: atmospheric and hydraulic residence times have been maximized. For air this is achieved by specifying an extremely low wind speed of 10^{-10} m/s, and for water by (i) specifying an extremely low value for the "sum of the discharges crossing the system boundaries" of 10^{-10} m^3/s, (ii) specifying an extremely low value for the "fraction of rainwater that runs off from soil" of 10^{-10}, and (iii) setting the STP capacity to the value of 10^6 pop.eq. (the minimum value allowed by USES 1.0).

While the primary objective (*viz.* to keep the LCA world "closed") is met by setting extremely long air and water residence times, the implicit (unwanted) consequences of this choice should be noted at this point. The result of setting the run-off of rain water to nearly zero is not only that the water compartment is refreshed at the desired low rate, but also that the transport of chemical from soil to water is underestimated. Also, the water compartment is modelled as a typical freshwater system, and the transport of chemical from air to water by atmospheric deposition is consequently computed too low. However, the hydraulic residence time is set to a more "oceanic" value, allowing time for removal processes (volatilization, degradation) to take place. Depending on the properties of the chemical and the compartment to which release takes place, the net consequence may either be over- or underestimation of the concentration in continental freshwater.

Entering inorganic chemicals in USES 1.0

For chemicals other than the non-ionic organic chemicals for which USES 1.0 was primarily designed (SO_2, NO_2, NH_3, heavy metals[2]), chemical-specific physico-chemical properties, partition coefficients and bioconcentration factors must be entered.

- For inorganic metals (for which no measured vapour pressure is available, except for mercury) an extreme small vapour pressure (10^{-10} Pa) must be entered to force USES 1.0 to estimate the fraction of the chemical associated with aerosol particles in air as nearly 1. This is correct for most metals.

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[1] These values differ from those of USES 1.0, but are in accordance with the Technical Guidance Document [47] which is the basis of EUSES, a fact which will probably lead to broader acceptance of the model.

[2] For heavy metals, the main route of immobilization is through sedimentation (burial), since degradation of heavy metals is not relevant and export (refreshment) is set to almost zero in the LCA country file.

- Realistic values should be entered for the air-water partition coefficient. For metals (for which no air-water partition coefficients are generally available), an extremely low value should be entered. The estimate offered by USES 1.0 (based on vapour pressure and solubility) must be rejected. However, no realistic values could be found for the air-water partition coefficients of inorganic chemicals.[1]
- Realistic values must be entered for solids-water partition coefficients in any case. The estimate offered by USES 1.0 (based on the octanol-water partition coefficient of the chemical and organic carbon fraction of the solids) must be rejected. This estimate can only be rejected if measured values are available. For almost all metals measured values are available.
- Realistic values must be entered for bioconcentration factors. The estimation procedures offered by USES 1.0 must be rejected. This estimate can only be rejected if measured values are available. For almost all metals measured values are available.
- Realistic values must be entered for all degradation half-lives. The values estimated in USES 1.0 (on the basis of biodegradation screening tests) have little meaning for these chemicals. In the new calculations, degradation half-life values are maximized for all metals. No measured values are used.

Other model settings in USES 1.0

In addition to reconfiguring the standard regional USES 1.0 environment by loading the LCA country file, several more chemical-specific parameters must be set in USES 1.0.

- Release of the chemical into the redefined "LCA world" must be specified in LCA terms. Therefore, the built-in estimation procedures of USES 1.0 are overruled by entering standard amounts (1000 kg/d) to the different environmental compartments. Separate computations are performed for the cases of releases to air, water, agricultural soil and industrial soil.
- Import of the chemical with air and water from the continental scale into the regional "LCA world" should be set to zero by attributing the value zero to releases at the continental scale.

3.3 FUTURE PERSPECTIVES

The RIVM, supervised by a working group consisting of member states, European Commission and chemical industry, is preparing a *European Union System for the Evaluation of Substances* (EUSES), to implement the terms of the harmonized Technical Guidance Document for the assessment of new and existing chemicals [50]. Most of the present features of USES 1.0 and a number of adaptations will be incorporated in this new system. Two of these new features are relevant to LCA:

- EUSES will contain a "nested" version of the present Simplebox. Whereas in the present USES 1.0 model computations for the continental scale and regional scale are performed sequentially (with the chemical passing from the continental to the regional scale, and not

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[1] The estimate of USES 1.0 for the air-water partition coefficient of metals is very low, because the vapour pressure is also extremely low.

vice versa*), in the new EUSES the computations are carried out simultaneously by nesting the regional scale inside the continental scale. This nested approach offers greater scope for resolving the incompatibilities of the LCA and RA approaches.

- **In the new EUSES system, it will be possible for the user to change all the default settings; a specific LCA country file will no longer be necessary. It is expected that the parameters of the country file developed in this project will also be useful in EUSES once it is released.**

Chapter 4

SOLUTIONS FOR THE FLUX-PULSE PROBLEM

4.1 DESCRIPTION OF THE PROBLEM

One of the problems with the application of environmental models within the framework of life cycle assessment is an incompatibility of dimensions. This chapter defines the problem, gives eight possible solutions, and makes a choice from these eight.

In LCA, a product is assessed from the cradle to the grave. The cradle and grave may be separated by many years. If one concentrates on the emissions of a particular substance as a function of time, one observes a very irregular pattern (Figure 4.1).

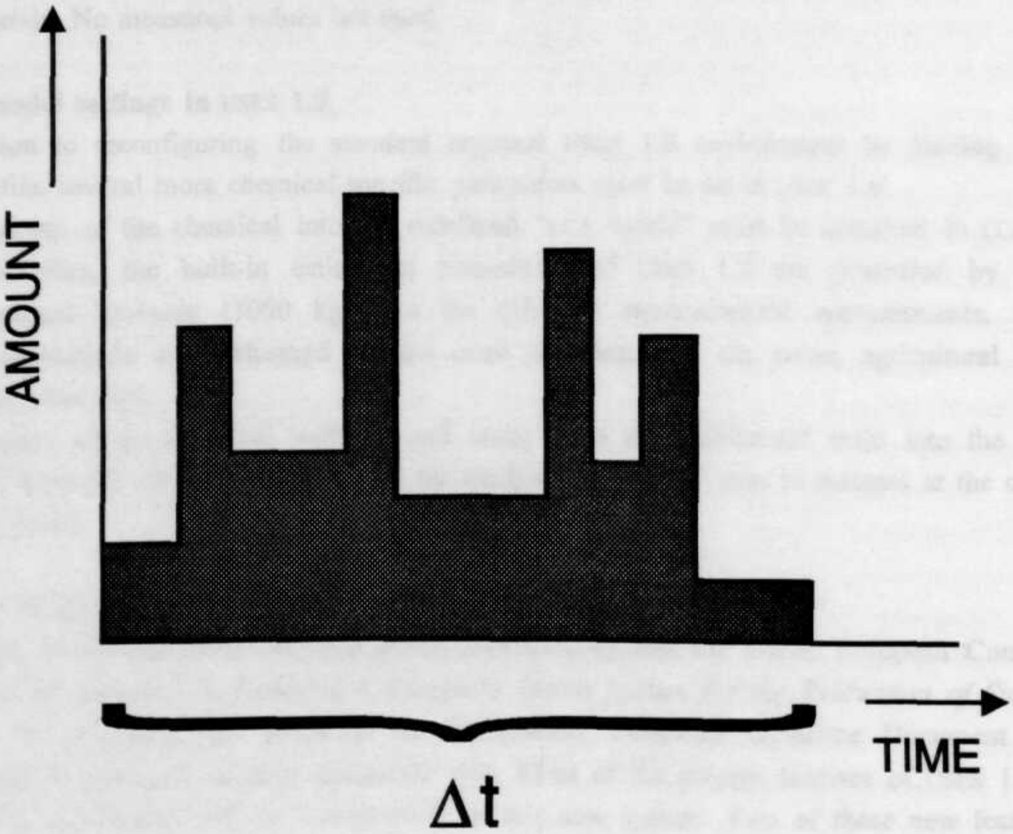

FIGURE 4.1: Time pattern of the releases of a certain substance during the life cycle of a product.

Since this irregularity cannot itself be modelled in LCA (cf. §3.2), it is necessary to consider the problem of what actually needs to be assessed. Is it the average rate of emission which is of interest? Or is it the total amount of pollutant which matters?

In fact the period during which the life cycle takes place (Δt in the Figure) is difficult to estimate, owing to the contribution of capital goods on the cradle side and of waste management on the grave side. For instance, a life cycle lasts for one month if production, use and disposal of the product are taken into account. If the production of the machinery is included as well, the life cycle may easily extend over 20 years. And if the machinery which produced this machinery is included, the life cycle could be expanded by another factor three. On the grave side there is an analogous phenomenon. Disposal of the waste-incinerating equipment may increase the duration of the life cycle substantially. The point is that the total emission of a certain chemical usually converges quite rapidly to an approximate answer, while the time span of the life cycle does not converge at all. Inclusion of the production of capital goods involved in producing capital goods will not have very much influence on the amount of pollutant emitted. The time span of the life cycle is greatly affected by this operation, however. This means that the average rate of emission cannot be established.

A solution to this problem is to estimate the total amount of substance emitted during the life cycle without estimating the time span of the life cycle. This is a quantity in mass terms (unit: kg), not in flow terms (unit: kg/hr). It corresponds to the shaded area in Figure 4.1. It is assumed that this total amount of substance is emitted in an unspecified time period, perhaps in an irregular way. Two extremes here are:

- the substance is released in one instantaneous pulse;
- the substance is released smoothly over a very long time period.

In the former case, there could be a short exposure to a very high concentration, while the latter case yields a very long exposure to a low concentration. From a toxicological point of view, these two extreme situations are by no means equivalent. The toxic impact of a substance is highly dependent on the exposure time and the exposure concentration. It is clear that a substance policy cannot be based on total amounts of an emitted substance. Nevertheless, these aggregated amounts have their own relevance in the context of pollution prevention, for which LCA is a tool. As the two extremes are considered equivalent in the context of LCA, it does not matter which option is chosen. The option that is most frequently seen in current LCA practice is the pulse option. The result of a life cycle inventory is then an inventory table which lists, amongst other things, some dozens of emitted substances. The quantities are expressed in terms of mass loadings, i.e. in kg or some derived unit thereof, like g, mg, μg or tonne. Below, these will be indicated by Δm.

Most environmental multi-media models [38,46,51,52] are concerned with steady-state modelling: a constant input flow of pollutants gives rise to a steady-state concentration of these pollutants in the various different media. Constant input flows bear the dimension of mass per time unit: kg/hr (or related units, such as μg/s or tonne/yr). The models calculate the steady-state concentration *PEC* (= predicted environmental concentration) as a function of a continuous inflow Φ:

$$PEC = K \times \Phi \qquad (4.1)$$

where K is a modelling constant[1] of dimension $\mathrm{hr{\cdot}m^{-3}}$. The steady-state concentration is related to a concentration that is assumed to be safe, the *PNEC* (= predicted no-effect concentration), to yield a dimensionless risk quotient R:

$$R \equiv \frac{PEC}{PNEC} \tag{4.2}$$

In the discussion below, it is useful to combine K and *PNEC* into one parameter G:

$$R = \frac{K}{PNEC} \times \Phi \equiv G \times \Phi \tag{4.3}$$

The problem, known as the flux-pulse problem, is how to reconcile the dimensions of the output of the inventory analysis and the input of the impact assessment models: how can we insert a Δm in the only available equation $R = G \times \Phi$? The problem was first observed in [36] and in [53]; a first solution was provided in [53] and [29]; more general treatments can be found in [54] and [45].

In Appendix C, eight possible solutions to this problem are described in quite some detail. All eight solutions have some disadvantages, but, remarkably, all of them yield the same results. The choice of one solution from these eight is therefore a question of taste.

4.2 CURRENT SITUATION: THE REFERENCE SUBSTANCE

The flux-pulse problem can be solved in at least eight ways; see Appendix C. All of these possible solutions have certain advantages and disadvantages. In principle any of these solutions could be chosen. In this report, based on criteria explained in Appendix C, we have opted for comparison with a reference substance (method *c1* in the appendix).

Having opted for this method, one or more reference substances need to be chosen. One possibility is to choose one reference substance per impact category, such as carbon dioxide for global warming and ethylene for photochemical oxidant formation. However, we may also strive for one single reference substance for all the different categories. In principle, any substance with a finite and non-zero K and *PNEC* is appropriate for this purpose. This already excludes persistent and non-toxic chemicals as a reference substance. For reasons of numerical stability it is appropriate to choose a well-studied substance. If the physico-chemical or toxicological properties of the reference substance change, all equivalency factors change. Additional, psychological reasons may guide us here. It seems attractive to choose a substance which satisfies a number of criteria related to appeal:

- preferably a substance that is clearly associated with toxicity (thus, a fairly toxic substance);
- preferably a substance that is exclusively associated with toxicity (thus, not a substance that is mainly notorious for, say, acidification);

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[1] For a one-compartment model with a simple decay law characterized by the decay rate κ, we have $K = 1/(V \times \kappa)$, where V is the volume of the compartment. For a multi-media model, the expressions become more complicated; see Heijungs (1995) for a general multi-linear treatment.

- preferably a substance for which emissions are well-known and regular (thus, not a substance that is rarely emitted).

Considering all these arguments and the fact that we have chosen the impact categories human toxicity, aquatic ecotoxicity and terrestrial ecotoxicity (see §7.2), we propose the choice of the substance 1,4-dichlorobenzene for all three impact categories. This reference substance is moderately persistent (several weeks to months) and moderately toxic. For the reference compartment, we propose to use air for human toxicity, water for aquatic ecotoxicity and industrial soil for terrestrial ecotoxicity.

Table 4.1: Overview of reference substances and reference compartments for the three impact categories.

target group	reference substance	reference compartment
aquatic ecosystems	1,4-dichlorobenzene	water
terrestrial ecosystems	1,4-dichlorobenzene	industrial soil
humans	1,4-dichlorobenzene	air

4.3 FUTURE PERSPECTIVES

The choice of the reference substance was now limited to one of the 94 chemicals studied in this report. When, in the future, more chemicals are included, the choice of the reference substance 1,4-dichlorobenzene may be reconsidered with regard to the criteria discussed above. In the future, the choice of the reference substance might also have to be adapted because of developments concerning spatial differentiation (Chapter 5), choice of toxicity parameter (Chapter 6) and distinctions between toxicity impact categories (Chapter 7).

Chapter 5

DEALING WITH SPATIAL DIFFERENTIATION IN LCA

5.1 DESCRIPTION OF THE PROBLEM

This chapter deals with the problem of spatial differentiation of emissions and/or impacts in LCA. First a brief overview of arguments for and against spatial differentiation will be given, and some previous attempts discussed.

Environmental life cycle assessment deals with the environmental impacts of a product in its entire life cycle. A life cycle consists of all the processes related to the functioning of the product: from the extraction of raw materials, through the production and use of the product to the reuse and disposal of the final waste. The main aim of LCA is to provide a systematic framework for the comparison of environmental impacts of different products with the same function. Another important purpose of LCA is to identify the most dominant stage in a product's life cycle and hence to indicate the main routes towards environmental improvements of existing products.

The aim of LCA is not to predict the actual concentrations of substances in the environment or to predict actual environmental impacts. There are several reasons why LCA deals with potential impacts and cannot predict actual concentrations and impacts (see also §2.3):

- LCA considers emissions which can be attributed to the functional unit of the product studied. Therefore LCA does not deal with the emission rate of a process. In the case of multi-input/output processes, moreover, LCA allocates only part of the emissions to the product system studied.
- LCA does not deal with background concentrations caused by other processes which are not part of the product system studied.
- LCA focuses mainly on gathering a complete relevant set of processes which represent the entire life cycle of the system. As a consequence, the number of processes can be very large. If detailed site-specific relations were to be incorporated in LCA, this would set extremely high demands on data in both the inventory analysis and the classification/characterization step. The inventory analysis should then include data on the geographical specification of each process and the classification/characterization data on the geographical distribution of relevant environments.

As stated in §2.3, LCA is not concerned with impact prediction but with environmental valuation of product alternatives using (generic) knowledge on fate, exposure and toxicity. In reality, however, the fate, exposure and toxicity of an intervention depend upon spatial aspects. So, although site-specific prediction of fate, exposure, or toxicity is not possible nor aimed for in LCA, one should try to include as much geographical information as is useful and practically feasible.

Until now, geographical information has not yet been used in LCA impact assessment methods, but the need to do so has been widely recognized [55,56,57]. In its final report the SETAC-Europe Working Group on Life Cycle Impact Assessment (WIA) states that for some impact categories including toxicity there "seems to be a great need for further development of the procedure for site-dependent impact assessment. A main challenge then is to prepare relevant maps for the different impact categories, preferably at a world level, with a fair balance between resolving power and feasibility" [25].

Following this site-dependent approach, in the literature several proposals for improvement of spatial differentiation in LCA methods are being introduced.

The site-dependent approach is based upon the following principles [14,55,56,57]:

- instead of one unit world, a number of standard environments are introduced; each impact category may require its own standard environments;
- use is made of generic, average information on each defined environment and, accompanying generic models, new characterization factors are calculated which represent this unique typical environment;
- the geographical site of the process or the type of process is matched with a defined standard environment or situation; once the process is typified, the emissions can be converted using the characterization factors for the defined standard environment.

In general, two procedures are described for introducing the site-dependent approach:

- a prospective procedure: differences in spatial aspects are taken directly into account during data-gathering in the inventory analysis; data explosion is to be avoided by choosing large areas (continents or subcontinents) or large environmental categories (land vs. sea or indoor vs. outdoor emissions);
- a retrospective procedure: it is argued that an integral introduction of a site-dependent approach in LCA (i.e. the prospective procedure) may complicate the procedure and will be resource-demanding. A two-step procedure is therefore proposed, consisting firstly of a screening LCA followed by some sort of sensitivity analysis to identify the most critical processes of the study and secondly of a detailed LCA that concentrates on the most important processes for which site-dependent information can be introduced.

Spatial information may play a role in both fate/exposure assessment and toxicity assessment. The partitioning and degradation of a chemical in the environment depends upon the physico-chemical properties of the environment. For example, the differences in humidity and organic matter content between peat, sand or clay will lead to different distribution and degradation characteristics. An urban environment may have a different distribution pattern from the rural/natural environment. Also, the distribution characteristics of the sea will differ from those of the land. And, of course, indoor emissions have a different distribution pattern from outdoor emissions.

Besides fate, the intrinsic toxicity of a chemical to the environment depends also on physical/chemical parameters (e.g. buffer capacity) and on biological/ecosystem parameters (e.g. sensitivity of vegetation to acidification). The impact of acid deposition on the sea will be less than the same deposition on natural land. Exposure to a human-toxic chemical will be greater in a region with a high population density (like a city) than in a region of low density (like a natural or rural environment or the sea).

There are various different parameters of a specific environment that can be spatially differentiated [58]. These will now be briefly discussed:

- *Compartment to which the substance is emitted.* The distribution and toxicity of an emission depends upon the compartment to which the substance is emitted. Generally, a distinction is made between emissions to air, water and soil. For LCA it may be relevant to add emissions indoors and "direct" emissions to human beings during use of a product (for example, exposure to solvents during painting).
- *Ratio of volumes of the compartments (air, water and soil).* Partitioning of substances between air, water and soil depends on the ratio between the amount of air, water and soil available in the region. The ratio between the amount of air and the amount of soil + water is assumed to be the same in all parts of the world; the height of the air column above the earth's surface is the same everywhere. The ratio between the amount of soil and the amount of water may differ significantly from region to region, however. In regions where the amount of water is relatively large, there will be more transport from air to water (and less from air to soil) then in regions where there is more soil and less water.
- *Physico-chemical properties.* In general, the physico-chemical properties of the environment are of influence on the distribution and toxicity of an emission. For instance, in the case of acidification the differences in buffer capacity between clay soils and sandy soils will lead to different acidifying impacts in practice. The potential of an emission to have acidifying impacts is much lower on clayey soils. And in the case of eutrophication, because of differences in binding capacity for phosphorus, distribution will differ between peat or clay soils and sandy soils. The physico-chemical properties of the environment also play an important role in the distribution and toxicity of toxic substances. For example, owing to the adsorption of cadmium to organic particles, distribution to other compartments and exposure of soil organisms will differ between clay and sandy soils.
- *Ecological properties.* Ecological properties differ from region to region. Some regions may contain vulnerable (or highly valued ecosystems), while in other regions the ecosystems may be less vulnerable (or less valued). For example, heathland is more vulnerable to eutrophication than a forest. Such a distinction can also be made for toxic impacts, because different organisms react in different ways. Therefore, some ecosystems can be characterized as more vulnerable to disruption due to toxic impacts then others. Another option is to argue that ecotoxic impacts are undesirable anywhere, regardless of the type of ecosystem.
- *Human population density.* Human population densities vary substantially from region to region. Regional population density can have an enormous influence on the extent to which an emission will lead to human exposure. For example, an emission at sea of a human-toxic substance will generally give rise to a much lower human exposure than an

equal emission in the middle of a large city. Another possibility is to argue that the world should be habitable everywhere, obviating the need for spatial differentiation.

- *Background concentrations (in relation to threshold values).* The background concentration of a substance may vary from area to area owing to differences in historical emissions and emissions caused by other product systems than the one considered in the LCA.

5.2 CURRENT SITUATION: DIFFERENTIATION FOR TWO TYPES OF SOILS

The input values of USES 1.0 for the spatial parameters are given in the so-called country file. This file contains information concerning meteorological parameters, amounts of air, water and soil, and soil characteristics (such as mixing depth, porosity, moisture and organic matter content). By means of the country file, therefore, the present version, USES 1.0, has various options for differentiating between geographical regions.

However, in current calculations of the characterization factors with USES 1.0 no distinction is made between different regions (e.g. different geographical regions or different environments such as sea, coastal area and land). The spatial parameters which influence the distribution and toxicity of a substance are based on world averages or world-representative data, described in the country file.

In the present calculations, however, some differentiation regarding the type of direct emission to the soil is incorporated. At present USES 1.0 has the potential to differentiate an emission to the soil, based upon soil use. With respect to direct emissions to the soil, a distinction is made between natural soil, receiving no direct emissions, and agricultural soil and industrial soil. This differentiation can be considered a first step towards spatial differentiation.

5.3 FUTURE PERSPECTIVES

There is great need for further development of site-dependent impact assessment. In the first section of this chapter some recent developments regarding incorporation of spatial differentiation in LCA have been mentioned.

The future perspectives of the site-dependent approach may be sketched with reference to the basic research questions to be dealt with. These basic questions include:

- *Which of the spatial aspects are relevant for each of the impact categories?* The distribution of human-toxic substances depends on the type of emission (e.g. indoor vs. outdoor). Physico-chemical properties may also play a role in the distribution of toxic substances. The impacts of human-toxic substances may be considered density-dependent (e.g. urban, rural, sea). Another argument may be that the impacts are not density-dependent, on the assumption that the world should be habitable everywhere.
- *Given an impact category and a specific substance, what is the relevant scale for implementation of spatial differentiation?* The deposition of ammonia occurs mainly within a radius of one kilometre from the emitting source. The impacts of sulphur dioxide will extend over 100 kilometres.
- *Given an impact category and a spatial aspect, what is the most relevant differentiation in*

standard environments; which different categories should be defined? What level of detail is relevant? (e.g. different soil types (clay vs. peat vs. sand), different geographical regions (e.g. continents, each with its own soil composition), different types of environment (urban areas, rural areas, sea), different sensitivity (sensitive vs. insensitive). In order to keep the number of categories limited, the site-dependent approach should be developed integrally for all impact categories. This means that categories should be developed that are appropriate for several or all impacts.

- *Given the different categories, how can reliable parameters be constructed?* Which distribution models and toxicity (dose-response) models should be used? And what role can USES 1.0 play?
- *What information is needed for implementation of the various spatial parameters, and is implementation of this information feasible (considering the goal of LCA)?* If human population densities are taken into account, data on average population densities in different parts of the world or in different environments are needed.

The above questions should lead to several typical standard environments for which distinctive characterization factors are calculated. Each method developed to include spatial information in LCA will have to make due allowance for the already extensive amount of data required in LCA and remain practically feasible.

Chapter 6

TOXICITY PARAMETERS IN LCA

6.1 DESCRIPTION OF THE PROBLEM

Besides fate and exposure data, toxicity data on individual chemicals are needed to develop equivalency factors for human toxicity and ecotoxicity for use in LCA. Fate, exposure and toxicity together determine the impact that a given amount of chemical has on the environment.

In §2.3 it was stated that the objective of LCA is to clarify the relationship between a product life cycle and its potential for contributing to toxic impacts. It is not so much the actual occurrence of toxic impacts that is of interest in LCA, but the potential contribution to such occurrence.

In risk assessment, the risk quotient PEC/PNEC is regarded as an indicator of the actual or predicted occurrence of toxic impacts. If LCA is supposed to quantify a life cycle's contribution to a PEC/PNEC ratio, it has to be established how a product life cycle can be linked to a PEC-like quantity. To this end, Vollebregt [36], for instance, has introduced the term product-related environmental concentration (PREC), and sought to establish PREC/PNEC ratios.

All these ideas presume that the PNEC can be used as a parameter for toxicity. However, in the fields of both RA and LCA there are ongoing discussions on the justification of this presumption. It is the choice of this toxicity parameter that is the topic of this chapter.

There are several possible parameters that can be used for toxicity data. Discussions on this issue are in progress the field of RA [59,60,61]. As stated earlier, it is important that these discussions are followed by LCA scientists and that the results of these discussion are considered for implementation in updated versions of LCA impact assessment methodologies. However, the difference in objective between LCA and RA may mean that the "ultimate" toxicity parameters for LCA and for RA may differ. After all, LCA equivalency factors are designed not to predict impacts, but to serve as generic impact information for evaluating product alternatives with respect to environmental aspects.

Two of the possibilities currently being discussed by RA experts are:

- PEC/PNEC ratio;
- Fu[1] approach.[2]

The main differences between these possibilities can be illustrated by drawing a typical

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[1] Fu stands for unprotected fraction of the species, and corresponds to the damage percentage in the concentration-damage curve at the present environmental concentration C_{env}.

[2] The use of Fu as a basis for aggregation of toxic emissions in RA is so new that it is only discussed in draft reports.

concentration-damage curve[1] (see Figure 6.1).

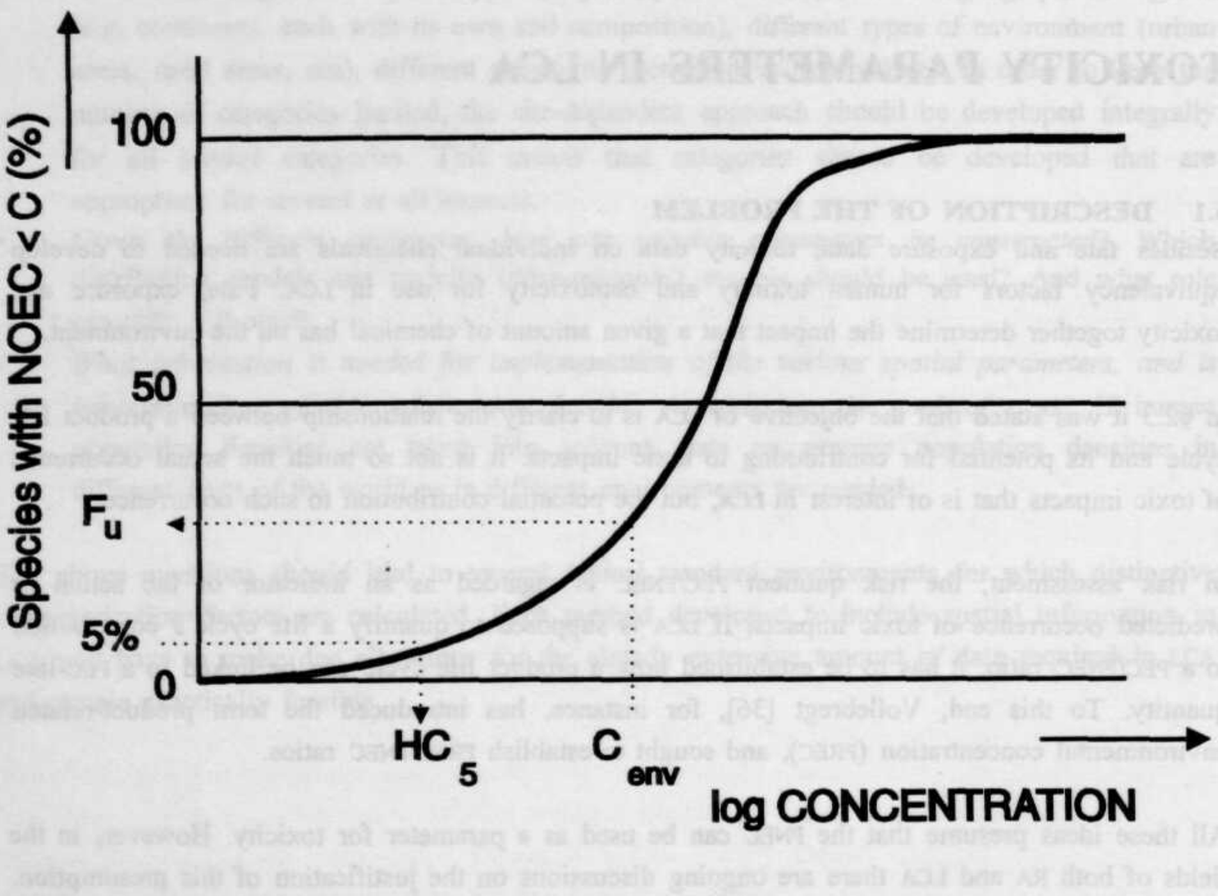

Figure 6.1: The cumulative distribution of laboratory-derived no-observed-effect concentrations (NOEC) is used as a concentration-damage curve to measure ecotoxicological risk.

This concentration-damage curve is valid for the impacts of most toxic chemicals. There is a concentration area in which there is no observable impact, then there is an area in which there is an almost linear relationship between the concentration and the effect, and finally there is an area above which any concentration will lead to a 100% effect. For mutagenic and carcinogenic chemicals a fully linear type of concentration-damage curve going through the origin appears to hold, for which a distinction between different concentration-damage areas is not therefore useful.

A PNEC for ecosystems is determined by limiting the percentage of species that is not fully protected to a maximum permissible level of 5%. The concentration above which this is the case is determined from the cumulative distribution of NOECs for single species (see Figure 6.1). All kinds of variations on this principle are possible, depending on the assumed form of the concentration-damage curve (log-logistic, straight line, etc.) and on the definition of the acceptable damage level. For instance, the former use in LCA of semi-political standards (such as

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[1] Where the term concentration-damage curve is used in this report, the term dose-response or concentration-response curve could also be used.

MAC-, MIC- and OVD-values) are basically a variant of the NEC-approach. The PNEC is taken as the indicator of the toxicity of an emission, and the PEC/PNEC ratio is considered to be a measure of toxic impacts.

The course of the concentration-damage curve can also be used in estimating the toxic impact of an emission. If the concentration-damage curve is known, the percentage of species damaged can be estimated for each PEC. This percentage can also be estimated if only a limited number of toxicity data are available [62]. This percentage could be used as the basis for aggregating toxic emissions in LCA. One could also make some calculation using the slope of the concentration-damage curve, but this would actually come down to the same principle. The advantage of this approach is that it indicates to what extent an impact occurs at any concentration value calculated, in contrast to the PEC/PNEC ratio. The disadvantage of this approach is that the required data are not (yet) sufficiently available.

6.2 CURRENT SITUATION: PNEC

In USES 1.0 the PNEC has been taken as the indicator of the toxicity of an emission. Therefore, the PNEC is also applied in this study. For the extrapolation methods used to derive the PNEC values for the various different chemicals, the reader is referred to USES 1.0 [38].

6.3 FUTURE PERSPECTIVES

The various different approaches and the associated (dis)advantages mentioned above are being discussed by the RA scientific community. LCA scientists should follow these results closely and see if and how the results of these debates can be applied in updated versions of LCA impact assessment methodologies. It should be emphasized that the LCA scientific community could examine similar questions in part independently of the RA community. What is best for RA need not be optimal for LCA as well.

Chapter 7

DEFINITION OF AND AGGREGATION WITHIN IMPACT CATEGORIES

7.1 DESCRIPTION OF THE PROBLEM

In §2.3 it was stated that life cycle inventory analysis performs an aggregation of emissions of the same substance, while life cycle impact assessment aggregates emissions of different substances. In the classification step of LCA impact assessment, impact categories are defined. These categories are defined in terms of environmental mechanisms or impacts to which a group of different chemicals contribute to in a similar way, for example global warming, acidification, etc.

For toxicity there is no single overall endpoint and thus no single overall impact category to which all toxic chemicals contribute. In some sense, all toxic chemicals act in a unique way. That is to say, besides specific behaviour in the environment (fate and exposure aspects), they can all have an impact on different toxicological endpoints in terms of target species and target organs. This argument might lead one to believe that there should be a very high number of impact categories: if there are 1 million relevant chemicals and 1 million relevant organisms, then there could be as many as 1 thousand billion (10^{12}!) impact categories. Although this provides some scientific justification for the impact assessment of toxic pollutants, and although it surely satisfies the impact assessment's aim of interpretation, in no way does it meet the other aim of impact assessment: aggregation. On the contrary, the original number of inventory items is expanded by basing the interpretation on many different species.

As discussed in §2.3, LCA is a decision support tool, weighting product alternatives with respect to their environmental aspect through the whole life cycle of these alternatives, and not a tool for predicting actual impacts or risks. For this aim of decision support, some form of aggregation is essential, resulting in a small number of impact categories for toxicity.

This aggregation problem is also an issue of concern in RA [63] and in developing environmental indicators [64]. The question here, of importance for both RA and LCA, is: which toxicological endpoints can be used as a basis for distinguishing different impact categories for aggregating toxic emissions? This question demands an explicit statement of an "equivalency principle". In the document of the SETAC-Europe subgroup on toxicity [26] it is stated that "the equivalency principle defines in words the conditions for which two toxic emissions are considered to have an equivalent effect." In other words: *What emission of chemical A to compartment I has an impact on impact category X equivalent to 1 kg emission of chemical B to compartment J?* Or, phrased differently: *How much additional emission of chemical A to compartment I is one willing to tolerate for a reduction of 1 kg emission of chemical B to* *compartment J with respect to impact category X?*

7.2 CURRENT SITUATION: ALL IMPACTS AGGREGATED 1-TO-1

Virtually no current quantitative LCA methods that assess human health distinguish between different endpoints such as carcinogenicity, mutagenicity, decline of reproductive capacity, etc. In most methods, the lowest ADI (or one of the other reference values) is determined, so in fact the first impact that occurs is determined and this value is used as a weighting factor to aggregate emissions into one score.

The present version of USES 1.0 distinguishes impacts on the following categories:
- humans;
- aquatic ecosystems;
- terrestrial ecosystems;
- predators (birds and mammals);
- wastewater treatment plants.

In USES 1.0 no aggregation of different substances takes places into these categories.

Given the lack of alternatives currently available from the field of RA, in this report the USES 1.0 categories are taken and a one-to-one aggregation of the scores within the different categories will be applied. Thus, all hazard quotients (PEC/PNEC) and the reciprocal of all margins of safety (MOS) are considered equally important. This implies a choice for the following equivalency principle: *A concentration of x times the PNEC makes a contribution to the impact score that is x times as large as a concentration of the PNEC.* This assumption is evidently not true, of course, but it is the best possibility currently available.

Not all categories of USES 1.0 are useful for the LCA equivalency factors: some categories have been left out for reasons of principle (the wastewater treatment plant, because it does not represent an ecosystem), others for practical reasons (predators, because the availability of data is very limited).

In conclusion, the impact categories that are chosen are:
- humans;
- aquatic ecosystems;
- terrestrial ecosystems.

The aggregation of substances within these impact categories takes place on a one-to-one basis: the PEC/PNEC forms the principle of aggregation.

7.3 FUTURE PERSPECTIVES

In the future, it may be preferable to distinguish more categories than those described above. At the least, a distinction between carcinogenic and non-carcinogenic chemicals and impacts could be introduced without too much effort.

As stated above and in previous chapters, discussions about impact categories for toxic emissions are in progress in RA. It seems best for LCA scientists to wait for the results of these discussions and use them in updated versions of LCA impact assessment methodologies. However, as these discussions are only just starting, for the time being consideration may be given to allowing some panel of RA experts to decide on the toxic impact categories. Such a proposal is currently being developed by a US expert panel, distinguishing such impact categories as irreversible/life-shortening effects, generally reversible but possibly life-threatening effects, and reversible but generally not life-threatening effects, with expert-based valuation factors of 100, 10, and 1 [65].

Another possibility is to distinguish, for a start, between carcinogens and non-carcinogens [35]. All these proposals require that additional information is available: the substance data used to produce equivalency factors with USES 1.0 contains information on NECs, ADIs, LC_{50}s, etc., but *not on the type of impact (cancer, irritation, etc.) that can be observed above those values.*

Still another option is to base the impact score not on the concentration or intake at which the first adverse effect occurs, but on the concentration or intake at which the most severe effect occurs (personal communication with M. Hauschild).

Chapter 8

CALCULATION

8.1 THEORY

For each of the 94 substances and the compartments air, surface water, agricultural soil and industrial soil, a regional assessment with USES 1.0 has been made. In calculating an equivalency factor for atmospheric emissions, the emission to air is set at 1000 kg/d, while emissions to the other compartments are set at 0 kg/d.

For aquatic ecotoxicity USES 1.0 then calculates – among other things – the PEC/PNEC ratio. The same procedure should be repeated for the reference substance emitted to the reference compartment, *viz.* 1,4-dichlorobenzene emitted to water. The equivalency factor for the chemical at stake emitted to air is now calculated by dividing its PEC/PNEC ratio by the same quantity of 1,4-dichlorobenzene emitted to water:

$$AETP_{subs,comp} = \frac{\left\{\dfrac{PEC_{\text{water},subs,comp}}{PNEC_{\text{aquatic ecosystems},subs}}\right\}}{\left\{\dfrac{PEC_{\text{water},1,4\text{-dichlorobenzene},\text{water}}}{PNEC_{\text{aquatic ecosystems},1,4\text{-dichlorobenzene}}}\right\}} \qquad (8.1)$$

In this formula, $PEC_{\text{water},subs,comp}$ denotes the predicted concentration of substance *subs* in water as a result of the emission of 1000 kg/d *subs* to the release compartment *comp*.[1] $PNEC_{\text{aquatic ecosystems},subs}$ denotes the predicted no-effect concentration of substance *subs* for aquatic ecosystems. The equivalency factors are called aquatic ecotoxicity potentials, abbreviated as AETP.

A similar procedure can be used to calculate equivalency factors for terrestrial ecotoxicity, the terrestrial ecotoxicity potentials (TETP). The reference substance is again 1,4-dichlorobenzene, but the reference compartment is industrial soil. The formula is then:

$$TETP_{subs,comp} = \frac{\left\{\dfrac{PEC_{\text{agricultural soil},subs,comp}}{PNEC_{\text{terrestrial ecosystems},subs}}\right\}}{\left\{\dfrac{PEC_{\text{agricultural soil},1,4\text{-dichlorobenzene},\text{industrial soil}}}{PNEC_{\text{terrestrial ecosystems},1,4\text{-dichlorobenzene}}}\right\}} \qquad (8.2)$$

The procedure for the calculation of equivalency factors for human toxicity is slightly different. USES 1.0 does not calculate a PEC/PNEC for humans, but a margin of safety (MOS). The reciprocal

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[1] Observe that there are two subscripts relating to compartments: one for the compartment in which the PEC can be found, and one for the compartment to which the substance was initially released.

of this quantity can be considered as the analogue of the PEC/PNEC; in fact the MOS is defined as a kind of acceptable daily intake divided by the predicted daily intake (ADI/"PDI").

$$HTP_{subs,comp} = \frac{MOS_{1,4\text{-dichlorobenzene},air}}{MOS_{subs,comp}} \qquad (8.3)$$

The equivalency factors are termed human toxicity potentials (HTP).

The equivalency factors obtained for the aquatic or terrestrial compartment and for humans are listed in Appendix A. For the water and soil compartment these factors are based on PEC/PNEC calculations, and for humans on the margin of safety (1/MOS) calculated with an ADI or TDI.

The choice of a reference compartment may require some further explanation. The AETP, for emission of 1,4-dichlorobenzene to water is by definition 1. The AETP of an atmospheric emission of the same substance turns out to be $1.1 \cdot 10^{-2}$. This means that an emission of 1 kg 1,4-dichlorobenzene to air is considered to be much less harmful to aquatic ecosystems than the same emission to water.

Selection of substances

Most of the 94 substances were available in a USES 1.0 database used previously for screening chemical substances with USES 1.0 [66]. Heavy metals (10), ammonia (anhydrous), nitrogen dioxide and sulphur dioxide have been added to this database.

As discussed earlier (§2.2), USES 1.0 is not designed for risk assessment of inorganic substances such as heavy metals. An assessment for metals was made by:

- entering an extremely low vapour pressure of 10^{-10} Pa, with the exception of mercury, for which a real value was used. With a vapour pressure of $1 \cdot 10^{-10}$ Pa and an estimated solubility in water, the Henry's law constant is accordingly calculated in USES 1.0 to be extremely small, resulting in a low volatility of the metal (as intended);
- setting the octanol-water partition coefficient (K_{oc}) at a value with which USES 1.0 calculates the real (measured) value for the solids-water partition coefficient in soil (K_p). For metals a K_{oc} cannot normally be derived from a K_p, but it is the best option within USES 1.0;
- not entering a value for the solubility, except for mercury. The solubility is calculated by USES 1.0 from the vapour pressure, the molecular weight and the Henry's law constant. A real value for the solubility of metals in water is difficult to determine, because of chemical speciation.
- entering a low Henry's law constant of 10^{-15}, except for mercury. The Henry's law constant for mercury is calculated by USES 1.0 with a real value for the water solubility and the vapour pressure;
- entering real values for K_p of sediment and suspended matter (when available);
- furthermore, all DT_{50} values [d] are maximized: photodeg. in air = 10^{-4}, hydrolysis in water = 10^{-6}, biodeg. in water = 10^{-4}, biodeg. in soil = 10^{-4};
- entering real (measured) values for the BCF for fish, worm and plant.

Best estimates of the soil-water and sediment-water partition coefficients (based on experimentally measured values reported in the literature) were entered in USES 1.0, since the hydrophobicity-based estimation routines are not applicable to metals. However, the standard hydrophobicity-based estimation routines of USES 1.0 were used to "fake" BCFs, since no literature data were available: K_{oc} values for metals were set to a value that produced a reasonable estimate for the soil-water and sediment-water partition coefficients. For all metals, except mercury, the toxicity values used for the terrestrial ecosystem are lower than background levels in the Netherlands. The terrestrial equivalency factors for metals are therefore not based on soil background concentrations. The data sources used for metals are [67,68,69,70,71,72,73, 74,75,76,77,78].

For ammonia (anhydrous), nitrogen dioxide and sulphur dioxide there are no toxicity values available for the aquatic and terrestrial compartment. The human equivalency factors for these substances are not based on the margin of safety, but were calculated by hand. USES 1.0 was used only for calculating the regional concentration in air. In this case the equivalency factor is the concentration in air divided by the WHO guideline value (24-hour average). The data sources used for ammonia (anhydrous), nitrogen dioxide and sulphur dioxide are [74,78,79,80,81, 82,83]. Furthermore, the atmospheric degradation of nitrogen dioxide and sulphur dioxide has been introduced in the computations by setting the parameter for photodegradation to the estimated value for oxidation. For SO_2 an estimated residence time of 1 day [84] suggests a DT_{50} of 0.7 day. For lack of a better estimate for NO_2, the same value has been used for this substance.

Further data sources are [38,66,85,86,87,88,89,90].

8.2 WHAT IS NEW: COMPARISON OF OLD AND NEW EQUIVALENCY FACTORS

The main difference between the equivalency factors calculated by USES 1.0 and by the NOH method [4] concerns the influence of the fate, i.e. distribution and degradation, of a substance. These fate aspects are taken into account in the calculations using USES 1.0, while being neglected in the NOH method. Comparison of the equivalency factors calculated by USES and by the NOH method provides some information about the sensitivity of the effect scores to the fate aspects. By confronting the results of the comparison with qualitative expert judgement of the characteristics concerning the persistence and distribution of the substances, the new set of equivalency factors can be roughly validated. This section gives an overview of the method used to compare the lists of equivalency factors. For convenience, these are denoted as USES LCA, NOH OLD, and NOH NEW (see below for the meaning of the last).

Updated equivalency factors according to the NOH method

In order to make a clear comparison between the equivalency factors calculated by USES 1.0 and by the NOH method, the equivalency factors of the NOH method first had to be updated. As these factors were generated in 1992, many toxicity data such as MTR, LC_{50}, NOEC, ADI/TDI and NOAEL may have since changed. To ensure that any differences between the equivalency factors calculated by USES 1.0 and by the NOH method are due strictly to fate aspects and not to changes in toxicity data, new equivalency factors were calculated with the old NOH method using current toxicity data. To calculate these updated equivalency factors, formulae were used which are described in the Backgrounds report of Heijungs *et al.* [4, pp. 93, 94, and 99]. Furthermore, the differentiation of two soil types has been abandoned in the comparison, with only the average generic soil being used here.

Use of a reference substance for comparing the values

The order of magnitude of the equivalency factors calculated by USES 1.0 and by the NOH method may differ substantially, simply because the dimensions are different. For convenience of comparison, the values have been converted to the same order of magnitude by describing the equivalency factors as a value relative to a defined reference substance and emission. Each equivalency factor is thus divided by an equivalency factor for a reference emission. The substance 1,4-dichlorobenzene has been selected for this purpose, as it is one of the only substances for which all possible equivalency factors are present.[1] For all data sets, the equivalency factor of 1,4-dichlorobenzene to some emission compartment is set to 1 and all the other data are given as values relative to 1,4-dichlorobenzene. The reference emission compartments are water for aquatic ecotoxicity, generic soil for terrestrial ecotoxicity and air for human toxicity. As concrete examples, the value of the entry in the column denoted as "NOH NEW/NOH OLD; water" and the row denoted as "AETP" is calculated as

$$\frac{\left[\dfrac{ECA_{\mathrm{new},subs}}{ECA_{\mathrm{new,1,4-dichlorobenzene}}}\right]}{\left[\dfrac{ECA_{\mathrm{old},subs}}{ECA_{\mathrm{old,1,4-dichlorobenzene}}}\right]} \tag{8.4}$$

and the value of the entry in the column denoted as "USES LCA/NOH NEW; water" and the row denoted as "AETP" is calculated as

$$\frac{AETP_{subs,\mathrm{water}}}{\left[\dfrac{ECA_{\mathrm{new},subs}}{ECA_{\mathrm{new,1,4-dichlorobenzene}}}\right]} \tag{8.5}$$

The results

The equivalency-factor calculations resulted in three data sets containing equivalency factors for aquatic, terrestrial and human toxicity for emissions to air, water and generic soil. The three data sets are mentioned after the method and update of the toxicity data from which they are calculated:

- NOH OLD, containing the equivalency factors calculated by the NOH method as described in the Dutch Guidelines [4], with the toxicity data available in 1992;
- NOH NEW, containing the equivalency factors calculated by the same NOH method, with up-

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[1] "By chance", it is also the reference substance for the equivalency factors of Appendix A.

to-date toxicity data as used for the USES calculations;

- USES LCA, containing the equivalency factors calculated by USES 1.0, with fate, exposure and up-to-date toxicity data.

Table 8.1 gives a selection of some interesting results. Not all entries have a value because, for instance, there is no value in NOH NEW or NOH OLD for impacts on aquatic ecosystems by emissions to air.

Comparing NOH NEW and NOH OLD

In the three columns denoted as "NOH NEW/NOH OLD", the equivalency factors as calculated by the NOH method are compared by dividing the NOH NEW by the NOH OLD factors. If the quotient is equal to one or close to one, the equivalency factors have remained the same, which means that the toxicity data (MTR, ADI/TDI) have not changed since 1992. If the quotient exceeds one, the toxicity standard has decreased since 1992, which means that the substance is now considered more toxic.[1] The overall conclusion is that many quotients are one or close to one, signifying that many toxic standards have remained the same or nearly the same. However, it is also clear that quite a few standards have been changed. Some have undergone moderate alteration, by a factor 2 or 3, but there have also been some major changes. For example, the human toxicity of an emission to air of hexachlorobenzene has changed by a factor 350.

To gain insight into the sensitivity of the equivalency factors to fate aspects such as distribution and degradation, these changes in toxicity standards have to be filtered out. Calculation of the equivalency factors should be based on the same toxicity standards. Therefore, the equivalency factors of USES LCA should be compared with the equivalency factors of NOH NEW.

Comparing USES LCA and NOH NEW

The comparison is made by calculating a fate-sensitivity indicator. The fate-sensitivity indicator of a substance emitted to a compartment is the quotient of the equivalency factor calculated by USES LCA and the relative equivalency factor calculated by the NOH method according to NOH NEW. This indicator tells us something about the increase or decrease in the relative equivalency factor due to fate aspects which are considered in USES LCA but not in NOH NEW. If the quotient is less than 1, the relative equivalency factor calculated by USES LCA is lower than the relative equivalency factor calculated by NOH NEW. For example, a decrease in the equivalency factor of a substance which degrades quickly is due to the fact that degradation of the substance was not considered in the NOH method. The magnitude of the quotient tells us something about the magnitude of increase or decrease.[2] If the quotient is 100, the equivalency factor has changed by a factor 100 compared to the equivalency factor of the reference substance. If the quotient is 2, the equivalency factor has changed by a factor 2 compared to the equivalency factor of the

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[1] More toxic here means that the PNEC is lower; see Chapter 6 for a discussion of the choice of toxicity parameter.

[2] Note that all the changes are given as relative changes to the equivalency factor of 1,4-dichlorobenzene (for the various reference compartments). The changes for 1,4-dichlorobenzene are thus 1 by definition. If a different reference substance were to be chosen, all the indicators would change, but the ratios between the indicators would remain the same. If a very persistent substance were chosen, for example, all indicators would be less than 1, but the ratio between the indicators of two substance would remain the same.

Table 8.1: Comparison of old and new equivalency factors; see text for explanation.

		NOH NEW/NOH OLD			USES LCA/NOH NEW		
Substance	Type	air	water	soil	air	water	soil
1,4-dichlorobenzene	AETP	—	$2.4\cdot10^{-2}$	—	—	1.0	—
	TETP	—	—	3.0	—	—	1.0
	HTP	1.7	1.0	—	1.0	8.6	—
hexachlorobenzene	AETP	—	$7.9\cdot10^{-3}$	—	—	1.4	—
	TETP	—	—	3.8	—	—	$4.0\cdot10^{3}$
	HTP	$3.5\cdot10^{2}$	1.0	—	$1.1\cdot10^{1}$	2.1	—
trichloroethylene	AETP	—	$9.0\cdot10^{-3}$	—	—	1.5	—
	TETP	—	—	—	—	—	$4.8\cdot10^{-1}$
	HTP	1.0	1.0	—	$2.0\cdot10^{-1}$	3.4	—
PCB	AETP	—	—	—	—	$9.9\cdot10^{1}$	—
	TETP	—	—	—	—	—	—
	HTP	—	—	—	$1.1\cdot10^{2}$	$7.4\cdot10^{2}$	—
2,3,7,8-TCDD	AETP	—	—	—	—	$6.8\cdot10^{-1}$	—
	TETP	—	—	$1.5\cdot10^{-1}$	—	—	$3.4\cdot10^{5}$
	HTP	1.0	1.0	—	$1.3\cdot10^{3}$	$1.9\cdot10^{3}$	—
cadmium	AETP	—	$1.4\cdot10^{-2}$	—	—	6.0	—
	TETP	—	—	22	—	—	$1.6\cdot10^{3}$
	HTP	$5.7\cdot10^{-2}$	1.0	—	$1.1\cdot10^{2}$	7.8	—
copper	AETP	—	$1.5\cdot10^{-1}$	—	—	1.2	—
	TETP	—	—	2.4	—	—	$1.8\cdot10^{3}$
	HTP	1.0	1.0	—	$2.5\cdot10^{2}$	9.1	—
lead	AETP	—	$5.0\cdot10^{-2}$	—	—	1.6	—
	TETP	—	—	$4.7\cdot10^{-2}$	—	—	$1.9\cdot10^{3}$
	HTP	$5.8\cdot10^{-2}$	1.0	—	$1.2\cdot10^{3}$	$5.4\cdot10^{1}$	—
mercury	AETP	—	1.1	—	—	$9.8\cdot10^{-1}$	—
	TETP	—	—	$1.0\cdot10^{1}$	—	—	$7.4\cdot10^{1}$
	HTP	$6.9\cdot10^{-2}$	$1.5\cdot10^{-1}$	—	$5.9\cdot10^{2}$	$4.3\cdot10^{3}$	—
nitrogen dioxide	AETP	—	—	—	—	—	—
	TETP	—	—	—	—	—	—
	HTP	$1.4\cdot10^{-2}$	—	—	3.9	—	—
sulphur dioxide	AETP	—	—	—	—	—	—
	TETP	—	—	—	—	—	—
	HTP	$5.6\cdot10^{-3}$	—	—	3.9	—	—

reference substance. Note that this indicator should not be confused with the (relative) equivalency factor itself. The (relative) equivalency factor tells us something about the toxic potential of a substance (compared to the toxic potential of a reference substance). The fate-sensitivity indicator tells us something about the changes that occur in the equivalency factor if fate aspects are considered. For example, according to the fate-sensitivity indicator an equivalency factor may have been increased substantially, but the equivalency factor of that substance may still be smaller than the equivalency factor of a substance with a low fate-sensitivity indicator.

In the columns entitled "USES LCA/NOH NEW" the fate-sensitivity indicator is given for the various substances. In the present context a few general remarks can be made.

- Compared with many other substances, persistent substances like 2,3,7,8-TCDD, PCB and heavy metals generally have high fate-sensitivity indicators. This illustrates that, owing to the low degradation rates of these substances, the equivalency factors will increase more relative to substances which are less persistent.
- On the other hand, a substance with a high degradation rate such as trichloroethylene has a low fate-sensitivity indicator. Note that the fate-sensitivity indicator for aquatic ecosystems due to emissions to water is low for these substances. This is due to sediment burial; see also Chapter 3.
- The fate-sensitivity indicators for NO_2 and SO_2 are low compared with those for persistent substances. In LCA studies following the NOH method, these substances were often the main cause of human toxicity. According to the results of this project the influence of these substances in LCA will decrease in comparison with persistent chemicals like heavy metals and PCBs.

Chapter 9

PRACTICAL GUIDELINES AND CONCLUDING DISCUSSION

9.1 PRACTICAL GUIDELINES

So far, the discussion has concentrated on the procedure, the model and the data used to obtain equivalency factors for toxic releases in LCA. This section is devoted to two very practical topics related to making an LCA:

- how to apply these equivalency factors in LCA impact assessment;
- what additional knowledge can USES 1.0 offer an LCA practitioner.

Applying the newly developed equivalency factors

Appendix A of this report contains a large number of equivalency factors for assessing the impacts of toxic releases in an LCA. Three impact categories are distinguished: human toxicity, aquatic ecotoxicity and terrestrial ecotoxicity. Calculation of the impact scores now proceeds according to the following formulae:

$$\begin{aligned} \textit{impact score}_{\text{human toxicity}}\ (\text{kg}) = {} & \sum_{subs} HTP_{subs,\text{air}} \times emission_{subs,\text{air}}\ (\text{kg}) + \\ & \sum_{subs} HTP_{subs,\text{water}} \times emission_{subs,\text{water}}\ (\text{kg}) + \\ & \sum_{subs} HTP_{subs,\text{industrial soil}} \times emission_{subs,\text{industrial soil}}\ (\text{kg}) + \\ & \sum_{subs} HTP_{subs,\text{agricultural soil}} \times emission_{subs,\text{agricultural soil}}\ (\text{kg}) \end{aligned} \tag{9.1}$$

for human toxicity,

$$\begin{aligned} \textit{impact score}_{\text{aquatic ecotoxicity}}\ (\text{kg}) = {} & \sum_{subs} AETP_{subs,\text{air}} \times emission_{subs,\text{air}}\ (\text{kg}) + \\ & \sum_{subs} AETP_{subs,\text{water}} \times emission_{subs,\text{water}}\ (\text{kg}) + \\ & \sum_{subs} AETP_{subs,\text{industrial soil}} \times emission_{subs,\text{industrial soil}}\ (\text{kg}) + \\ & \sum_{subs} AETP_{subs,\text{agricultural soil}} \times emission_{subs,\text{agricultural soil}}\ (\text{kg}) \end{aligned} \tag{9.2}$$

for aquatic ecotoxicity, and

$$\begin{aligned} \textit{impact score}_{\text{terrestrial ecotoxicity}}\ (\text{kg}) = {} & \sum_{subs} TETP_{subs,\text{air}} \times emission_{subs,\text{air}}\ (\text{kg}) + \\ & \sum_{subs} TETP_{subs,\text{water}} \times emission_{subs,\text{water}}\ (\text{kg}) + \\ & \sum_{subs} TETP_{subs,\text{industrial soil}} \times emission_{subs,\text{industrial soil}}\ (\text{kg}) + \\ & \sum_{subs} TETP_{subs,\text{agricultural soil}} \times emission_{subs,\text{agricultural soil}}\ (\text{kg}) \end{aligned} \tag{9.3}$$

for terrestrial ecotoxicity.

The units in these formulae deserve special attention: the equivalency factors (HTP, AETP, and TETP) are all expressed in kg reference substance per kg of toxic substance.[1] This means that the unit "kg" on the left-hand side of the above three formulae is in fact "kg reference substance", while the "kg" on the right-hand side is "kg toxic substance". Including this in the notation makes the formulae more difficult to read, but facilitates interpretation. The final expressions on the left-hand side represent the amount of reference substance that would yield a toxic impact to the endpoint (humans, aquatic ecosystems and terrestrial ecosystems) which – under the LCA conditions described in this report – is considered to be equivalent.

Readers interested in the absolute PEC/PNEC and MOS values can construct these with the absolute value for the reference substance emitted to the reference compartment. These values are:

- aquatic ecotoxicity (1000 kg/d 1,4-dichlorobenzene emitted to (surface) water): PEC/PNEC = $2.078 \cdot 10^{-5}$;
- terrestrial ecotoxicity (1000 kg/d 1,4-dichlorobenzene emitted to industrial soil: PEC/PNEC = $2.709 \cdot 10^{-8}$;
- human toxicity (1000 kg/d 1,4-dichlorobenzene emitted to air): MOS = $1.379 \cdot 10^{5}$.

Emissions to soil

For emissions to soil, there are two lists of equivalency factors: emissions to industrial soil and emissions to agricultural soil. If it is not known to which of those soils a substance is emitted, one can either choose the most probable soil, or use some generic distribution.

This generic distribution could be based on a weighted average of the occurrence of the soil types. The LCA country file models a world in which 10% of the soil is industrial and 27% is agricultural. From this one could derive generic toxicity potentials, e.g.:

$$HTP_{subs,\text{generic soil}} = \frac{10}{37} \times HTP_{subs,\text{industrial soil}} + \frac{27}{37} \times HTP_{subs,\text{agricultural soil}} \tag{9.4}$$

One should be careful in assigning an (initial) emission to a soil as a default emission to the generic soil. If there is reasonable information that the emission will take place to an industrial soil, the emission should be assigned to industrial soil, and a similar reasoning applies to agricultural soil. For instance: pesticides will most probably be emitted to agricultural soil, and organic solvents to industrial soil. If the type of process or the type of substance is such that reasonable estimates can be made, one should do so. For some chemicals, especially immobile heavy metals, there may be a difference of 6 orders of magnitude between the HTPs for industrial and agricultural soil. This should warn the user to make a careful choice.

Knowledge of the in- and effluent of a sewage treatment plant in USES 1.0

The in- and effluent of a sewage treatment plant (STP) are part of the distribution module of

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[1] This subtlety is not commonly denoted: in most books and papers global warming potentials are described as dimensionless, and not as having the dimension kg CO_2 per kg greenhouse gas.

USES 1.0. In LCA the STP is considered to be an economic process. The STP is then part of the process tree and information about the in- and effluent of the STP is process information, which means that the inventory table is already adjusted for a possible STP. For calculating toxicity factors for LCA, therefore, this part of the USES 1.0 model should be switched off.

However, when executing an LCA the information on the STP in USES 1.0 may be very useful, as the required process data is often not available. The model in USES 1.0 which deals with the STP is Simpletreat. This model can be used to estimate the effluent of the STP given an influent as input. When collecting the process data in the inventory step of an LCA, therefore, these USES 1.0 models should be kept in mind for estimating the effluent if specific process data are lacking.

Knowledge of the emission of pesticides during application in USES 1.0
Application of pesticides (and other substances) in the agricultural sector are also considered economic processes and should therefore be dealt with in the inventory step of an LCA. Pesticide emission estimation should therefore also be switched off when using USES 1.0 for calculating equivalency factors for LCA. The models in USES 1.0 for estimating pesticides emissions to soil, water and air due to pesticide application may however be useful in the inventory step of an LCA, when collecting process data.

9.2 CONCLUDING DISCUSSION

In this report equivalency factors for toxic emissions have been calculated applying the USES 1.0 model. In this way, fate and exposure data of chemicals have been included in addition to toxicity data. Inclusion of fate and exposure aspects is new compared with previous methods. Particularly new is the inclusion in the equivalency factors of fate parameters such as persistence, (bio)degradation and intermedia transport and, for human toxicity, data on exposure routes such as on respiration volume and consumption of drinking water, fish, meat, dairy products and vegetables. These parameters and data are part of an integrated model – USES 1.0 – which has been developed by the Dutch institute RIVM for risk assessment of chemicals, and has served as basis for calculating LCA equivalency factors for toxic releases.

It has been shown that there are significant differences between the "old" equivalency factors, based only on toxicity data, and the "new" equivalency factors, which also include fate and exposure data. The equivalency factors of persistent chemicals such as metals and dioxins now have a much higher value than before (§8.2). Thus, it can be concluded that inclusion of fate and exposure data is worth the effort.

However, in this report equivalency factors have been calculated for only 94 toxic chemicals, while the "old" list included almost 300 chemicals. The reason for this huge difference is that it is by no means an easy job to obtain the data on each chemical required to calculate the MOS for human toxicity and the PEC/PNEC for aquatic and terrestrial ecotoxicity. The EC Council Regulation 793/93 on the Evaluation and Control of the Risks of Existing Substances requires that in due course available fate, exposure and toxicity data be submitted by industry for all high production volume chemicals (HPCV; > 1000 tonne/year) listed in EINECS, the *European*

INventory of Existing Chemical Substances (about 100,000 chemicals), and a more limited data set for all chemicals with production volumes between 10 and 1000 tonne/year [91]. These data will be included in a database called IUCLID, a public version of which will be issued. This development in data gathering may be very helpful in calculating LCA equivalency factors applying USES 1.0 for more chemicals than the current total of 94. However, these activities have not yet resulted in a public database. Consequently, data availability will remain an important focus of attention in the development of LCA equivalency factors applying USES 1.0.

Furthermore, a number of research topics have been identified for further improvement of the LCA equivalency factors based on USES 1.0. Some of these topics are being addressed by RA experts in currently ongoing discussions and the results of these discussions should be followed by LCA researchers and assessed on their usefulness for LCA. These topics include:

- improvements of the USES 1.0 model itself (first update will be EUSES, to be released in 1996);
- discussions on toxicity parameter (cf. Chapter 6);
- impact categories for toxicity (cf. Chapter 7).

A specific LCA research topic is the inclusion of spatial information in the impact assessment component (cf. Chapter 5). Within RIVM, the feasibility of a nested local-continental-global NL-version of EUSES (cf. §3.3) is currently being investigated and this could be a very useful input for this research work. However, there are many more possibilities for including spatial information in LCA impact assessment and these should be evaluated as to their theoretical relevance and, particularly, their practical feasibility. This dilemma is typical for LCA, and not for RA, resulting in a specific LCA research need. The first form of spatial differentiation introduced in this report – differentiating emissions to soil into emissions to industrial soil and emissions to agricultural soil – already appeared to create a problem in calculating normalization data, as most national emission accounts do not make this distinction. Any further differentiation will only increase those problems.

Other topics of interest include the incorporation of toxic or other impacts of decay products (metabolites) and how to deal with synergistic and antagonistic effects.

References

1. Ministry of Housing, Spatial Planning and Environment (VROM), 1994: *Policy document on products and the environment*. VROM, The Hague.
2. Berg, N.W. van den, C.E. Dutilh & G. Huppes: *Beginning LCA. A guide to environmental life cycle assessment.* NOH, Utrecht, 1995.
3. Consoli, F., D. Allen, I. Boustead, J. Fava, W. Franklin, A.A. Jensen, N. de Oude, R. Parrish, R. Perriman, D. Postlethwaite, B. Quay, J. Seguin & B. Vigon, 1993: *Guidelines for life-cycle assessment: a "Code of Practice". Edition 1.* SETAC, Brussels/Pensacola.
4. Heijungs, R., J.B. Guinée, G. Huppes, R.M. Lankreijer, H.A. Udo de Haes, A. Wegener Sleeswijk, A.M.M. Ansems, P.G. Eggels, R. van Duin & H.P. de Goede, 1992: *Environmental life cycle assessment of products. Guide & Backgrounds – October 1992.* Centre of Environmental Science, Leiden, The Netherlands.
5. Guinée, J.B., R. Heijungs, H.A. Udo de Haes & G. Huppes, 1993: *Quantitative life cycle assessment of products: classification, valuation and improvement analysis*. J. Cleaner Prod. 1:81-91.
6. Wenzel, H. & Hauschild, M., 1993: *Key issues for toxicity assessment of a product life cycle*. Technical University of Denmark, Lyngby, Denmark.
7. Fava, J.A., R. Denison, B. Jones, M.A. Curran, B. Vigon, S. Selke & J. Barnum (eds.), 1991: *A technical framework for life-cycle assessments*. Workshop Report. Society of Environmental Toxicology and Chemistry, Smugglers Notch, VT, August 18-23, 1990.
8. Anonymous, 1992: *Product Life Cycle Assessment - Principles and Methodology*. Nord, Copenhagen, Denmark.
9. Pedersen, B. (ed.), 1993: *Environmental Assessment of products - A course on Life Cycle Assessment*. The University-Enterprise Training Partnership in Environmental Engineering Education (UETP-EEE), Helsinki, Finland.
10. Vigon, B.W., D.A. Tolle, B.W. Cornaby, H.C. Latham, C.L. Harrison, T.L. Boguski, R.G. Hunt & J.D. Sellers, 1993: *Life-cycle assessment: inventory guidelines and principles*. EPA/600/R-92/245, Environmental Protection Agency, Washington DC, USA.
11. Lindfors, L.-G., Christiansen, K., Hoffmann, L., Virtanen, Y., Juntilla, V., Leskinen, A., Hanssen, O.-J., Rønning, A., Ekvall, T. & Finnveden, G., 1995: *LCA-Nordic. Technical reports and Special reports*. Nord, Copenhagen, Denmark.
12. Guinée, J.B., 1995: *Development of a methodology for the environmental life-cycle assessment of products - with a case study on margarines.* Ph. D. thesis. Leiden University, Leiden, The Netherlands.
13. Guinée, J.B., 1992: *Headings for Classification*. Proceedings, SETAC-Europe workshop on Environmental Life-Cycle Assessment of Products, Leiden, The Netherlands, December 2-3 1991, pp. 81-85.
14. Baumann, H., T. Ekvall, G. Svensson, T. Rydberg & A.-M. Tillman, 1992: *Aggregation and operative units*. Proceedings, SETAC-Europe workshop on Environmental Life-Cycle Assessment of Products, Leiden, The Netherlands, December 2-3 1991, pp. 87-94.
15. Finnveden, G., Y. Andersson-Sköld, M.-O. Samuelsson, L. Zetterberg & L.-G. Lindfors, 1992: *Classification (Impact Analysis) in connection with Life Cycle Assessments*. In: [8], pp. 172-231.
16. Udo de Haes, H.A., Jensen, A.A., Klöpffer, W. & Lindfors, L.-G., 1994: *Integrating impact assessment into LCA.* SETAC, Brussels, Belgium.
17. Anonymous, 1995: *Impact assessment.* In: [11].
18. Houghton, J.T., G.J. Jenkins & J.J. Ephraums (eds.), 1991: *Climate change. The IPCC scientific assessment.* Cambridge University Press, Cambridge, UK.

19. World Meteorological Organization, 1989: *Scientific assessment of stratospheric ozone, Vol. 1*. Report 20. Geneva, Switzerland.

20. Derwent, R.G. & M.E. Jenkin, 1990: *Hydrocarbon involvement in photochemical ozone formation in Europe*. AERE-R13736. Harwell Laboratory, Oxfordshire, UK.

21. Vermeire, T.G., A.A.J. van Iersel, F.A.A.M. de Leeuw, W.J.G.M. Peijnenburg, P. van der Poel, R.D.F.M. Taalman & C. Toet, 1992: *Initial assessment of the hazards and risks of new chemicals to man and the environment*. Report 679102006. National Institute of Public Health and Environmental Protection, Bilthoven, The Netherlands.

22. Anonymous, 1984: *Ökobilanzen von Packstoffen*. Schriftenreihe Umweltschutz no. 24. Bundesamt für Umweltschutz, Bern.

23. Druijff, E.A., 1984: *Milieurelevante produktinformatie (Environmental information on products)*. CML-mededelingen 15. Leiden, the Netherlands.

24. Rapp, K. & F. Schönborn, 1994: *Human- und Ökotoxizität in auswirkungsorientierten Ökobilanzen. Diplomarbeit.* ETH, Zürich.

25. Udo de Haes, H.A. (ed.), 1996: *Towards a Methodology for Life Cycle Impact Assessment*. Report of the SETAC-Europe Workgroup on Life Cycle Impact Assessment (WIA). Final Draft (February 1996).

26. Jolliet, O. (ed.), 1996: *Impact assessment of human and eco-toxicity in life cycle assessment.* Report of the SETAC-Europe Workgroup on Life Cycle Impact Assessment (WIA). 4th Draft (February 1996).

27. Assies, J.A., 1994: *Assessment of toxic emissions in life-cycle impact assessment*. In: H.A. Udo de Haes, A.A. Jensen, W. Klöpffer and L.-G. Lindfors (eds.), *Integrating Impact Assessment in LCA*, Proceedings of the LCA symposium held at the Fourth SETAC-Europe Congress 11-14 April 1994, The Free University, Brussels (Belgium). SETAC-Europe Brussels.

28. Gebler, W., 1992: *Ökobilanzen in der Abfallwirtschaft.* Stuttgarter Berichte zur Abfallwirtschaft, Bericht 41, 2. Auflage, Bielefeld.

29. Guinée, J. & R. Heijungs, 1993: *A Proposal for the Classification of Toxic Substances within the Framework of Life Cycle Assessment of Products*. Chemosphere 26, 1925-1944.

30. Hauschild, M, H. Wenzel, A. Damborg & J. Tørsløv, 1993: *Methods for screening and quantitative assessment of ecotoxicity in life cycle analysis of products*. Paper presented at the SETAC/SECOTOX workshop on ecotoxicity, Lyngby, January 7-8 1993, Technical University of Denmark, Lyngby.

31. Herrchen, M., 1993: *Methodology for classification and evaluation of the environmental impact of incinerated and landfilled plastics*. Paper presented at the SETAC/SECOTOX workshop on ecotoxicity, Lyngby, January 7-8 1993, Technical University of Denmark, Lyngby.

32. Hunt, R.G., W.E Franklin, R.O. Welch, J.A. Cross & A.E. Woodal, 1974: *Resource and environmental profile analysis of nine beverage container alternatives*. US Environmental Protection Agency, Washington DC, USA.

33. Jolliet, O., 1994: *Critical surface-time: an evaluation method for LCA*. In: H.A. Udo de Haes, A.A. Jensen, W. Klöpffer and L.-G. Lindfors (eds.), *Integrating Impact Assessment in LCA*, Proceedings of the LCA symposium held at the Fourth SETAC-Europe Congress, 11-14 April 1994, The Free University, Brussels (Belgium). SETAC-Europe Brussels.

34. Mekel, O.C.L., G. Huppes, R. Huele & J.B. Guinée, 1990: *Environmental effects of different package systems for fresh milk.* CML report 70, Leiden.

35. Tellus Institute, 1992: *The Tellus packaging study.* The Tellus Institute, Boston, MA, USA.

36. Vollebregt, L., 1994: *De PEC/NEC in een LCA. Ontwikkeling van een module voor de verspreiding en effecten van toxische stoffen in een levenscyclusanalyse.* Chemiewinkel UvA, Amsterdam.

37. EPA, 1984: *Estimating concern levels for concentrations of chemical substances in the*

environment. US-EPA, Environmental Effects Branch, Washington.

38. RIVM, VROM, WVC, 1994: *Uniform system for the evaluation of substances (USES). Version 1.0.* National Institute of Public Health and Environmental Protection (RIVM), Ministry of Housing, Spatial Planning and Environment (VROM), Ministry of Welfare, Health and Cultural Affairs (WVC). The Hague, Ministry of Housing, Spatial Planning and Environment. Distribution No. 11144/150.
39. Jager, D.T., C.J.M. Visser & D. van de Meent, 1994: *Uniform system for the evaluation of substances IV: distribution and intake.* Chemosphere Vol. 29, No. 2, pp. 353-369.
40. Vermeire, T.G., P.T.J. van der Zandt, H. Roelfzema & C.J. van Leeuwen, 1994: *Uniform system for the evaluation of substances I: principles and structure.* Chemosphere Vol. 29, No. 1, pp. 23-38.
41. Voet, E. van der, L. van Egmond, R. Kleijn & G. Huppes, 994: *Cadmium in the European Community: a policy-oriented analysis.* Waste Management & Research **12**, 507-526.
42. Udo de Haes, H.A. & G. Huppes, 1994: *The positioning of LCA in relation to other environmental decision support tools.* In: Proceedings of fourth SETAC-Europe Congress, Integration of Impact Assessment in LCA, April 11-14 1994, Brussels.
43. Heijungs, R., G. Huppes & H.A. Udo de Haes, forthcoming: *LCA in environmental decision making; what it is, how it functions and what it means for governments, firms and NGOs in developed, transition and developing countries.* UNEP, Paris.
44. Heijungs, R. & J.B. Guinée, 1993: *CML on actual versus potential risks.* In: SETAC Europe News (LCA News), Vol. 3, No. 4, p. 4.
45. Heijungs, R., 1995: *Harmonization of methods for impact assessment.* Environmental Science and Pollution Research **2**: 4, 217-224.
46. Meent, D. van de: *Simplebox: a generic multimedia fate evaluation model.* Report 672720001. National Institute of Public Health and Environmental Protection, Bilthoven, The Netherlands.
47. EC, 1993: *Risk assessment of notified new substances; Technical Guidance Document.* Commission of the European Communities, Directorate-General for Environment, Nuclear Safety and Civil Protection. Brussels.
48. Slooff, W., 1992: *Guidance document; Ecotoxicological effect assessment: deriving Maximum Tolerable Concentrations (MTC) from single-species toxicity data.* RIVM, Report No. 719102018. Bilthoven.
49. Noesen, S. & H.A. Udo de Haes, 1996: *SETAC and the ISO 14000 process.* LCA News **6**:2, p.3.
50. Anonymous, 1995: *Environmental Risk Assessment of new and existing substances. Technical Guidance Document. Draft. October 1995.*
51. Mackay, D., 1991: *Multimedia environmental models, the fugacity approach.* Lewis Publ. Inc. Chelsea.
52. Cowan, C.E., D. Mackay, T.C.J. Feytel, D. van de Meent, A. di Gurdo, J. Davies & N. Mackay, 1995: *The multi-media fate model: a vital tool for predicting the fate of chemicals.* SETAC Press, Pensacola.
53. Guinée, J.B. & R. Heijungs, 1992: *Classification factors for toxic substances within the framework of life cycle assessment of products.* CML paper 11, Leiden.
54. Heijungs, R. & J.B. Guinée, 1994: *Using environmental multi-media models in LCA. The flux-pulse problem.* CML paper 18, Leiden.
55. Potting, J. & K. Blok, 1994: *Spatial aspects of life-cycle impact assessment.* In: H.A. Udo de Haes, A.A. Jensen, W. Klöpffer & L.-G. Lindfors (eds.), *Integrating Impact Assessment in LCA*, Proceedings of the LCA symposium held at the Fourth SETAC-Europe Congress, 11-14 April 1994, Free University of Brussels (Belgium). SETAC-Europe Brussels.
56. Finnveden, G., 1994: *Some comments on the level of spatial detail in the characterisation.* In: Udo de Haes, H.A. *et al.*, First Working Document on Life-Cycle Impact Assessment

Methodology. Report of a workshop held at ETH Zürich from July 8-9, 1994, organized by the SETAC-Europe Working Group on Life-Cycle Impact Assessment.

57. Nichols, P. (ed.), 1995: *First generation impact categories*. Discussion document of SETAC sub Working Group on 'First generation impact categories'. PIRA, Leatherhead, UK.
58. Wegener Sleeswijk, A., R. Huele, M.C.Th. Scholten & H.P.M. Schobben, 1995: *Risk Analysis and Life Cycle Assessment. A comparison of methods*. CML, Leiden and TNO Environmental Sciences, Den Helder, the Netherlands.
59. Crump, K.S., 1984: *A new method for determining Allowable Daily Intakes*. Fundamental and applied toxicology **4**, pp. 854-871.
60. Straalen, N.M. van & J.A.C. Verkleij (eds.), 1991: *Leerboek Oecotoxicologie*. VU uitgeverij, Amsterdam.
61. Renwick, A.G. & R. Walker, 1993: *An analysis of the risk of exceeding the Acceptable or Tolerable Daily Intake*. Regulatory toxicology and pharmacology **18**, pp. 463-480.
62. Straalen, N.M. van & Denneman, C.A.J., 1989: *Ecotoxicological evaluation of soil quality criteria*. Ecotox. Environ. Saf., No. 18, 241-251.
63. Farland, W. & M. Dourson, 1993: *Noncancer health endpoints: approaches to quantitative Risk Assessment*. In: Cothern, C.R. (ed.), 1993: Comparative environmental Risk Assessment, pp. 87-106. Lewis Publishers, Boca Raton (Florida).
64. Adriaanse, A., 1993: *Environmental policy performance indicators*. SDU uitgeverij, The Hague.
65. Burke, Th., J. Doull, Th. McKone, D. Paustenbach, R. Scheuplein, H.A. Udo de Haes & J. Young, 1995: *Human health impact assessment in life cycle assessments: analysis by an expert panel. Draft*. Washington D.C.
66. Gingnagel, P. & T.G. Vermeire, 1995: *Screening of chemical substances; Application of the Uniform System for the Evaluation of Substances, USES 1.0*. RIVM report No. 601014009, Bilthoven.
67. Plassche, E.J. v.d., J.H.M. de Bruijn, 1992: *Towards integrated environmental quality objectives for surface water, ground water, sediment and soil for nine trace metals*. RIVM report No. 679101005, Bilthoven.
68. Ros J.P.M., Slooff W. (eds.), Apeldoorn M.E. van, Boer K.F. de, Canton J.H., Gestel C.A.M. van, Heijden C.A. van der, Heijna-Merkus E., Janus J.A., Knaap A.G.A.C., Knoop J., Kranjc E.I., Leeuwen F.X.R. van, Loch J.P.G., Meulen A. van der, Minderhoud A., Ros J.P.M., Wiel H.J. van de, Besemer A.C., Blokzijl P.J., Feron V.J., Guicherit R., Huldy H.J., Huigen C., Most P.F.J. van der, Mulder H.C.M., Schoot-Uiterkamp A., Sinkeldam E.J., Vink G.T.J. & Vrijer F. de, 1988: *Integrated criteria document cadmium*. RIVM report No. 758476004, Bilthoven.
69. Slooff W., Cleven R.F.M.J., Janus J.A., Poel P. van der (eds.), Beelen P. van, Boumans L.J.M., Canton J.H., Eerens H.C., Krajnc E.I., Leeuw F.A.A.M. de, Matthijsen A.J.C.M., Meent D. van de, Meulen A. van der, Mohn G.R., Wijland G.C., Bruijn P.J. de, Keulen A. van, Verburgh J.J. & Woerd K.F. van der, 1990): *Integrated criteria document chromium*. RIVM report No. 710401002, Bilthoven.
70. Slooff W., Cleven R.F.M.J., Janus J.A., Ros J.P.M. (eds.), Aalst R.M. van, Beugelink G.P., Boumans L.J.M., Canton JH, Eerens H.C., Gestel C.A.M. van, Heijna-Merkus E., Matthijsen A.J.C.M., Meent D. van de, Meulen A. van der, Staps J.J. & Woerd K.F. van der, 1989: *Integrated criteria document copper*. RIVM report No. 758474009, Bilthoven.
71. Slooff W., Haring B.J.A., Hesse J.M., Janus J.A., Thomas R. (eds.), Beelen, P. van, Boer J.L.M. de, Boumans L.J.M., Buijsman E., Canton J.H., Cremers, P.M.A., Heijden C.A. van der, Knaap A.G.A.C., Krajnc E.I., Kramers P.G.N., Kreis I.A., Kroese E.D., Lebret E., Matthijsen A.J.C.M., Meent D. van de, Meulen A. van der, Meulenbelt J., Taalman R.D.F.M., Bijstra D., Bril J., Salomons W. & Woerd K.F. van der, 1990: *Basisdocument Arseen*. RIVM report No. 758701002, Bilthoven.

72. Slooff W., Beelen P. van, Annema J.A., Janus J.A. (eds.), 1994: *Basisdocument kwik.* RIVM report No. 710401023, Bilthoven.

73. Slooff W., Bont P.F.H., Janus J.A. & Loos B., 1992: *Exploratory report nickel and nickel compounds.* RIVM report No. 710401017, Bilthoven.

74. Weast, R.C., M.J. Astle & W.H. Beyer, 1985-1986: *CRC handbook of chemistry and chemics, 66th edition, A ready reference book of chemical and physical data.* CRC Press Inc., Boca Raton, Florida.

75. Bockting G.J.M., E.J. van de Plassche, J. Struijs & J.H. Canton, 1992: *Soil-water partition coefficients for some trace metals.* RIVM report No. 679101003, Bilthoven.

76. Bockting G.J.M. & R. van den Berg, 1992: *De accumulatie van sporenmetalen in groenten geteeld op verontreinigde bodems.* RIVM report No. 725201009, Bilthoven.

77. Koolenbrander, J.G.M., 1995: *Urgentie van bodemsanering, de handleiding.* SDU, The Hague.

78. Janus, J.A., J.M. Hesse & M.G.J. Rikken (eds.), 1994: *Aandachtstoffen in het Nederlandse milieubeleid – overzicht 1994.* RIVM report No. 601014006, Bilthoven.

79. WHO, 1977: *Oxides of nitrogen.* Environmental Health Criteria 4, United Kingdom.

80. WHO, 1979: *Sulphur oxides and suspended particulate matter.* Environmental Health Criteria 8, United Kingdom.

81. WHO, 1986: *Ammonia.* Environmental Health Criteria 54, International Programme on Chemical Safety (IPCS), Geneva.

82. ATSDR, 1990: *Toxicological profile for ammonia.* Agency for toxic substances and disease registry, US department of health and human services, ATSDR/TP-90-03.

83. ATSDR, 1992: *Toxicological profile for vanadium.* Agency for toxic substances and disease registry, US department of health and human services, ATSDR/TP-91/29.

84. National Research Council, 1978: *Commission on Sulfur Dioxide.* National Academy of Science, Washington.

85. Cleven R.F.M.J., Janus J.A., Annema J.A.& Slooff W. (eds.), 1992: *Basisdocument zink.* RIVM report No. 710401019, Bilthoven.

86. Janus J.A., Annema J.A., Slooff W. & Cleven R.F.M.J., 1996: *Evaluatiedocument lood (concept).*, RIVM report No. 601014003, Bilthoven.

87. Kalf, D.F., G.H. Crommentuijn, R. Posthumus & E.J. van de Plassche, 1995: *Integrated environmental quality objectives for polycyclic aromatic hydrocarbons (PAHs).*, RIVM report No. 679101018, Bilthoven.

88. Meent, D. van de, T. Aldenberg & J.H. Canton, 1990: *Streven naar waarden. Achtergrondstudie ten behoeve van de nota milieu-kwaliteitsnormering water en bodem.* RIVM report No. 670101001, Bilthoven.

89. Peijnenburg, W.J.G.M., M. van Ewijk, M.W.A. de Haan, J.A. Janus, J.P.M. Ros, W. Slooff & E.G. van de Velde, 1991: *Update of exploratory report phtalates.* RIVM report No. 710401008, Bilthoven.

90. Plassche, E.J. v.d., 1994: *Towards integrated environmental quality objectives for several compounds with a potential for secondary poisoning.* RIVM report No. 679101011, Bilthoven.

91. Bruijn, J. de & K. Grein, 1995: *EU Risk Assessment Update.* SETAC-Europe News, Vol. 6, No. 4, pp. 8-9.

Appendix A

EQUIVALENCY FACTORS

Substance			Type	Initial emission compartment				
No.	Name	CAS No.		air	(surface) water	agricultural soil	industrial soil	generic soil
1	1,1,1-trichloroethane	71-55-6	AETP	$3.0\cdot10^{-3}$	$1.8\cdot10^{-1}$	$2.9\cdot10^{-3}$	$3.0\cdot10^{-3}$	$3.0\cdot10^{-3}$
			TETP	2.0	2.0	$1.6\cdot10^{1}$	2.0	$1.2\cdot10^{1}$
			HTP	$1.2\cdot10^{3}$	$1.2\cdot10^{3}$	$1.2\cdot10^{3}$	$1.2\cdot10^{3}$	$1.2\cdot10^{3}$
2	1,2,3,4-tetrachlorobenzene	634-66-2	AETP	$2.1\cdot10^{-1}$	$1.8\cdot10^{1}$	$1.9\cdot10^{-1}$	$2.0\cdot10^{-1}$	$1.9\cdot10^{-1}$
			TETP	$3.1\cdot10^{3}$	$3.0\cdot10^{3}$	$5.8\cdot10^{5}$	$3.0\cdot10^{3}$	$4.3\cdot10^{5}$
			HTP	$8.5\cdot10^{1}$	$1.3\cdot10^{2}$	$1.9\cdot10^{2}$	$8.3\cdot10^{1}$	$1.6\cdot10^{2}$
3	1,2,3,5-tetrachlorobenzene	634-90-2	AETP	$8.9\cdot10^{-2}$	$1.7\cdot10^{1}$	$8.5\cdot10^{-2}$	$8.8\cdot10^{-2}$	$8.6\cdot10^{-2}$
			TETP	$3.7\cdot10^{4}$	$3.6\cdot10^{4}$	$7.2\cdot10^{6}$	$3.6\cdot10^{4}$	$5.3\cdot10^{6}$
			HTP	$8.2\cdot10^{1}$	$1.2\cdot10^{2}$	$1.3\cdot10^{2}$	$8.1\cdot10^{1}$	$1.1\cdot10^{2}$
4	1,2,3-trichlorobenzene	87-61-6	AETP	$3.8\cdot10^{-1}$	6.6	$3.5\cdot10^{-1}$	$3.7\cdot10^{-1}$	$3.6\cdot10^{-1}$
			TETP	$1.9\cdot10^{5}$	$1.9\cdot10^{5}$	$6.5\cdot10^{6}$	$1.9\cdot10^{5}$	$4.8\cdot10^{6}$
			HTP	$9.7\cdot10^{1}$	$9.9\cdot10^{1}$	$1.0\cdot10^{2}$	$9.4\cdot10^{1}$	$9.9\cdot10^{1}$
5	1,2-dichlorobenzene	95-50-1	AETP	$1.4\cdot10^{-2}$	1.6	$1.3\cdot10^{-2}$	$1.4\cdot10^{-2}$	$1.3\cdot10^{-2}$
			TETP	$1.2\cdot10^{2}$	$1.2\cdot10^{2}$	$3.6\cdot10^{4}$	$1.1\cdot10^{2}$	$2.6\cdot10^{4}$
			HTP	$3.4\cdot10^{-1}$	$3.9\cdot10^{-1}$	$6.6\cdot10^{-1}$	$3.2\cdot10^{-1}$	$5.7\cdot10^{-1}$
6	1,2-dichloroethane	107-06-2	AETP	$1.2\cdot10^{-2}$	$5.7\cdot10^{-1}$	$1.1\cdot10^{-2}$	$1.2\cdot10^{-2}$	$1.2\cdot10^{-2}$
			TETP	4.2	4.2	$2.8\cdot10^{2}$	4.1	$2.0\cdot10^{2}$
			HTP	$6.9\cdot10^{1}$	$6.9\cdot10^{1}$	$6.9\cdot10^{1}$	$6.7\cdot10^{1}$	$6.8\cdot10^{1}$
7	1,3-butadiene	106-99-0	AETP	5.3	$1.7\cdot10^{1}$	2.2	3.6	2.5
			TETP	$2.6\cdot10^{3}$	$2.6\cdot10^{3}$	$6.0\cdot10^{4}$	$1.8\cdot10^{3}$	$4.4\cdot10^{4}$
			HTP	2.8	2.9	2.1	1.9	2.0
8	1,4-dichloro-2-nitrobenzene	89-61-2	AETP	$6.8\cdot10^{2}$	$1.9\cdot10^{3}$	$8.8\cdot10^{1}$	$2.1\cdot10^{2}$	$1.2\cdot10^{2}$
			TETP	$4.9\cdot10^{3}$	$4.7\cdot10^{3}$	$5.5\cdot10^{4}$	$1.5\cdot10^{3}$	$4.1\cdot10^{4}$
			HTP	$1.9\cdot10^{2}$	$2.1\cdot10^{2}$	$1.6\cdot10^{2}$	$5.9\cdot10^{1}$	$1.3\cdot10^{2}$
9	1,4-dichlorobenzene	106-46-7	AETP	$1.1\cdot10^{-2}$	1.0	$3.5\cdot10^{-4}$	$1.3\cdot10^{-3}$	$6.1\cdot10^{-4}$
			TETP	8.5	5.1	$2.6\cdot10^{3}$	1.0	$1.9\cdot10^{3}$
			HTP	1.0	$7.4\cdot10^{-1}$	$9.0\cdot10^{-2}$	$1.2\cdot10^{-1}$	$9.8\cdot10^{-2}$
10	1-chloro-4-nitrobenzene	100-00-5	AETP	$1.2\cdot10^{3}$	$1.0\cdot10^{4}$	$1.8\cdot10^{1}$	$5.4\cdot10^{1}$	$2.8\cdot10^{1}$
			TETP	$5.2\cdot10^{5}$	$3.0\cdot10^{5}$	$2.2\cdot10^{6}$	$2.3\cdot10^{4}$	$1.6\cdot10^{6}$
			HTP	$9.1\cdot10^{2}$	$3.2\cdot10^{3}$	$1.1\cdot10^{3}$	$4.1\cdot10^{1}$	$8.4\cdot10^{2}$

Substance			Type	Initial emission compartment				
No.	Name	CAS No.		air	(surface) water	agricultural soil	industrial soil	generic soil
11	2,3,7,8-TCDD	1746-01-6	AETP	$7.2\cdot10^{6}$	$1.5\cdot10^{8}$	$1.6\cdot10^{6}$	$3.3\cdot10^{6}$	$2.1\cdot10^{6}$
			TETP	$2.6\cdot10^{8}$	$2.9\cdot10^{7}$	$6.5\cdot10^{8}$	$1.2\cdot10^{8}$	$5.1\cdot10^{8}$
			HTP	$2.6\cdot10^{10}$	$3.2\cdot10^{9}$	$6.0\cdot10^{10}$	$1.2\cdot10^{10}$	$4.7\cdot10^{10}$
12	2,4,6-trichloroaniline	634-93-5	AETP	$6.3\cdot10^{2}$	$1.9\cdot10^{4}$	4.9	$1.5\cdot10^{1}$	7.5
			TETP	$1.6\cdot10^{4}$	$3.7\cdot10^{2}$	$5.8\cdot10^{4}$	$3.7\cdot10^{2}$	$4.2\cdot10^{4}$
			HTP	—	—	—	—	—
13	2,4,6-trichlorophenol	88-06-2	AETP	$6.6\cdot10^{1}$	$2.0\cdot10^{2}$	$1.2\cdot10^{-1}$	$4.6\cdot10^{-1}$	$2.1\cdot10^{-1}$
			TETP	$1.0\cdot10^{2}$	$3.1\cdot10^{1}$	$2.4\cdot10^{3}$	$7.1\cdot10^{-1}$	$1.7\cdot10^{3}$
			HTP	$5.4\cdot10^{3}$	$1.9\cdot10^{3}$	$5.7\cdot10^{1}$	$3.8\cdot10^{1}$	$5.2\cdot10^{1}$
14	2,4-dichlorophenol	120-83-2	AETP	8.9	$2.9\cdot10^{1}$	$2.8\cdot10^{-2}$	$1.1\cdot10^{-1}$	$5.0\cdot10^{-2}$
			TETP	$3.5\cdot10^{1}$	$1.4\cdot10^{1}$	$1.0\cdot10^{3}$	$4.4\cdot10^{-1}$	$7.4\cdot10^{2}$
			HTP	$4.4\cdot10^{3}$	$1.9\cdot10^{3}$	$3.9\cdot10^{1}$	$5.5\cdot10^{1}$	$4.3\cdot10^{1}$
15	2-chlorophenol	95-57-8	AETP	6.7	$2.0\cdot10^{1}$	$1.1\cdot10^{-2}$	$4.5\cdot10^{-2}$	$2.0\cdot10^{-2}$
			TETP	$1.4\cdot10^{1}$	4.1	$3.2\cdot10^{2}$	$9.1\cdot10^{-2}$	$2.4\cdot10^{2}$
			HTP	$3.3\cdot10^{1}$	$1.1\cdot10^{1}$	$2.3\cdot10^{-1}$	$2.2\cdot10^{-1}$	$2.2\cdot10^{-1}$
16	3,4-dichloroaniline	95-76-1	AETP	$2.7\cdot10^{1}$	$1.0\cdot10^{2}$	2.7	$2.7\cdot10^{1}$	9.2
			TETP	$3.5\cdot10^{-3}$	$3.5\cdot10^{-3}$	$4.6\cdot10^{-3}$	$3.5\cdot10^{-3}$	$4.3\cdot10^{-3}$
			HTP	$9.5\cdot10^{3}$	$9.4\cdot10^{3}$	$9.5\cdot10^{3}$	$9.5\cdot10^{3}$	$9.5\cdot10^{3}$
17	3,5-dichloroaniline	626-43-7	AETP	$4.2\cdot10^{2}$	$1.4\cdot10^{4}$	1.1	3.5	1.8
			TETP	$5.5\cdot10^{3}$	$1.8\cdot10^{1}$	$2.0\cdot10^{4}$	$4.6\cdot10^{1}$	$1.5\cdot10^{4}$
			HTP	—	—	—	—	—
18	3-monochloroaniline	108-42-9	AETP	6.7	$2.5\cdot10^{1}$	6.7	6.7	6.7
			TETP	$3.0\cdot10^{-4}$	$3.0\cdot10^{-4}$	$3.9\cdot10^{-4}$	$3.0\cdot10^{-4}$	$3.6\cdot10^{-4}$
			HTP	$7.6\cdot10^{4}$	$7.5\cdot10^{4}$	$7.6\cdot10^{4}$	$7.6\cdot10^{4}$	$7.6\cdot10^{4}$
19	4-monochloroaniline	106-47-8	AETP	6.7	$2.5\cdot10^{1}$	6.7	6.7	6.7
			TETP	$3.8\cdot10^{-4}$	$3.8\cdot10^{-4}$	$4.9\cdot10^{-4}$	$3.8\cdot10^{-4}$	$4.6\cdot10^{-4}$
			HTP	$3.8\cdot10^{5}$	$3.8\cdot10^{5}$	$3.8\cdot10^{5}$	$3.8\cdot10^{5}$	$3.8\cdot10^{5}$
20	acrolein	107-02-8	AETP	$1.6\cdot10^{2}$	$5.0\cdot10^{2}$	$3.0\cdot10^{-1}$	1.2	$5.3\cdot10^{-1}$
			TETP	$6.8\cdot10^{2}$	$2.1\cdot10^{2}$	$1.7\cdot10^{4}$	4.9	$1.2\cdot10^{4}$
			HTP	$2.3\cdot10^{3}$	$8.0\cdot10^{2}$	$1.4\cdot10^{1}$	$1.7\cdot10^{1}$	$1.5\cdot10^{1}$
21	acrylonitrile	107-13-1	AETP	4.9	$3.9\cdot10^{1}$	$9.8\cdot10^{-2}$	$3.7\cdot10^{-1}$	$1.7\cdot10^{-1}$
			TETP	$4.8\cdot10^{2}$	$2.8\cdot10^{2}$	$1.7\cdot10^{4}$	$3.6\cdot10^{1}$	$1.3\cdot10^{4}$
			HTP	$2.1\cdot10^{3}$	$1.2\cdot10^{2}$	$4.6\cdot10^{1}$	$1.5\cdot10^{2}$	$7.5\cdot10^{1}$
22	aldrin	309-00-2	AETP	$1.3\cdot10^{3}$	$9.6\cdot10^{3}$	$1.1\cdot10^{3}$	$1.2\cdot10^{3}$	$1.1\cdot10^{3}$
			TETP	$2.3\cdot10^{8}$	$8.4\cdot10^{7}$	$9.0\cdot10^{8}$	$2.2\cdot10^{8}$	$7.2\cdot10^{8}$
			HTP	$1.4\cdot10^{6}$	$6.0\cdot10^{5}$	$1.6\cdot10^{6}$	$1.3\cdot10^{6}$	$1.5\cdot10^{6}$

Substance			Type	Initial emission compartment				
No.	Name	CAS No.		air	(surface) water	agricultural soil	industrial soil	generic soil
23	α,α,α-trichlorotoluene	98-07-7	AETP	$1.8\cdot10^{-2}$	$1.5\cdot10^{1}$	$1.8\cdot10^{-2}$	$1.8\cdot10^{-2}$	$1.8\cdot10^{-2}$
			TETP	$1.8\cdot10^{-7}$	$1.7\cdot10^{-7}$	$4.6\cdot10^{-6}$	$1.8\cdot10^{-7}$	$3.4\cdot10^{-6}$
			HTP	$2.0\cdot10^{3}$	$2.0\cdot10^{3}$	$2.0\cdot10^{3}$	$2.0\cdot10^{3}$	$2.0\cdot10^{3}$
24	α,α-dichlorotoluene	98-87-3	AETP	$1.5\cdot10^{-5}$	1.7	$1.5\cdot10^{-5}$	$1.5\cdot10^{-5}$	$1.5\cdot10^{-5}$
			TETP	$1.8\cdot10^{-10}$	$1.1\cdot10^{-10}$	$6.3\cdot10^{-9}$	$1.8\cdot10^{-10}$	$4.6\cdot10^{-9}$
			HTP	$1.9\cdot10^{3}$	$1.2\cdot10^{3}$	$1.9\cdot10^{3}$	$1.9\cdot10^{3}$	$1.9\cdot10^{3}$
25	α-chlorotoluene	100-44-7	AETP	$5.2\cdot10^{-8}$	$6.5\cdot10^{-1}$	$5.2\cdot10^{-8}$	$5.2\cdot10^{-8}$	$5.2\cdot10^{-8}$
			TETP	$3.6\cdot10^{-13}$	$2.3\cdot10^{-13}$	$4.5\cdot10^{-10}$	$3.6\cdot10^{-13}$	$3.3\cdot10^{-10}$
			HTP	1.3	1.1	1.3	1.3	1.3
26	ammonia (anhydrous)	7664-41-7	AETP	—	—	—	—	—
			TETP	—	—	—	—	—
			HTP	$1.6\cdot10^{1}$	$1.4\cdot10^{1}$	$5.5\cdot10^{-1}$	1.6	$8.3\cdot10^{-1}$
27	arsenic	7440-38-2	AETP	5.6	$1.9\cdot10^{2}$	$1.8\cdot10^{-8}$	$6.4\cdot10^{-8}$	$3.0\cdot10^{-8}$
			TETP	$7.2\cdot10^{4}$	$9.7\cdot10^{-6}$	$2.7\cdot10^{5}$	$7.0\cdot10^{-4}$	$2.0\cdot10^{5}$
			HTP	$4.2\cdot10^{4}$	$5.1\cdot10^{1}$	$9.1\cdot10^{2}$	$4.1\cdot10^{-4}$	$6.7\cdot10^{2}$
28	atrazine	1912-24-9	AETP	$9.2\cdot10^{1}$	$3.6\cdot10^{2}$	$5.0\cdot10^{1}$	$7.3\cdot10^{1}$	$5.6\cdot10^{1}$
			TETP	$6.9\cdot10^{3}$	$6.5\cdot10^{3}$	$1.9\cdot10^{5}$	$5.5\cdot10^{3}$	$1.4\cdot10^{5}$
			HTP	$9.2\cdot10$	$8.9\cdot10^{2}$	$7.9\cdot10^{2}$	$7.3\cdot10^{2}$	$7.7\cdot10^{2}$
29	azinfos-methyl	86-50-0	AETP	$6.3\cdot10$	$3.0\cdot10^{4}$	$1.8\cdot10^{2}$	$5.2\cdot10^{2}$	$2.7\cdot10^{2}$
			TETP	$7.2\cdot10^{6}$	$1.1\cdot10^{6}$	$4.3\cdot10^{7}$	$5.9\cdot10^{5}$	$3.1\cdot10^{7}$
			HTP	$5.9\cdot10^{2}$	$1.6\cdot10^{2}$	$4.6\cdot10^{2}$	$4.8\cdot10^{1}$	$3.5\cdot10^{2}$
30	bentazone	25057-89-0	AETP	$3.4\cdot10^{1}$	$1.1\cdot10^{3}$	$2.0\cdot10^{-7}$	$6.0\cdot10^{-7}$	$3.1\cdot10^{-7}$
			TETP	$3.0\cdot10^{4}$	$1.2\cdot10^{-4}$	$1.1\cdot10^{5}$	$4.2\cdot10^{-4}$	$8.1\cdot10^{4}$
			HTP	6.7	$6.3\cdot10^{1}$	$1.2\cdot10^{1}$	$9.6\cdot10^{-8}$	8.5
31	benzene	71-43-2	AETP	$1.3\cdot10^{-3}$	1.0	$1.4\cdot10^{-4}$	$4.2\cdot10^{-4}$	$2.2\cdot10^{-4}$
			TETP	$6.3\cdot10^{-2}$	$3.9\cdot10^{-2}$	$5.3\cdot10^{1}$	$2.1\cdot10^{-2}$	$3.9\cdot10^{1}$
			HTP	$2.9\cdot10^{1}$	$2.2\cdot10^{1}$	5.2	9.4	6.3
32	benzo[a]pyrene	50-32-8	AETP	$3.2\cdot10^{2}$	$1.0\cdot10^{4}$	2.9	8.8	4.5
			TETP	$6.4\cdot10^{7}$	$8.1\cdot10^{4}$	$2.3\cdot10^{8}$	$1.8\cdot10^{6}$	$1.7\cdot10^{8}$
			HTP	$3.7\cdot10^{3}$	$1.7\cdot10^{3}$	$1.1\cdot10^{4}$	$1.0\cdot10^{2}$	$8.3\cdot10^{3}$
33	benzylbutylphthalate	85-68-7	AETP	$3.1\cdot10^{1}$	$4.8\cdot10^{2}$	$4.2\cdot10^{-1}$	1.3	$6.4\cdot10^{-1}$
			TETP	$1.2\cdot10^{5}$	$7.6\cdot10^{4}$	$4.9\cdot10^{5}$	$5.0\cdot10^{3}$	$3.6\cdot10^{5}$
			HTP	$4.3\cdot10^{2}$	$1.0\cdot10^{2}$	$1.1\cdot10^{2}$	$1.7\cdot10^{1}$	$8.3\cdot10^{1}$
34	butyl(2-ethylhexyl) phthalate	85-69-8	AETP	6.3	$9.1\cdot10^{1}$	$6.1\cdot10^{-4}$	$2.4\cdot10^{-3}$	$1.1\cdot10^{-3}$
			TETP	$1.6\cdot10^{3}$	$2.2\cdot10^{1}$	$6.6\cdot10^{3}$	$6.2\cdot10^{-1}$	$4.8\cdot10^{3}$
			HTP	—	—	—	—	—

Substance			Type	Initial emission compartment				
No.	Name	CAS No.		air	(surface) water	agricultural soil	industrial soil	generic soil
35	cadmium	7440-43-9	AETP	$1.3\cdot10^{2}$	$4.5\cdot10^{3}$	$2.7\cdot10^{-6}$	$7.1\cdot10^{-6}$	$3.9\cdot10^{-6}$
			TETP	$1.3\cdot10^{8}$	$2.5\cdot10^{-2}$	$4.7\cdot10^{8}$	6.0	$3.4\cdot10^{8}$
			HTP	$2.3\cdot10^{4}$	$1.3\cdot10^{2}$	$2.8\cdot10^{4}$	$1.1\cdot10^{-3}$	$2.0\cdot10^{4}$
36	carbon disulphide	75-15-0	AETP	$5.1\cdot10^{-2}$	4.0	$5.0\cdot10^{-2}$	$5.1\cdot10^{-2}$	$5.0\cdot10^{-2}$
			TETP	$3.9\cdot10^{1}$	$3.9\cdot10^{1}$	$1.3\cdot10^{3}$	$3.9\cdot10^{1}$	$9.8\cdot10^{2}$
			HTP	$1.5\cdot10^{2}$	$1.5\cdot10^{2}$	$1.5\cdot10^{-1}$	$1.5\cdot10^{-1}$	$1.5\cdot10^{-1}$
37	chromium III	7440-47-3	AETP	2.5	$8.4\cdot10^{1}$	$7.6\cdot10^{-10}$	$3.0\cdot10^{-9}$	$1.4\cdot10^{-9}$
			TETP	$2.2\cdot10^{5}$	$1.1\cdot10^{-5}$	$8.2\cdot10^{5}$	$2.3\cdot10^{-4}$	$6.0\cdot10^{5}$
			HTP	$4.9\cdot10^{5}$	9.3	$4.7\cdot10^{2}$	$5.2\cdot10^{-4}$	$3.4\cdot10^{2}$
38	chromium VI	7440-47-3	AETP	2.5	$8.4\cdot10^{1}$	$7.6\cdot10^{-10}$	$3.0\cdot10^{-9}$	$1.4\cdot10^{-9}$
			TETP	$2.2\cdot10^{5}$	$1.1\cdot10^{-5}$	$8.2\cdot10^{5}$	$2.3\cdot10^{-4}$	$6.0\cdot10^{5}$
			HTP	$3.5\cdot10^{9}$	$6.7\cdot10^{4}$	$3.4\cdot10^{6}$	3.7	$2.5\cdot10^{6}$
39	cobalt	7440-48-4	AETP	2.6	$8.8\cdot10^{1}$	$4.4\cdot10^{-8}$	$1.0\cdot10^{-7}$	$6.0\cdot10^{-8}$
			TETP	$1.7\cdot10^{4}$	$2.0\cdot10^{-7}$	$6.2\cdot10^{4}$	$5.2\cdot10^{-4}$	$4.5\cdot10^{4}$
			HTP	$7.6\cdot10^{3}$	$3.1\cdot10^{1}$	$2.1\cdot10^{3}$	$2.4\cdot10^{-4}$	$1.5\cdot10^{3}$
40	copper	7440-50-8	AETP	2.9	$9.6\cdot10^{1}$	$8.4\cdot10^{-9}$	$2.8\cdot10^{-8}$	$1.4\cdot10^{-8}$
			TETP	$9.1\cdot10^{5}$	$1.0\cdot10^{-5}$	$3.4\cdot10^{6}$	$6.0\cdot10^{-3}$	$2.4\cdot10^{6}$
			HTP	$3.5\cdot10^{2}$	1.1	$4.2\cdot10^{1}$	$2.3\cdot10^{-6}$	$3.0\cdot10^{1}$
41	di(2-ethylhexyl)phthalate	117-81-7	AETP	$2.9\cdot10^{-1}$	$4.7\cdot10^{1}$	$4.6\cdot10^{-4}$	$1.8\cdot10^{-3}$	$8.3\cdot10^{-4}$
			TETP	$1.1\cdot10^{2}$	$2.6\cdot10^{1}$	$4.9\cdot10^{3}$	$6.9\cdot10^{-1}$	$3.6\cdot10^{3}$
			HTP	$1.4\cdot10^{1}$	$5.9\cdot10^{1}$	3.9	$8.8\cdot10^{-2}$	2.9
42	di(n-hexyl,n-octyl,n-decyl) phthalate	25724-58-7	AETP	3.8	$5.5\cdot10^{1}$	$3.7\cdot10^{-4}$	$1.5\cdot10^{-3}$	$6.6\cdot10^{-4}$
			TETP	$9.7\cdot10^{2}$	$1.3\cdot10^{1}$	$4.0\cdot10^{3}$	$3.7\cdot10^{-1}$	$2.9\cdot10^{3}$
			HTP	—	—	—	—	—
43	dibutylphthalate	84-74-2	AETP	2.2	$1.8\cdot10^{1}$	$2.2\cdot10^{-4}$	$8.6\cdot10^{-4}$	$3.9\cdot10^{-4}$
			TETP	$2.5\cdot10^{2}$	4.0	$1.2\cdot10^{3}$	$1.0\cdot10^{-1}$	$8.7\cdot10^{2}$
			HTP	$6.9\cdot10^{2}$	$2.4\cdot10^{1}$	$9.5\cdot10^{-1}$	$2.7\cdot10^{-1}$	$7.6\cdot10^{-1}$
44	dichloromethane	75-09-2	AETP	$4.4\cdot10^{-4}$	$2.1\cdot10^{-2}$	$4.0\cdot10^{-4}$	$4.3\cdot10^{-4}$	$4.1\cdot10^{-4}$
			TETP	$7.8\cdot10^{-2}$	$7.8\cdot10^{-2}$	7.2	$7.6\cdot10^{-2}$	5.2
			HTP	$1.1\cdot10^{1}$	$1.2\cdot10^{1}$	$1.2\cdot10^{1}$	$1.1\cdot10^{1}$	$1.2\cdot10^{1}$
45	dichlorvos	62-73-7	AETP	$1.5\cdot10^{1}$	$2.9\cdot10^{2}$	$1.5\cdot10^{-1}$	$4.5\cdot10^{-1}$	$2.3\cdot10^{-1}$
			TETP	$9.4\cdot10^{3}$	$2.1\cdot10^{3}$	$3.5\cdot10^{4}$	$2.8\cdot10^{2}$	$2.6\cdot10^{4}$
			HTP	$1.2\cdot10^{2}$	$1.2\cdot10^{3}$	$2.5\cdot10^{2}$	3.6	$1.8\cdot10^{2}$
46	dieldrin	60-57-1	AETP	$1.2\cdot10^{3}$	$2.0\cdot10^{4}$	$4.4\cdot10^{1}$	$1.3\cdot10^{2}$	$6.6\cdot10^{1}$
			TETP	$5.1\cdot10^{8}$	$1.7\cdot10^{7}$	$1.9\cdot10^{9}$	$5.6\cdot10^{7}$	$1.4\cdot10^{9}$
			HTP	$2.3\cdot10^{6}$	$2.0\cdot10^{5}$	$1.2\cdot10^{6}$	$2.5\cdot10^{5}$	$9.3\cdot10^{5}$

Substance			Type	Initial emission compartment				
No.	Name	CAS No.		air	(surface) water	agricultural soil	industrial soil	generic soil
47	diethylphthalate	84-66-2	AETP	$9.4\cdot10^{-3}$	$2.6\cdot10^{-1}$	$4.5\cdot10^{-7}$	$1.8\cdot10^{-6}$	$8.1\cdot10^{-7}$
			TETP	2.9	$2.4\cdot10^{-3}$	$1.1\cdot10^{1}$	$5.6\cdot10^{-4}$	8.1
			HTP	1.8	$2.9\cdot10^{-1}$	$3.3\cdot10^{-2}$	$3.3\cdot10^{-4}$	$2.4\cdot10^{-2}$
48	diheptylphthalate	3648-21-3	AETP	—	—	—	—	—
			TETP	$8.2\cdot10^{2}$	$1.1\cdot10^{1}$	$3.4\cdot10^{3}$	$3.2\cdot10^{-1}$	$2.5\cdot10^{3}$
			HTP	—	—	—	—	—
49	dihexylphthalate	84-75-3	AETP	4.7	$4.2\cdot10^{1}$	$2.8\cdot10^{-3}$	$1.1\cdot10^{-2}$	$5.1\cdot10^{-3}$
			TETP	$1.1\cdot10^{3}$	$9.7\cdot10^{1}$	$4.9\cdot10^{3}$	2.6	$3.6\cdot10^{3}$
			HTP	—	—	—	—	—
50	diisooctylphthalate	27554-26-3	AETP	$2.6\cdot10^{1}$	$3.1\cdot10^{2}$	3.0	7.5	4.2
			TETP	$3.4\cdot10^{5}$	$1.9\cdot10^{5}$	$1.1\cdot10^{6}$	$9.7\cdot10^{4}$	$8.2\cdot10^{5}$
			HTP	$8.0\cdot10^{2}$	$7.9\cdot10^{2}$	$1.1\cdot10^{3}$	$2.3\cdot10^{2}$	$8.4\cdot10^{2}$
51	diisodecylphthalate	26761-40-0	AETP	$4.5\cdot10^{1}$	$1.5\cdot10^{3}$	$5.9\cdot10^{-2}$	$1.8\cdot10^{-1}$	$9.2\cdot10^{-2}$
			TETP	$6.4\cdot10^{5}$	$5.3\cdot10^{1}$	$2.4\cdot10^{6}$	$2.5\cdot10^{3}$	$1.7\cdot10^{6}$
			HTP	$4.6\cdot10^{2}$	$1.6\cdot10^{2}$	$2.1\cdot10^{2}$	1.8	$1.5\cdot10^{2}$
52	dimethylphthalate	131-11-3	AETP	$2.7\cdot10^{-2}$	$6.5\cdot10^{-1}$	$1.4\cdot10^{-6}$	$5.5\cdot10^{-6}$	$2.5\cdot10^{-6}$
			TETP	$5.8\cdot10^{3}$	8.6	$2.2\cdot10^{4}$	1.2	$1.6\cdot10^{4}$
			HTP	—	—	—	—	—
53	dioctylphthalate	117-84-0	AETP	$7.9\cdot10^{-1}$	$1.3\cdot10^{1}$	$6.0\cdot10^{-5}$	$2.4\cdot10^{-4}$	$1.1\cdot10^{-4}$
			TETP	$3.1\cdot10^{2}$	1.8	$1.2\cdot10^{3}$	$9.3\cdot10^{-2}$	$9.0\cdot10^{2}$
			HTP	—	—	—	—	—
54	endosulfan	115-29-7	AETP	$8.6\cdot10^{5}$	$9.0\cdot10^{6}$	$8.5\cdot10^{4}$	$2.2\cdot10^{5}$	$1.2\cdot10^{5}$
			TETP	$2.3\cdot10^{6}$	$2.1\cdot10^{6}$	$7.6\cdot10^{6}$	$5.9\cdot10^{5}$	$5.7\cdot10^{6}$
			HTP	$4.9\cdot10^{2}$	$5.3\cdot10^{2}$	$4.8\cdot10^{2}$	$1.2\cdot10^{2}$	$3.8\cdot10^{2}$
55	endrin	72-20-8	AETP	$2.7\cdot10^{4}$	$8.1\cdot10^{5}$	$2.9\cdot10^{2}$	$8.6\cdot10^{2}$	$4.4\cdot10^{2}$
			TETP	$9.0\cdot10^{8}$	$1.5\cdot10^{7}$	$3.3\cdot10^{9}$	$2.9\cdot10^{7}$	$2.4\cdot10^{9}$
			HTP	$8.5\cdot10^{4}$	$4.2\cdot10^{4}$	$8.1\cdot10^{4}$	$2.8\cdot10^{3}$	$6.0\cdot10^{4}$
56	ethylene	74-85-1	AETP	$2.2\cdot10^{-3}$	$7.6\cdot10^{-2}$	$1.7\cdot10^{-8}$	$6.9\cdot10^{-8}$	$3.1\cdot10^{-8}$
			TETP	$1.7\cdot10^{1}$	$2.2\cdot10^{-4}$	$6.5\cdot10^{1}$	$5.3\cdot10^{-4}$	$4.7\cdot10^{1}$
			HTP	—	—	—	—	—
57	fenitrothion	122-14-5	AETP	$1.4\cdot10^{3}$	$4.1\cdot10^{4}$	$1.1\cdot10^{1}$	$3.4\cdot10^{1}$	$1.7\cdot10^{1}$
			TETP	$1.9\cdot10^{6}$	$6.5\cdot10^{4}$	$7.1\cdot10^{6}$	$4.7\cdot10^{3}$	$5.2\cdot10^{6}$
			HTP	$9.2\cdot10^{2}$	$1.4\cdot10^{3}$	$4.7\cdot10^{2}$	$2.2\cdot10^{1}$	$3.5\cdot10^{2}$
58	fenthion	55-38-9	AETP	$2.2\cdot10^{5}$	$5.6\cdot10^{6}$	$2.1\cdot10^{3}$	$6.3\cdot10^{3}$	$3.2\cdot10^{3}$
			TETP	$7.4\cdot10^{8}$	$3.5\cdot10^{7}$	$2.7\cdot10^{9}$	$2.1\cdot10^{7}$	$2.0\cdot10^{9}$
			HTP	$1.2\cdot10^{4}$	$7.1\cdot10^{3}$	$4.2\cdot10^{3}$	$3.3\cdot10^{2}$	$3.2\cdot10^{3}$

Substance			Type	Initial emission compartment				
No.	Name	CAS No.		air	(surface) water	agricultural soil	industrial soil	generic soil
59	fentinacetate	900-95-8	AETP	$3.6\cdot10^{5}$	$1.1\cdot10^{7}$	$2.6\cdot10^{3}$	$7.8\cdot10^{3}$	$4.0\cdot10^{3}$
			TETP	$3.9\cdot10^{8}$	$8.8\cdot10^{6}$	$1.4\cdot10^{9}$	$8.3\cdot10^{6}$	$1.0\cdot10^{9}$
			HTP	$4.3\cdot10^{3}$	$1.3\cdot10^{4}$	$3.5\cdot10^{3}$	$9.3\cdot10^{1}$	$2.6\cdot10^{3}$
60	fentinchloride	639-58-7	AETP	$2.1\cdot10^{5}$	$5.8\cdot10^{5}$	$3.4\cdot10^{4}$	$7.8\cdot10^{4}$	$4.6\cdot10^{4}$
			TETP	$8.9\cdot10^{7}$	$8.1\cdot10^{7}$	$1.2\cdot10^{9}$	$3.4\cdot10^{7}$	$8.9\cdot10^{8}$
			HTP	$8.7\cdot10^{3}$	$9.1\cdot10^{3}$	$7.7\cdot10^{3}$	$3.3\cdot10^{3}$	$6.5\cdot10^{3}$
61	fentinhydroxide	76-87-9	AETP	$2.1\cdot10^{5}$	$6.5\cdot10^{6}$	$1.8\cdot10^{3}$	$5.3\cdot10^{3}$	$2.7\cdot10^{3}$
			TETP	$3.9\cdot10^{8}$	$1.4\cdot10^{7}$	$1.4\cdot10^{9}$	$9.8\cdot10^{6}$	$1.0\cdot10^{9}$
			HTP	$8.1\cdot10^{3}$	$1.4\cdot10^{4}$	$5.6\cdot10^{3}$	$2.0\cdot10^{2}$	$4.2\cdot10^{3}$
62	formaldehyde	50-00-0	AETP	6.1	$1.6\cdot10^{2}$	$2.9\cdot10^{-4}$	$1.2\cdot10^{-3}$	$5.3\cdot10^{-4}$
			TETP	$2.6\cdot10^{3}$	2.5	$9.5\cdot10^{3}$	$5.1\cdot10^{-1}$	$7.2\cdot10^{3}$
			HTP	$4.2\cdot10^{-1}$	$3.5\cdot10^{-1}$	$3.1\cdot10^{-2}$	$8.2\cdot10^{-5}$	$2.3\cdot10^{-2}$
63	hexachlorobenzene	118-74-1	AETP	4.3	$1.6\cdot10^{2}$	3.3	3.9	3.4
			TETP	$4.0\cdot10^{5}$	$3.1\cdot10^{5}$	$3.1\cdot10^{6}$	$3.7\cdot10^{5}$	$2.4\cdot10^{6}$
			HTP	$4.4\cdot10^{3}$	$7.3\cdot10^{3}$	$1.4\cdot10^{4}$	$4.0\cdot10^{3}$	$1.1\cdot10^{4}$
64	hexachlorobutadiene	87-68-3	AETP	$1.4\cdot10^{2}$	$1.2\cdot10^{4}$	$1.4\cdot10^{2}$	$1.4\cdot10^{2}$	$1.4\cdot10^{2}$
			TETP	$1.2\cdot10^{5}$	$1.1\cdot10^{5}$	$3.9\cdot10^{6}$	$1.1\cdot10^{5}$	$2.9\cdot10^{6}$
			HTP	$1.0\cdot10^{4}$	$2.3\cdot10^{4}$	$1.1\cdot10^{4}$	$1.0\cdot10^{4}$	$1.1\cdot10^{4}$
65	hexachlorocyclohexane (γ)	58-89-9	AETP	$2.2\cdot10^{3}$	$4.1\cdot10^{4}$	$2.3\cdot10^{1}$	$6.8\cdot10^{1}$	$3.5\cdot10^{1}$
			TETP	$1.6\cdot10^{7}$	$2.8\cdot10^{6}$	$5.9\cdot10^{7}$	$4.9\cdot10^{5}$	$4.3\cdot10^{7}$
			HTP	$6.1\cdot10^{3}$	$3.2\cdot10^{4}$	$2.6\cdot10^{3}$	$1.9\cdot10^{2}$	$1.9\cdot10^{3}$
66	isodrin	465-73-6	AETP	—	—	—	—	—
			TETP	—	—	—	—	—
			HTP	$1.8\cdot10^{5}$	$1.4\cdot10^{5}$	$2.4\cdot10^{5}$	$9.7\cdot10^{4}$	$2.0\cdot10^{5}$
67	lead	7439-92-1	AETP	1.2	$4.0\cdot10^{1}$	$1.0\cdot10^{-9}$	$3.9\cdot10^{-9}$	$1.8\cdot10^{-9}$
			TETP	$1.1\cdot10^{4}$	$2.0\cdot10^{-7}$	$4.0\cdot10^{4}$	$2.5\cdot10^{-5}$	$2.9\cdot10^{4}$
			HTP	$6.7\cdot10^{4}$	$2.6\cdot10^{2}$	$4.8\cdot10^{2}$	$1.6\cdot10^{-4}$	$3.5\cdot10^{2}$
68	malathion	121-75-5	AETP	$5.3\cdot10^{5}$	$1.4\cdot10^{7}$	$4.5\cdot10^{3}$	$1.4\cdot10^{4}$	$7.0\cdot10^{3}$
			TETP	$3.3\cdot10^{5}$	$2.7\cdot10^{4}$	$1.2\cdot10^{6}$	$8.6\cdot10^{3}$	$8.9\cdot10^{5}$
			HTP	$6.4\cdot10^{1}$	$3.0\cdot10^{2}$	$7.2\cdot10^{1}$	1.7	$5.3\cdot10^{1}$
69	mercury	7430-97-6	AETP	$1.6\cdot10^{4}$	$1.3\cdot10^{5}$	$1.6\cdot10^{4}$	$1.6\cdot10^{4}$	$1.6\cdot10^{4}$
			TETP	$1.3\cdot10^{7}$	$8.2\cdot10^{6}$	$1.8\cdot10^{7}$	$1.3\cdot10^{7}$	$1.7\cdot10^{7}$
			HTP	$2.9\cdot10^{4}$	$1.8\cdot10^{4}$	$2.9\cdot10^{4}$	$2.9\cdot10^{4}$	$2.9\cdot10^{4}$
70	methylbromide	74-83-9	AETP	2.2	$1.4\cdot10^{2}$	2.1	2.2	2.2
			TETP	$1.7\cdot10^{3}$	$1.7\cdot10^{3}$	$5.7\cdot10^{4}$	$1.7\cdot10^{3}$	$4.2\cdot10^{4}$
			HTP	1.9	1.9	1.9	1.9	1.9

Substance			Type	Initial emission compartment				
No.	Name	CAS No.		air	(surface) water	agricul-tural soil	industrial soil	generic soil
71	methylparathion	298-00-0	AETP	$6.8\cdot10^{4}$	$2.0\cdot10^{6}$	$5.2\cdot10^{2}$	$1.6\cdot10^{3}$	$8.1\cdot10^{2}$
			TETP	$8.0\cdot10^{7}$	$2.5\cdot10^{6}$	$2.9\cdot10^{8}$	$1.9\cdot10^{6}$	$2.2\cdot10^{8}$
			HTP	$1.6\cdot10^{2}$	$3.4\cdot10^{2}$	$1.0\cdot10^{2}$	3.8	$7.6\cdot10^{1}$
72	monochlorobenzene	108-90-7	AETP	$9.9\cdot10^{-4}$	$3.6\cdot10^{-1}$	$6.8\cdot10^{-5}$	$2.3\cdot10^{-4}$	$1.1\cdot10^{-4}$
			TETP	$4.5\cdot10^{-2}$	$2.8\cdot10^{-2}$	$2.7\cdot10^{1}$	$1.0\cdot10^{-2}$	$2.0\cdot10^{1}$
			HTP	$3.4\cdot10^{-1}$	$2.5\cdot10^{-1}$	$4.7\cdot10^{-2}$	$7.7\cdot10^{-2}$	$5.5\cdot10^{-2}$
73	nickel	7440-02-0	AETP	$8.0\cdot10^{1}$	$2.7\cdot10^{3}$	$3.6\cdot10^{-7}$	$1.2\cdot10^{-6}$	$5.8\cdot10^{-7}$
			TETP	$1.9\cdot10^{5}$	$3.1\cdot10^{-5}$	$7.1\cdot10^{5}$	$2.3\cdot10^{-3}$	$5.2\cdot10^{5}$
			HTP	$9.8\cdot10^{3}$	$6.3\cdot10^{1}$	$1.1\cdot10^{3}$	$1.2\cdot10^{-4}$	$8.0\cdot10^{2}$
74	nitrogen dioxide	10102-44-0	AETP	—	—	—	—	—
			TETP	—	—	—	—	—
			HTP	$2.6\cdot10^{-1}$	$2.5\cdot10^{-1}$	$4.0\cdot10^{-2}$	$9.3\cdot10^{-3}$	$3.2\cdot10^{-2}$
75	parathion	56-38-2	AETP	$1.3\cdot10^{5}$	$3.8\cdot10^{6}$	$9.7\cdot10^{2}$	$2.9\cdot10^{3}$	$1.5\cdot10^{3}$
			TETP	$8.1\cdot10^{6}$	$2.3\cdot10^{5}$	$3.0\cdot10^{7}$	$1.9\cdot10^{5}$	$2.2\cdot10^{7}$
			HTP	$6.2\cdot10^{2}$	6.7	$4.0\cdot10^{2}$	$1.4\cdot10^{1}$	$2.9\cdot10^{2}$
76	PCB	1336-36-3	AETP	$4.9\cdot10^{4}$	$3.2\cdot10^{5}$	$2.7\cdot10^{3}$	$7.5\cdot10^{3}$	$4.0\cdot10^{3}$
			TETP	$1.9\cdot10^{8}$	$6.8\cdot10^{7}$	$8.5\cdot10^{8}$	$3.0\cdot10^{7}$	$6.3\cdot10^{8}$
			HTP	$2.4\cdot10^{5}$	$1.4\cdot10^{5}$	$1.4\cdot10^{5}$	$3.7\cdot10^{4}$	$1.1\cdot10^{5}$
77	pentachloroaniline	527-20-8	AETP	$1.1\cdot10^{3}$	$1.4\cdot10^{4}$	$2.1\cdot10^{1}$	$6.2\cdot10^{1}$	$3.2\cdot10^{1}$
			TETP	$1.8\cdot10^{7}$	$1.7\cdot10^{6}$	$7.2\cdot10^{7}$	$1.0\cdot10^{6}$	$5.3\cdot10^{7}$
			HTP	—	—	—	—	—
78	pentachlorobenzene	608-93-5	AETP	$9.5\cdot10^{-1}$	$4.9\cdot10^{1}$	$9.2\cdot10^{-1}$	$9.4\cdot10^{-1}$	$9.3\cdot10^{-1}$
			TETP	$1.1\cdot10^{4}$	$1.0\cdot10^{4}$	$3.5\cdot10^{5}$	$1.1\cdot10^{5}$	$2.8\cdot10^{5}$
			HTP	$2.5\cdot10^{2}$	$3.0\cdot10^{2}$	$2.8\cdot10^{2}$	$2.5\cdot10^{2}$	$2.7\cdot10^{2}$
79	pentachlorophenol	87-86-5	AETP	$1.0\cdot10^{2}$	$4.2\cdot10^{2}$	$4.9\cdot10^{1}$	$7.5\cdot10^{1}$	$5.6\cdot10^{1}$
			TETP	$2.4\cdot10^{6}$	$2.2\cdot10^{6}$	$1.3\cdot10^{7}$	$1.8\cdot10^{6}$	$9.8\cdot10^{6}$
			HTP	$2.0\cdot10^{2}$	$2.0\cdot10^{2}$	$2.5\cdot10^{2}$	$1.5\cdot10^{2}$	$2.2\cdot10^{2}$
80	phenol	108-95-2	AETP	$3.9\cdot10^{1}$	$7.2\cdot10^{2}$	$2.2\cdot10^{-3}$	$8.9\cdot10^{-3}$	$4.0\cdot10^{-3}$
			TETP	$1.1\cdot10^{4}$	$3.4\cdot10^{1}$	$4.4\cdot10^{4}$	2.5	$3.2\cdot10^{4}$
			HTP	2.2	$8.9\cdot10^{-1}$	$8.7\cdot10^{-2}$	$5.0\cdot10^{-4}$	$6.3\cdot10^{-2}$
81	phthalic anhydride	85-44-9	AETP	—	—	—	—	—
			TETP	—	—	—	—	—
			HTP	$2.2\cdot10^{-1}$	$2.9\cdot10^{-5}$	$1.4\cdot10^{-2}$	$1.7\cdot10^{-5}$	$1.0\cdot10^{-2}$
82	propyleneoxide	75-56-9	AETP	1.6	5.0	$2.9\cdot10^{-3}$	$1.2\cdot10^{-2}$	$5.3\cdot10^{-3}$
			TETP	$1.8\cdot10^{1}$	5.0	$4.4\cdot10^{2}$	$1.3\cdot10^{-1}$	$3.2\cdot10^{2}$
			HTP	$6.0\cdot10^{1}$	$1.8\cdot10^{1}$	$3.4\cdot10^{-1}$	$4.2\cdot10^{-1}$	$3.6\cdot10^{-1}$

Substance			Type	Initial emission compartment				
No.	Name	CAS No.		air	(surface) water	agricultural soil	industrial soil	generic soil
83	simazine	122-34-9	AETP	$2.7\cdot10^{4}$	$5.6\cdot10^{5}$	$2.7\cdot10^{2}$	$8.1\cdot10^{2}$	$4.2\cdot10^{2}$
			TETP	$1.9\cdot10^{7}$	$4.7\cdot10^{6}$	$7.1\cdot10^{7}$	$5.7\cdot10^{5}$	$5.2\cdot10^{7}$
			HTP	$4.5\cdot10^{2}$	$2.5\cdot10^{3}$	$5.3\cdot10^{2}$	$1.3\cdot10^{1}$	$3.9\cdot10^{2}$
84	sulphur dioxide	7446-09-5	AETP	—	—	—	—	—
			TETP	—	—	—	—	—
			HTP	$1.6\cdot10^{-1}$	$1.6\cdot10^{-1}$	$1.4\cdot10^{-1}$	$1.5\cdot10^{-1}$	$1.4\cdot10^{-1}$
85	tetrachloroethene	127-18-4	AETP	$3.3\cdot10^{-3}$	1.1	$3.3\cdot10^{-3}$	$3.3\cdot10^{-3}$	$3.3\cdot10^{-3}$
			TETP	$1.1\cdot10^{2}$	$1.1\cdot10^{2}$	$1.3\cdot10^{4}$	$1.1\cdot10^{2}$	$9.5\cdot10^{3}$
			HTP	$3.5\cdot10^{1}$	$3.7\cdot10^{1}$	$3.7\cdot10^{1}$	$3.5\cdot10^{1}$	$3.6\cdot10^{1}$
86	tetrachloromethane	56-23-5	AETP	$2.9\cdot10^{-3}$	$3.5\cdot10^{-1}$	$2.9\cdot10^{-3}$	$2.9\cdot10^{-3}$	$2.9\cdot10^{-3}$
			TETP	$2.1\cdot10^{-1}$	$2.1\cdot10^{-1}$	7.2	$2.1\cdot10^{-1}$	5.3
			HTP	$4.8\cdot10^{2}$	$4.8\cdot10^{2}$	$4.8\cdot10^{2}$	$4.8\cdot10^{2}$	$4.8\cdot10^{2}$
87	toluene	108-88-3	AETP	$9.7\cdot10^{-5}$	$3.3\cdot10^{-1}$	$9.5\cdot10^{-6}$	$2.9\cdot10^{-5}$	$1.5\cdot10^{-5}$
			TETP	$3.5\cdot10^{-2}$	$2.2\cdot10^{-2}$	$1.4\cdot10^{2}$	$1.0\cdot10^{-2}$	$1.0\cdot10^{2}$
			HTP	$3.6\cdot10^{-2}$	$5.3\cdot10^{-2}$	$1.9\cdot10^{-2}$	$1.1\cdot10^{-2}$	$1.7\cdot10^{-2}$
88	tributyltinoxide	56-35-9	AETP	$1.0\cdot10^{6}$	$1.2\cdot10^{7}$	$1.3\cdot10^{4}$	$3.9\cdot10^{4}$	$2.0\cdot10^{4}$
			TETP	$5.9\cdot10^{8}$	$2.4\cdot10^{8}$	$2.3\cdot10^{9}$	$2.2\cdot10^{7}$	$1.7\cdot10^{9}$
			HTP	$7.4\cdot10^{3}$	$1.6\cdot10^{4}$	$5.8\cdot10^{3}$	$2.8\cdot10^{2}$	$4.3\cdot10^{3}$
89	trichloroethylene	79-01-6	AETP	$7.0\cdot10^{-5}$	$1.6\cdot10^{-1}$	$6.8\cdot10^{-5}$	$6.9\cdot10^{-5}$	$6.8\cdot10^{-5}$
			TETP	$2.5\cdot10^{-2}$	$2.4\cdot10^{-2}$	$3.8\cdot10^{1}$	$2.4\cdot10^{-2}$	$2.8\cdot10^{1}$
			HTP	$7.5\cdot10^{-2}$	$1.1\cdot10^{-1}$	$1.3\cdot10^{-1}$	$7.5\cdot10^{-2}$	$1.2\cdot10^{-1}$
90	trichloromethane	67-66-3	AETP	$2.0\cdot10^{-2}$	$7.0\cdot10^{-1}$	$1.9\cdot10^{-2}$	$2.0\cdot10^{-2}$	$1.9\cdot10^{-2}$
			TETP	5.2	5.2	$3.4\cdot10^{2}$	5.1	$2.5\cdot10^{2}$
			HTP	$3.2\cdot10^{1}$	$3.2\cdot10^{1}$	$3.2\cdot10^{1}$	$3.1\cdot10^{1}$	$3.2\cdot10^{1}$
91	trifluralin	1582-09-8	AETP	$1.2\cdot10^{1}$	$6.7\cdot10^{1}$	8.3	$1.0\cdot10^{1}$	8.8
			TETP	$2.6\cdot10^{6}$	$6.5\cdot10^{4}$	$1.3\cdot10^{7}$	$2.3\cdot10^{6}$	$9.8\cdot10^{6}$
			HTP	$1.0\cdot10^{3}$	$3.3\cdot10^{1}$	$1.5\cdot10^{3}$	$8.9\cdot10^{2}$	$1.3\cdot10^{3}$
92	vanadium	7440-62-2	AETP	$1.1\cdot10^{1}$	$3.8\cdot10^{2}$	$5.1\cdot10^{-8}$	$1.7\cdot10^{-7}$	$8.2\cdot10^{-8}$
			TETP	$4.5\cdot10^{5}$	$3.4\cdot10^{-5}$	$1.7\cdot10^{6}$	$5.1\cdot10^{-3}$	$1.2\cdot10^{6}$
			HTP	$4.9\cdot10^{3}$	$1.9\cdot10^{1}$	$2.2\cdot10^{2}$	$5.5\cdot10^{-5}$	$1.6\cdot10^{2}$
93	vinylchloride	75-01-4	AETP	$3.1\cdot10^{-3}$	$4.6\cdot10^{-1}$	$3.1\cdot10^{-3}$	$3.1\cdot10^{-3}$	$3.1\cdot10^{-3}$
			TETP	$4.5\cdot10^{-2}$	$4.4\cdot10^{-2}$	1.5	$4.4\cdot10^{-2}$	1.1
			HTP	$5.5\cdot10^{2}$	$5.5\cdot10^{2}$	$5.4\cdot10^{2}$	$5.4\cdot10^{2}$	$5.4\cdot10^{2}$
94	zinc	7440-66-6	AETP	2.6	$8.6\cdot10^{1}$	$2.6\cdot10^{-8}$	$7.4\cdot10^{-8}$	$3.9\cdot10^{-8}$
			TETP	$6.6\cdot10^{5}$	$2.5\cdot10^{-5}$	$2.4\cdot10^{6}$	$1.6\cdot10^{-2}$	$1.8\cdot10^{6}$
			HTP	$6.3\cdot10^{-1}$	$5.8\cdot10^{-2}$	$1.7\cdot10^{1}$	$1.5\cdot10^{-8}$	$1.2\cdot10^{1}$

Usage
The impact score for aquatic ecotoxicity is calculated as

$$\begin{aligned} \textit{impact score}_{\text{aquatic ecotoxicity}}\ (\text{kg}) = {} & \sum_{subs} \textit{AETP}_{subs,\text{air}} \times \textit{emission}_{subs,\text{air}}\ (\text{kg}) + \\ & \sum_{subs} \textit{AETP}_{subs,\text{water}} \times \textit{emission}_{subs,\text{water}}\ (\text{kg}) + \\ & \sum_{subs} \textit{AETP}_{subs,\text{industrial soil}} \times \textit{emission}_{subs,\text{industrial soil}}\ (\text{kg}) + \\ & \sum_{subs} \textit{AETP}_{subs,\text{agricultural soil}} \times \textit{emission}_{subs,\text{agricultural soil}}\ (\text{kg}) \end{aligned}$$

The impact score for terrestrial ecotoxicity is calculated as

$$\begin{aligned} \textit{impact score}_{\text{terrestrial ecotoxicity}}\ (\text{kg}) = {} & \sum_{subs} \textit{TETP}_{subs,\text{air}} \times \textit{emission}_{subs,\text{air}}\ (\text{kg}) + \\ & \sum_{subs} \textit{TETP}_{subs,\text{water}} \times \textit{emission}_{subs,\text{water}}\ (\text{kg}) + \\ & \sum_{subs} \textit{TETP}_{subs,\text{industrial soil}} \times \textit{emission}_{subs,\text{industrial soil}}\ (\text{kg}) + \\ & \sum_{subs} \textit{TETP}_{subs,\text{agricultural soil}} \times \textit{emission}_{subs,\text{agricultural soil}}\ (\text{kg}) \end{aligned}$$

The impact score for human toxicity is calculated as

$$\begin{aligned} \textit{impact score}_{\text{human toxicity}}\ (\text{kg}) = {} & \sum_{subs} \textit{HTP}_{subs,\text{air}} \times \textit{emission}_{subs,\text{air}}\ (\text{kg}) + \\ & \sum_{subs} \textit{HTP}_{subs,\text{water}} \times \textit{emission}_{subs,\text{water}}\ (\text{kg}) + \\ & \sum_{subs} \textit{HTP}_{subs,\text{industrial soil}} \times \textit{emission}_{subs,\text{industrial soil}}\ (\text{kg}) + \\ & \sum_{subs} \textit{HTP}_{subs,\text{agricultural soil}} \times \textit{emission}_{subs,\text{agricultural soil}}\ (\text{kg}) \end{aligned}$$

Use the column "generic soil" only after critical reflection; see page 63.

Example
Suppose that an inventory table lists an atmospheric emission of phenol of 3.0 kg and an emission of mercury to industrial soil of 10 mg. This results in an impact score for aquatic ecotoxicity of
$(3.0\ \text{kg} \times 3.9 \cdot 10^{1}) + (1.0 \cdot 10^{-2}\ \text{kg} \times 1.6 \cdot 10^{4}) = 2.8 \cdot 10^{2}$ kg,
in an impact score for terrestrial ecotoxicity of:
$(3.0\ \text{kg} \times 1.1 \cdot 10^{4}) + (1.0 \cdot 10^{-2}\ \text{kg} \times 5.6 \times 10^{6}) = 8.9 \cdot 10^{4}$ kg,
and in an impact score for human toxicity of:
$(3.0\ \text{kg} \times 2.2) + (1.0 \cdot 10^{-2}\ \text{kg} \times 2.0 \cdot 10^{3}) = 2.7 \cdot 10^{1}$ kg.

Appendix B

DATA USED FOR DETERMINATION OF THE PNEC

The following table lists the toxicity parameters used for calculating the equivalency factors with USES 1.0.

If a "—" is listed in the table, there is no toxicological data available for the aquatic or terrestrial compartment or for humans.

The abbreviations used in this table are explained below. The abbreviations are listed in brackets in bold type. In calculating the equivalency factors the single substance module of USES 1.0 has been used rather than the priority module. For the aquatic and terrestrial ecosystem, for the majority of the substances an MTR-value (maximum tolerable risk) has been used as PNEC **(MTR)**. For some substances the only value available was an MTR-value for the terrestrial ecosystem, which was derived from an aquatic MTR using equilibrium partitioning **(MTR (eq))**. For substances with no MTR, USES 1.0 calculates a PNEC-value using the $L(E)C_{50}$- or NOEC-values **(LC_{50}/NOEC)**. In USES 1.0 equilibrium partitioning is used for calculating PNEC-values if there are no toxicity values available for the soil compartment **(equil. part.)**. For the majority of the substances an ADI or TDI is used for calculating the human equivalency factor **(ADI/TDI)**. If an ADI or TDI is lacking, a NEL man is extrapolated from an inhalation or oral LOAEL **(LOAEL inh/oral)** or NOAEL **(NOAEL inh/oral)**, according to Table 10 of the USES 1.0 report [38]. For genotoxic or carcinogenic substances a NEL man is used **(NEL man)**. For the substances ammonia (anhydrous), nitrogen dioxide and sulphur dioxide only the inhalation route is used **(inh. route)**; see page 57.

Substance			Target	Toxicity parameter		
Nr.	Name	CAS nr.		type	value	unit
1	1,1,1-trichloroethane	71-55-6	aquatic ecosystem	MTR	2.1	mg/l
			terrestrial ecosystem	MTR (eq)	6.9	mg/kg
			human	LOAEL oral	81.43	mg/kg
2	1,2,3,4-tetrachlorobenzene	634-66-2	aquatic ecosystem	MTR	0.023	mg/l
			terrestrial ecosystem	MTR	0.2	mg/kg
			human	ADI/TDI	0.004	mg/(kg·d)
3	1,2,3,5-tetrachlorobenzene	634-90-2	aquatic ecosystem	MTR	0.022	mg/l
			terrestrial ecosystem	MTR	0.007	mg/kg
			human	ADI/TDI	0.004	mg/(kg·d)

Substance			Target	Toxicity parameter		
Nr.	Name	CAS nr.		type	value	unit
4	1,2,3-trichlorobenzene	87-61-6	aquatic ecosystem	MTR	0.064	mg/l
			terrestrial ecosystem	MTR	0.005	mg/kg
			human	ADI/TDI	0.02	mg/(kg·d)
5	1,2-dichlorobenzene	95-50-1	aquatic ecosystem	MTR	0.27	mg/l
			terrestrial ecosystem	MTR	0.4	mg/kg
			human	ADI/TDI	0.6	mg/(kg·d)
6	1,2-dichloroethane	107-06-2	aquatic ecosystem	MTR	0.7	mg/l
			terrestrial ecosystem	MTR (eq)	1.5	mg/kg
			human	ADI/TDI	0.014	mg/(kg·d)
7	1,3-butadiene	106-99-0	aquatic ecosystem	LC_{50}	71.3	mg/l
			terrestrial ecosystem	equil. part.		mg/kg
			human	NEL man oral	0.643	mg/(kg·d)
8	1,4-dichloro-2-nitrobenzene	89-61-2	aquatic ecosystem	LC_{50}	2.1	mg/l
			terrestrial ecosystem	LC_{50}/NOEC	9.6	mg/kg
			human	NOAEL oral	10	mg/(kg·d)
9	1,4-dichlorobenzene	106-46-7	aquatic ecosystem	MTR	0.26	mg/l
			terrestrial ecosystem	MTR	0.4	mg/kg
			human	ADI/TDI	0.2	mg/(kg·d)
10	1-chloro-4-nitrobenzene	100-00-5	aquatic ecosystem	LC_{50}/NOEC	2	mg/l
			terrestrial ecosystem	equil. part.		mg/kg
			human	NEL man oral	0.001	mg/(kg·d)
11	2,3,7,8-TCDD	1746-01-6	aquatic ecosystem	MTR	$1.2 \cdot 10^{-9}$	mg/l
			terrestrial ecosystem	MTR	0.5	mg/kg
			human	ADI/TDI	$1.0 \cdot 10^{-8}$	mg/(kg·d)
12	2,4,6-trichloroaniline	634-93-5	aquatic ecosystem	MTR	0.002	mg/l
			terrestrial ecosystem	MTR	5	mg/kg
			human	—	—	—
13	2,4,6-trichlorophenol	88-06-2	aquatic ecosystem	MTR	0.0025	mg/l
			terrestrial ecosystem	MTR	0.72	mg/kg
			human	NOAEL oral	0.3	mg/(kg·d)
14	2,4-dichlorophenol	120-83-2	aquatic ecosystem	MTR	0.015	mg/l
			terrestrial ecosystem	MTR	0.22	mg/kg
			human	NOAEL oral	0.3	mg/(kg·d)
15	2-chlorophenol	95-57-8	aquatic ecosystem	MTR	0.025	mg/l
			terrestrial ecosystem	MTR	0.2	mg/kg
			human	NOAEL oral	35	mg/(kg·d)

Substance			Target	Toxicity parameter		
Nr.	Name	CAS nr.		type	value	unit
16	3,4-dichloroaniline	95-76-1	aquatic ecosystem	MTR	0.005	mg/l
			terrestrial ecosystem	MTR	0.5	mg/kg
			human	NOAEL oral	0.2	mg/(kg·d)
17	3,5-dichloroaniline	626-43-7	aquatic ecosystem	MTR	0.005	mg/l
			terrestrial ecosystem	LC_{50}	1600	mg/kg
			human	—	—	—
18	3-monochloroaniline	108-42-9	aquatic ecosystem	MTR	0.02	mg/l
			terrestrial ecosystem	MTR	1.6	mg/kg
			human	NOAEL oral	0.25	mg/(kg·d)
19	4-monochloroaniline	106-47-8	aquatic ecosystem	MTR	0.02	mg/l
			terrestrial ecosystem	MTR	1.2	mg/kg
			human	ADI/TDI	0.00005	mg/(kg·d)
20	acrolein	107-02-8	aquatic ecosystem	MTR	0.001	mg/l
			terrestrial ecosystem	MTR (eq)	0.001	mg/kg
			human	ADI/TDI	0.0005	mg/(kg·d)
21	acrylonitrile	107-13-1	aquatic ecosystem	MTR	0.0076	mg/l
			terrestrial ecosystem	MTR (eq)	0.00068	mg/kg
			human	NEL man oral	0.00079	mg/(kg·d)
22	aldrin	309-00-2	aquatic ecosystem	MTR	0.00002	mg/l
			terrestrial ecosystem	MTR	0.05	mg/kg
			human	ADI/TDI	0.0001	mg/(kg·d)
23	α,α,α-trichlorotoluene	98-07-7	aquatic ecosystem	MTR	0.024	mg/l
			terrestrial ecosystem	MTR	8	mg/kg
			human	NEL man oral	0.001	mg/(kg·d)
24	α,α-dichlorotoluene	98-87-3	aquatic ecosystem	MTR	0.143	mg/l
			terrestrial ecosystem	MTR	7	mg/kg
			human	NEL man oral	0.001	mg/(kg·d)
25	α-chlorotoluene	100-44-7	aquatic ecosystem	MTR	0.365	mg/l
			terrestrial ecosystem	MTR	5.5	mg/kg
			human	NEL man ora	0.04	mg/(kg·d)
26	ammonia (anhydrous)	7664-41-7	aquatic ecosystem	—	—	—
			terrestrial ecosystem	—	—	—
			human	inh. route*	0.21	mg/m^3
27	arsenic	7440-38-2	aquatic ecosystem	MTR	0.0086	mg/l
			terrestrial ecosystem	MTR	7.1	mg/kg
			human	ADI/TDI	0.002	mg/(kg·d)

Substance			Target	Toxicity parameter		
Nr.	Name	CAS nr.		type	value	unit
28	atrazine	1912-24-9	aquatic ecosystem	MTR	0.0022	mg/l
			terrestrial ecosystem	MTR	0.065	mg/kg
			human	ADI/TDI	0.002	mg/(kg·d)
29	azinfos-methyl	86-50-0	aquatic ecosystem	MTR	0.00009	mg/l
			terrestrial ecosystem	MTR	0.005	mg/kg
			human	ADI/TDI	0.005	mg/(kg·d)
30	bentazone	25057-89-0	aquatic ecosystem	LC$_{50}$	64	mg/l
			terrestrial ecosystem	equil. part.		mg/kg
			human	ADI/TDI	0.1	mg/(kg·d)
31	benzene	71-43-2	aquatic ecosystem	MTR	0.24	mg/l
			terrestrial ecosystem	MTR (eq)	0.95	mg/kg
			human	NEL man oral	0.00257	mg/(kg·d)
32	benzo[a]pyrene	50-32-8	aquatic ecosystem	MTR	0.00005	mg/l
			terrestrial ecosystem	MTR (eq)	0.26	mg/kg
			human	NEL man oral	0.0063	mg/(kg·d)
33	benzylbutylphthalate	85-68-7	aquatic ecosystem	MTR	0.009	mg/l
			terrestrial ecosystem	LC$_{50}$	10000	mg/kg
			human	ADI/TDI	0.1	mg/(kg·d)
34	butyl(2-ethylhexyl)phthalate	85-69-8	aquatic ecosystem	MTR	0.006	mg/l
			terrestrial ecosystem	equil. part.		mg/kg
			human	—	—	—
35	cadmium	7440-43-9	aquatic ecosystem	MTR	0.00035	mg/l
			terrestrial ecosystem	MTR	0.0035	mg/kg
			human	ADI/TDI	0.001	mg/(kg·d)
36	carbon disulphide	75-15-0	aquatic ecosystem	LC$_{50}$	95	mg/l
			terrestrial ecosystem	equil. part.		mg/kg
			human	NOAEL oral	12.86	mg/(kg·d)
37	chromium III	7440-47-3	aquatic ecosystem	MTR	0.005	mg/l
			terrestrial ecosystem	MTR	2.4	mg/kg
			human	ADI/TDI	0.005	mg/(kg·d)
38	chromium VI	7440-47-3	aquatic ecosystem	MTR	0.005	mg/l
			terrestrial ecosystem	MTR	2.4	mg/kg
			human	NEL man oral	$7.0 \cdot 10^{-7}$	mg/(kg·d)
39	cobalt	7440-48-4	aquatic ecosystem	MTR	0.002	mg/l
			terrestrial ecosystem	MTR	24	mg/kg
			human	ADI/TDI	0.0014	mg/(kg·d)

Substance			Target	Toxicity parameter		
Nr.	Name	CAS nr.		type	value	unit
40	copper	7440-50-8	aquatic ecosystem	MTR	0.0033	mg/l
			terrestrial ecosystem	MTR	0.55	mg/kg
			human	ADI/TDI	0.14	mg/(kg·d)
41	di(2-ethylhexyl)phthalate	117-81-7	aquatic ecosystem	MTR	0.008	mg/l
			terrestrial ecosystem	equil. part.		mg/kg
			human	ADI/TDI	0.025	mg/(kg·d)
42	di(n-hexyl,n-octyl,n-decyl) phthalate	25724-58-7	aquatic ecosystem	MTR	0.01	mg/l
			terrestrial ecosystem	equil. part.		mg/kg
			human	—	—	—
43	dibutylphthalate	84-74-2	aquatic ecosystem	MTR	0.033	mg/l
			terrestrial ecosystem	equil. part.		mg/kg
			human	ADI/TDI	0.05	mg/(kg·d)
44	dichloromethane	75-09-2	aquatic ecosystem	MTR	20	mg/l
			terrestrial ecosystem	MTR (eq)	36	mg/kg
			human	ADI/TDI	0.06	mg/(kg·d)
45	dichlorvos	62-73-7	aquatic ecosystem	LC_{50}/NOEC	0.066	mg/l
			terrestrial ecosystem	equil. part.		mg/kg
			human	ADI/TDI	0.004	mg/(kg·d)
46	dieldrin	60-57-1	aquatic ecosystem	MTR	0.00002	mg/l
			terrestrial ecosystem	MTR	0.05	mg/kg
			human	ADI/TDI	0.0001	mg/(kg·d)
47	diethylphthalate	84-66-2	aquatic ecosystem	MTR	2.5	mg/l
			terrestrial ecosystem	MTR	10	mg/kg
			human	ADI/TDI	0.2	mg/(kg·d)
48	diheptylphthalate	3648-21-3	aquatic ecosystem	—	—	—
			terrestrial ecosystem	MTR	10	mg/kg
			human	—	—	—
49	dihexylphthalate	84-75-3	aquatic ecosystem	MTR	0.008	mg/l
			terrestrial ecosystem	equil. part.		mg/kg
			human	—	—	—
50	diisooctylphthalate	27554-26-3	aquatic ecosystem	MTR	0.006	mg/l
			terrestrial ecosystem	equil. part.	—	mg/kg
			human	LOAEL oral	100	mg/(kg·d)
51	diisodecylphthalate	26761-40-0	aquatic ecosystem	MTR	0.003	mg/l
			terrestrial ecosystem	equil. part.		mg/kg
			human	ADI/TDI	0.05	mg/(kg·d)

Substance			Target	Toxicity parameter		
Nr.	Name	CAS nr.		type	value	unit
52	dimethylphtalate	131-11-3	aquatic ecosystem	MTR	1	mg/l
			terrestrial ecosystem	LC_{50}/NOEC	1.065	mg/kg
			human	—	—	—
53	dioctylphthalate	117-84-0	aquatic ecosystem	MTR	0.032	mg/l
			terrestrial ecosystem	equil. part.		mg/kg
			human	—	—	—
54	endosulfan	115-29-7	aquatic ecosystem	MTR	$4.0\cdot10^{-7}$	mg/l
			terrestrial ecosystem	MTR	0.05	mg/kg
			human	ADI/TDI	0.006	mg/(kg·d)
55	endrin	72-20-8	aquatic ecosystem	MTR	$3.0\cdot10^{-6}$	mg/l
			terrestrial ecosystem	MTR (eq)	0.0029	mg/kg
			human	ADI/TDI	0.0002	mg/(kg·d)
56	ethylene	74-85-1	aquatic ecosystem	MTR	8.5	mg/l
			terrestrial ecosystem	MTR (eq)	5.8	mg/kg
			human	—	—	—
57	fenitrothion	122-14-5	aquatic ecosystem	LC_{50}/NOEC	0.0016	mg/l
			terrestrial ecosystem	equil. part.		mg/kg
			human	ADI/TDI	0.005	mg/(kg·d)
58	fenthion	55-38-9	aquatic ecosystem	MTR	$3.1\cdot10^{-6}$	mg/l
			terrestrial ecosystem	MTR (eq)	0.00035	mg/kg
			human	ADI/TDI	0.001	mg/(kg·d)
59	fentinacetate	900-95-8	aquatic ecosystem	MTR	$5.0\cdot10^{-6}$	mg/l
			terrestrial ecosystem	equil. part.		mg/kg
			human	ADI/TDI	0.0005	mg/(kg·d)
60	fentinchloride	639-58-7	aquatic ecosystem	MTR	$5.0\cdot10^{-6}$	mg/l
			terrestrial ecosystem	equil. part.		mg/kg
			human	ADI/TDI	0.0005	mg/(kg·d)
61	fentinhydroxide	76-87-9	aquatic ecosystem	MTR	$5.0\cdot10^{-6}$	mg/l
			terrestrial ecosystem	equil. part.		mg/kg
			human	ADI/TDI	0.0005	mg/(kg·d)
62	formaldehyde	50-00-0	aquatic ecosystem	MTR	0.004	mg/l
			terrestrial ecosystem	equil. part.		mg/kg
			human	ADI/TDI	0.15	mg/(kg·d)
63	hexachlorobenzene	118-74-1	aquatic ecosystem	MTR	0.0024	mg/l
			terrestrial ecosystem	MTR (eq)	1.3	mg/kg
			human	ADI/TDI	0.0005	mg/(kg·d)

Substance			Target	Toxicity parameter		
Nr.	Name	CAS nr.		type	value	unit
64	hexachlorobutadiene	87-68-3	aquatic ecosystem	LC$_{50}$/NOEC	0.09	mg/l
			terrestrial ecosystem	equil. part.		mg/kg
			human	ADI/TDI	0.0002	mg/(kg·d)
65	hexachlorocyclohexane (γ)	58-89-9	aquatic ecosystem	MTR	0.00077	mg/l
			terrestrial ecosystem	MTR	0.005	mg/kg
			human	ADI/TDI	0.001	mg/(kg·d)
66	isodrin	465-73-6	aquatic ecosystem	—	—	—
			terrestrial ecosystem	—	—	—
			human	ADI/TDI	0.0001	mg/(kg·d)
67	lead	7439-92-1	aquatic ecosystem	MTR	0.01	mg/l
			terrestrial ecosystem	MTR	49	mg/kg
			human	ADI/TDI	0.0036	mg/(kg·d)
68	malathion	121-75-5	aquatic ecosystem	MTR	$4.3\cdot10^{-6}$	mg/l
			terrestrial ecosystem	MTR	0.04	mg/kg
			human	ADI/TDI	0.02	mg/(kg·d)
69	mercury	7430-97-6	aquatic ecosystem	MTR	$1.9\cdot10^{-6}$	mg/l
			terrestrial ecosystem	MTR	0.0033	mg/kg
			human	ADI/TDI	0.004	mg/(kg·d)
70	methylbromide	74-83-9	aquatic ecosystem	LC$_{50}$/NOEC	0.3	mg/l
			terrestrial ecosystem	equil. part.		mg/kg
			human	ADI/TDI	1	mg/(kg·d)
71	methylparathion	298-00-0	aquatic ecosystem	MTR	0.00002	mg/l
			terrestrial ecosystem	equil. part.		mg/kg
			human	ADI/TDI	0.02	mg/(kg·d)
72	monochlorobenzene	108-90-7	aquatic ecosystem	MTR	0.69	mg/l
			terrestrial ecosystem	MTR (eq)	7.6	mg/kg
			human	ADI/TDI	0.3	mg/(kg·d)
73	nickel	7440-02-0	aquatic ecosystem	MTR	0.0009	mg/l
			terrestrial ecosystem	MTR	2.6	mg/kg
			human	ADI/TDI	0.005	mg/(kg·d)
74	nitrogen dioxide	10102-44-0	aquatic ecosystem	—	—	—
			terrestrial ecosystem	—	—	—
			human	inh. route*	0.15	mg/m^3
75	parathion	56-38-2	aquatic ecosystem	MTR	0.00001	mg/l
			terrestrial ecosystem	MTR	0.005	mg/kg
			human	ADI/TDI	0.005	mg/(kg·d)

Substance			Target	Toxicity parameter		
Nr.	Name	CAS nr.		type	value	unit
76	PCB	1336-36-3	aquatic ecosystem	LC_{50}/NOEC	0.008	mg/l
			terrestrial ecosystem	equil. part.		mg/kg
			human	ADI/TDI	0.00009	mg/(kg·d)
77	pentachloroaniline	527-20-8	aquatic ecosystem	MTR	0.0002	mg/l
			terrestrial ecosystem	MTR	0.1	mg/kg
			human	—	—	—
78	pentachlorobenzene	608-93-5	aquatic ecosystem	MTR	0.0075	mg/l
			terrestrial ecosystem	MTR	0.3	mg/kg
			human	NOAEL oral	8	mg/(kg·d)
79	pentachlorophenol	87-86-5	aquatic ecosystem	MTR	0.002	mg/l
			terrestrial ecosystem	MTR	0.17	mg/kg
			human	ADI/TDI	0.03	mg/(kg·d)
80	phenol	108-95-2	aquatic ecosystem	LC_{50}/NOEC	0.009	mg/l
			terrestrial ecosystem	equil. part.		mg/kg
			human	ADI/TDI	0.06	mg/(kg·d)
81	phthalic anhydride	85-44-9	aquatic ecosystem	—	—	—
			terrestrial ecosystem	—	—	—
			human	NOAEL oral	375	mg/(kg·d)
82	propyleneoxide	75-56-9	aquatic ecosystem	LC_{50}	89	mg/l
			terrestrial ecosystem	equil. part.		mg/kg
			human	NEL man oral	0.01929	mg/(kg·d)
83	simazine	122-34-9	aquatic ecosystem	MTR	0.0001	mg/l
			terrestrial ecosystem	equil. part.		mg/(kg·d)
			human	ADI/TDI	0.002	mg/(kg·d)
84	sulphur dioxide	7446-09-5	aquatic ecosystem	—	—	—
			terrestrial ecosystem	—	—	—
			human	inh. route*	0.25	mg/m^3
85	tetrachloroethene	127-18-4	aquatic ecosystem	MTR	0.33	mg/l
			terrestrial ecosystem	MTR	0.16	mg/kg
			human	ADI/TDI	0.016	mg/(kg·d)
86	tetrachloromethane	56-23-5	aquatic ecosystem	MTR	1.1	mg/l
			terrestrial ecosystem	MTR (eq)	37	mg/kg
			human	ADI/TDI	0.004	mg/(kg·d)
87	toluene	108-88-3	aquatic ecosystem	MTR	0.73	mg/l
			terrestrial ecosystem	MTR	1.4	mg/kg
			human	ADI/TDI	0.43	mg/(kg·d)

Substance			Target	Toxicity parameter		
Nr.	Name	CAS nr.		type	value	unit
88	tributyltinoxide	56-35-9	aquatic ecosystem	MTR	$3.0 \cdot 10^{-6}$	mg/l
			terrestrial ecosystem	equil. part.		mg/kg
			human	ADI/TDI	0.0003	mg/(kg·d)
89	trichloroethylene	79-01-6	aquatic ecosystem	MTR	2.4	mg/l
			terrestrial ecosystem	MTR (eq)	13	mg/kg
			human	ADI/TDI	0.54	mg/(kg·d)
90	trichloromethane	67-66-3	aquatic ecosystem	MTR	0.59	mg/l
			terrestrial ecosystem	MTR	1.9	mg/kg
			human	ADI/TDI	0.03	mg/(kg·d)
91	trifluralin	1582-09-8	aquatic ecosystem	MTR	0.00019	mg/l
			terrestrial ecosystem	equil. part.		mg/kg
			human	ADI/TDI	0.0075	mg/(kg·d)
92	vanadium	7440-62-2	aquatic ecosystem	MTR	0.0035	mg/l
			terrestrial ecosystem	MTR	1.1	mg/kg
			human	ADI/TDI	0.009	mg/(kg·d)
93	vinylchloride	75-01-4	aquatic ecosystem	MTR	0.82	mg/l
			terrestrial ecosystem	MTR	14	mg/kg
			human	NEL man oral	0.00351	mg/(kg·d)
94	zinc	7440-66-6	aquatic ecosystem	MTR	0.006	mg/l
			terrestrial ecosystem	MTR	0.7	mg/kg
			human	ADI/TDI	40	mg/(kg·d)

[*] See page 57.

Appendix C

DESCRIPTION AND DISCUSSION OF EIGHT SOLUTIONS FOR THE FLUX-PULSE PROBLEM

In Chapter 4, the flux-pulse problem was defined as an incompatibility of dimensions. The inventory table of an LCA contains emission numbers in terms of mass units with an unspecified release term. It was argued that these amounts of substances can be thought of as being released instantaneously, as pulses. On the other hand, the distribution model of the USES 1.0 model for risk assessment is based on an input of emission fluxes, i.e. mass per time.

Some solutions

There are several classes of possible solutions to this problem:

- the problem can be ignored or argued to be non-existent (*a1* and *a2*);
- life cycle inventories can be changed so as to produce emission fluxes (*b1, b2* and *b2*);
- environmental multi-media models can be changed so as to accept emission pulses (*c1*, *c2* and *c3*).

The eight possible solutions will now be discussed in detail. In doing so, the following structure will be employed:

- description;
- example (all methods will be illustrated by an example calculation: an emission of 3 kg of a hypothetical chemical with a *K* of 4 $\text{hr}\cdot\text{m}^{-3}$ and a *PNEC* of 2 $\text{kg}\cdot\text{m}^{-3}$ is used.)
- advantages (apart from solving the problem);
- disadvantages;
- scores on the criteria of consistency and correctness, realm of application (whether equivalency factors can be computed, and whether the approach is applicable for all types of LCA) and psychological appeal.

POSSIBILITY A1: IGNORING THE PROBLEM

Description

A PC version of an environmental multi-media model will ask:

```
    Emission of phenol to air [kg/hr] = _
```

and, after some calculations, will give a result:

```
    Risk quotient for phenol [-] = 0.1456872
```

The computation is performed using the formula

$$R = G\times\Phi \tag{C.1}$$

where $G = K/PNEC$, and where the values of *G*, *K*, and *PNEC* remain inside the PC. The flux-pulse problem can be ignored by just entering a pulse at in response to the query for a flux.

Example

If an inventory table gives an emission of 3 kg, one can simply type a 3 when prompted for input, ignoring the dimensions, and treat the risk quotient (= 6) as the resulting impact score for that emission. The dimension of this result remains somewhat obscure; it is left undefined here.

Advantages

An advantage of this procedure is that no adaption at all is needed.

Disadvantages

A disadvantage, of course, is that a problem is "solved" by ignoring it. This means that the original inconsistency remains. This comes down to misusing the model as a black box, having one target in mind: a number should be produced. A more practical disadvantage is that the model itself must be used when making an LCA: there are no lists of equivalency factors.

Scores on the criteria

Consistency and correctness: –
Realm of application: –
Psychological appeal: –

POSSIBILITY A2: EXTENDING THE DOMAIN OF THE MODEL

Description

G values are intended to link emission fluxes to risk quotients. Nevertheless, one might apply them as equivalency factors for pulse emissions Δm (in kg) as well:

$$r \equiv G \times \Delta m \tag{C.2}$$

where r is a kind of "degenerated" risk quotient. It has the dimension of time (in hr), which was one of the reasons for giving it a symbol different from R, which was after all dimensionless.

Example

The example emission of 3 kg yields a score of 6 hr:

$$r = \frac{4\ \mathrm{hr{\cdot}m^{-3}}}{2\ \mathrm{kg{\cdot}m^{-3}}} \times 3\ \mathrm{kg} = 6\ \mathrm{hr} \tag{C.3}$$

Advantages

The advantage of this approach is that no adaptation is necessary. The equivalency factors are simply the *G*-values.

Disadvantages

On the other hand, another problem has been created, as the validity of the extension of the formula can be doubted. The meaning and properties of an extension of the original domain and of the new quantity r must be investigated before it can be claimed to be a measure of what we are looking for. That the meaning is different should be clear from the fact that whereas R may assume the "magic value" of 1, the degenerated r has no special values.

Scores on the criteria

Consistency and correctness: –
Realm of application: +
Psychological appeal: +

POSSIBILITY B1: MANIPULATING THE INVENTORY TABLE

Description

Another approach is to take the inventory table that the LCI produced, and change the item:

`Emission of 3 kg phenol to air`

into:

`Emission of 3 kg/hr phenol to air`

and do so for all items in the inventory table. Now, the numbers can be input into the multi-media model, and the result can be interpreted. Or, alternatively, the G-values for different chemicals can be used to compile a list of equivalency factors, using

$$R = G \times \Phi \tag{C.4}$$

where Φ is the manipulated inventory item.

Example

The emission of 3 kg is now converted into 3 $\text{kg}\cdot\text{hr}^{-1}$. This gives a score of 6 (without dimension):

$$R = \frac{4\ \text{hr}\cdot\text{m}^{-3}}{2\ \text{kg}\cdot\text{m}^{-3}} \times 3\ \text{kg}\cdot\text{hr}^{-1} = 6 \tag{C.5}$$

Advantages

The only advantage of this approach is that it is quite simple.

Disadvantages

A disadvantage here is that at some stage of the procedure a completely arbitrary unit is added. It is difficult to answer the question why we did not use "per second" or "per year" instead of "per hour". A more psychological disadvantage is that the computation of a risk quotient suggests that an actual risk is computed, whereas only a small part of this risk is computed. If the computed R is, say, 0.001, it may well be that the total risk is above 1.

Scores on the criteria

Consistency and correctness: −
Realm of application: +
Psychological appeal: −

POSSIBILITY B2: ADAPTING THE FUNCTIONAL UNIT

Description

One could redefine the functional unit of the LCA such that a flow is implied. For instance, the functional unit "1000 litre milk" could be changed into "1000 litre milk per year". This modification means that the inventory table now produces emission fluxes, so that they can be neatly input in the multi-media model. Or, again, a list of equivalency factors could be produced. Calculation of a score then proceeds by

$$R = G \times \Phi \tag{C.6}$$

This approach is advocated in [27].

Example

By changing the functional unit, the inventory item of 3 kg is converted into 3 $\text{kg}\cdot\text{hr}^{-1}$, again producing a score of 6 (without dimension):

$$R = \frac{4\ \text{hr}\cdot\text{m}^{-3}}{2\ \text{kg}\cdot\text{m}^{-3}} \times 3\ \text{kg}\cdot\text{hr}^{-1} = 6 \tag{C.7}$$

Advantage

An advantage relative to the previous method (*b1*) is that the adaptation is very explicit: the functional unit which is the most explicit enunciation of the subject of the study is adapted.

Disadvantage

A disadvantage is that the choice "per year" is still arbitrary. It should be emphasized that the "1000 litres" is arbitrary as well. The arbitrariness might be reduced somewhat by conforming to a "real" flux, e.g. corresponding to the production volume, or to the consumption volume. The presumed reality of this modification is misleading, however. One has to choose between the production volume, the consumption volume, the packaging production volume, etc. The problem is that there is not one "real" gauge parameter here. Another disadvantage is associated with the fact that a flux that is input in a multi-media model can be assessed in terms of a concentration, and hence in terms of a risk quotient. As only a tiny fraction of the emission flux is due to the product studied, a tiny fraction of the concentration is calculated. The functional unit will most probably not give rise to problematic risk quotients near or above 1. The suggestion of a "real" concentration could be so strong that this might easily be overlooked. As a last disadvantage, it is noted that the majority of functional units are currently chosen according to the pulse approach. These inventories would be excluded by the requirement[1].

Scores on the criteria

Consistency and correctness: +
Realm of application: −
Psychological appeal: +

POSSIBILITY B3: INTRODUCING THE TIME SPAN OF THE LIFE CYCLE

Description

An approach which is somewhere intermediate between *b1* and *b2* is one in which the total emission of a substance throughout the life cycle is not considered to be released instantaneously, but as a pulse, but to be smoothly emitted over the time span of the life cycle, i.e the period between the cradle and the grave. Denoting this time span by Δt, the calculation of the average emissions flux is simply

$$\Phi = \frac{\Delta m}{\Delta t} \tag{C.8}$$

This flux can easily be inserted in the equation of the USES 1.0 model:

$$R = G \times \Phi \tag{C.9}$$

Example

Assuming that the time span of the life cycle Δt is 10^5 hr ($\approx$ 11 yr), we find a score of

$$R = \frac{4\ \mathrm{hr{\cdot}m^{-3}}}{2\ \mathrm{kg{\cdot}m^{-3}}} \times \frac{3\ \mathrm{kg}}{10^5\ \mathrm{hr}} = 6{\cdot}10^{-5} \tag{C.10}$$

Advantage

An advantage relative to method *b2* is that the choice of time period is at least theoretically solid, and that the interpretation of Φ as the average emission flux during the life cycle is straightforward.

---

[1] It might be thought that this can easily be solved by introducing a time. However, in doing so one is actually working more along the lines of *b1* than of *b2*.

Disadvantage

Although the choice of Δt is theoretically easy, it is impossible to find this value in practice. As discussed in §4.1, the influence of cutting off capital goods or landfilling waste is so large[1] that the time period of the life cycle has no meaning in practice.

Scores on the criteria

Consistency and correctness: +

Realm of application: −

Psychological appeal: +

POSSIBILITY C1: COMPARISON WITH A REFERENCE SUBSTANCE

Description

Similar to the GWP, ODP and POCP concepts, a reference substance can be introduced. A reference substance means that the impact scores are not expressed in impact terms, but in amounts of reference substance that would yield exactly the same impact. It is assumed that the emission takes place within a time interval Δt and that the reference substance is released during the same (but still unknown) release time. Thus, it can be argued that the two Δts cancel one another out. The risk quotient of the "constructed" flux of the emission pulse is

$$R = G \times \frac{\Delta m}{\Delta t} \tag{C.11}$$

For the reference substance (denoted by primed quantities) a similar expression holds:

$$R' = G' \times \frac{\Delta m'}{\Delta t} \tag{C.12}$$

This latter expression can be transformed to yield an expression for $\Delta m'$:

$$\Delta m' = \frac{R'}{G'} \Delta t \tag{C.13}$$

Requiring that the risk R due to the emission pulse Δm is equal to the risk R' due to the reference emission pulse $\Delta m'$, i.e. putting $R = R'$, leads to the following expression:

$$\Delta m' = \frac{G}{G'} \Delta m \tag{C.14}$$

The equivalency factors are therefore now dimensionless: G/G', and the impact score is now in terms of a mass of a reference substance. This approach is followed in [29].

Example

Assuming that a reference substance is chosen with a K' of 30 hr·m^{-3} and a *PNEC* of 10 kg·m^{-3}, a score of 2 kg toxic equivalent is found:

$$\Delta m' = \frac{4\ \text{hr}\cdot\text{m}^{-3}}{2\ \text{kg}\cdot\text{m}^{-3}} \times \frac{10\ \text{kg}\cdot\text{m}^{-3}}{30\ \text{hr}\cdot\text{m}^{-3}} \times 3\ \text{kg} = 2\ \text{kg} \tag{C.15}$$

Advantage

An advantage of this approach is that a certain extent of harmonization is achieved, as global

---

[1] A very strict reasoning of the principles of LCA would tell us that the life cycle of every product is infinitely long. This makes the expression $\Delta m/\Delta t$ undefined, in which case the pulse option (Δm) is again the only alternative basis for an assessment.

warming, ozone depletion and photochemical oxidant formation are already expressed in terms of reference substances. Another advantage is that it is attempted to derive an expression, instead of just postulating it, as in method *a2*.

Disadvantage

A disadvantage is that the expression in terms of a reference substance suggests that it is possible to express an amount of, say, cadmium in terms of an amount of, say, phenol, with the same amount of impact. It should be emphasized that any procedure which allows aggregation of emissions of cadmium and phenol implies this equivalency (see also Chapter 7); in fact the etymology of the term "equivalency factor" goes back to this. The psychological factor, apparently at stake here, must not be forgotten, though.

Scores on the criteria

Consistency and correctness: +

Realm of application: +

Psychological appeal: –

POSSIBILITY C2: USING RESIDENCE TIMES

Description

The residence time τ of a chemical in a compartment is defined as the ratio of the amount present in steady state m and the flux into that compartment Φ:

$$\tau \equiv \frac{m}{\Phi} \tag{C.16}$$

Because the amount present m is related to the concentration C by the volume of the compartment via

$$m = PEC \times V \tag{C.17}$$

an expression for the residence time is easily found:

$$\tau = K \times V \tag{C.18}$$

The residence time can be used to calculate an alternative risk quotient Q:

$$Q = \frac{\tau}{NEC} \times \Phi \tag{C.19}$$

The dimension of Q is that of a volume (m^3). It can now be argued that the residence time is a fundamental characteristic of a chemical in a certain environment, and that it may consequently be used for pulses as well. In that case an alternative but quite similar expression is used:

$$q = \frac{\tau}{NEC} \times \Delta m \tag{C.20}$$

where q is expressed in $\mathrm{hr \cdot m^3}$. In fact, this is a variant of possibility *a2*: a certain formula is derived and it is applied beyond its original domain. The equivalency factors are given by $\tau / PNEC$.

Example

An additional assumption concerning the volume of the compartment must be made: 10 m^3. This gives a score of :

$$R = \frac{4\ \mathrm{hr \cdot m^{-3}}}{2\ \mathrm{kg \cdot m^{-3}}} \times 3\ \mathrm{kg} = 6\ \mathrm{hr} \tag{C.21}$$

Advantages

The advantages and disadvantages of this method are clearly the same as for method *a2*, although some may feel that this represents a proof of method *a2*. So: no adaptation is necessary, and the equivalency factors are simply the *G*-values.

Disadvantages

Again, the validity of the extension of the formula may be doubted. The meaning and properties of an extension of the original domain must be investigated before it can be claimed to be a measure of what we are looking for.

Scores on the criteria

Consistency and correctness: –
Realm of application: +
Psychological appeal: +

POSSIBILITY C3: DYNAMIZATION OF THE MULTI-MEDIA MODEL

Description

Many multi-media models are conceived as steady-state models, expressing a relationship between continuous flux and steady-state concentration. There are also models that can deal with emission pulses. These models are much more complicated, because the steady-state concentration which is no longer calculated, but rather the entire time pattern in the concentration variation is modelled:

$$PEC(t) = f(t)\times\Delta m \tag{C.22}$$

where $f(t)$ is a function that depends in a non-linear way on t. From this the time-dependency of the risk quotient can be calculated:

$$R(t) = \frac{PEC(t)}{PNEC} = \frac{f(t)}{PNEC}\times\Delta m \tag{C.23}$$

These models do not give a single answer (the steady-state concentration or risk) but give a continuum of answers. A decision which of these answers must be presented as "the impact score" is needed. One obvious choice here is the time-integrated hazard quotient increase:

$$r \equiv \int_0^\infty \frac{PEC(t)}{PNEC}\mathrm{d}t = \frac{1}{PNEC}\int_0^\infty PEC(t)\,\mathrm{d}t \tag{C.24}$$

Other choices may be argued, however. This approach has been elaborated in [54,33] and more extensively in [45].

Example

As a basis for the calculation, a first-order differential equation has been used; it turns out that in this case $r = K\times\Delta m/PNEC$; see [54]. This leads to a score of 6 hr.

Advantage

An advantage of this approach is that pulse emissions are assessed properly as pulse emissions.

Disadvantage

The fact that there are several choices for r immediately points out the disadvantage of this approach: by turning to another model many fundamental questions emerge, and the mathematics becomes quite complicated. It is not clear to what extent equivalency factors can be compiled. Another problem is that this procedure allows one to characterize only pulse emissions, not fluxes. This would suggest that different procedures for impact assessment are required, depending on the dimension of the functional unit.

Scores on the criteria

Consistency and correctness: +

Realm of application: −

Psychological appeal: −

Discussion

The flux-pulse problem presents itself as a real problem: at least eight solutions are conceivable, and each solution has its advantages and disadvantages (see Table C.1).

Table C.1: Summary of scores on three criteria for the eight solutions for the flux-pulse problem.

method	consistency and correctness	realm of application	psychological appeal
a1	−	−	−
a2	−	+	+
b1	−	+	−
b2	+	−	−
b3	+	−	+
c1	+	+	−
c2	−	+	+
c3	+	−	−

A challenging question is to what extent the solutions give different results; see [54] for a discussion on methods *b2*, *c1* and *c3*. The present discussion is devoted to an investigation of this issue for all eight possibilities described here. It should be kept in mind that it is impossible to attribute an absolute meaning to the impact scores of LCA. Only relative interpretations make sense: in product comparisons, in comparing the impacts in different life cycle stages of one product, or in comparing the contributions from different pollutants in one life cycle. A proposed test for this is the following. Consider the emission of two chemicals A and B; Table C.2 summarizes the data and results.

It is clear that most of the possibilities give different results. Even if the numbers are the same, the unit is different. The remarkable thing is, however, that the ratio between the score for A and

Table C.2: Numerical example of two hypothetical chemicals and their scores according to the different solutions to the flux-pulse problem.

Quantity	Chemical A	Chemical B	Unit
Δm	3	20	kg
K	4	30	$\mathrm{hr \cdot m^{-3}}$
PNEC	2	10	$\mathrm{kg \cdot m^{-3}}$
V	10	20	$\mathrm{m^3}$
score according to *a1*	6	60	ill-defined[*]
score according to *a2*	6	60	hr
score according to *b1*	6	60	—
score according to *b2*	6	60	—
score according to *b3*[†]	$6 \cdot 10^{-5}$	$60 \cdot 10^{-5}$	—
score according to *c1*[‡]	2	20	kg B-equivalent
score according to *c2*	120	1200	$\mathrm{hr \cdot m^3}$
score according to *c3*[§]	6	60	hr

[*] The characteristic of solution *a1* is that the incompatibility of units is ignored. This makes the resulting unit ill-defined.

[†] The life spans are set to the same value (10^5 hr) for A and B.

[‡] Substance B is taken as reference substance.

[§] As a basis for the calculation, a first-order differential equation has been used; it turns out that in this case $r = K \times \Delta m / \mathrm{PNEC}$.

the score for B is the same for all[1] possibilities. And, since LCA is only concerned with relative scores, all the possibilities described here are equally good with respect to their result. So, the only criteria which remain are arguments of applicability on the one hand and of conceivability, appeal and harmonization on the other. With respect to these arguments, it can be said that *a1* and *b1* have a definite disadvantage in being untidy, that *b2*, *b3* and *c3* have the disadvantage of being inapplicable to all LCAs, that *a2* and *c2* are more a conjecture than a rigid method, and that *c1* appears to have psychological disadvantages [27].

The consistency and correctness of the approach is a serious point. However, as it can be shown that a consistent and correct approach (*c3*) gives identical answers to the other approaches, the consistency and correctness of these approaches may no longer be doubted. Next is the realm of application: we postulate here that this is of prime importance. The method should be applicable to both pulse-oriented and flux-oriented LCAs, and equivalency factors should be developed to

---

[1] It should be emphasized once more that the equivalency of possibility *c3* has only been verified for a one-compartment system. It can, however, be proven that the equivalency is valid for a general multi-linear multi-compartment system [45]. Furthermore, the ratio according to possibility *b3* is based on an equal time span of the life cycles. As stated above, this assumption is very difficult to verify.

avoid using the full model for every case study.

It is concluded here that the wide applicability and the effect of harmonization with other impact categories (such as global warming where the GWP is a measure on the basis of a comparison with a reference substance) of method *c1* makes this the best approach. This option is a good way to clearly demonstrate the equivalency principle explained in §7.1. Should one consider the psychological barriers unsurmountable, solutions *a2* and *c2* provide good alternatives.

Appendix D

LIST OF ABBREVIATIONS

ADI	acceptable daily intake
AETP	aquatic ecotoxicity potential
CML	*Centre of Environmental Science, Leiden University*
EUSES	*European Union System for the Evaluation of Substances*
HTP	human toxicity potential
LC_{50}	lethal concentration for 50% of the species
LCA	life cycle assessment
MAC	maximum accepted concentration
MOS	margin of safety
MTR	maximum tolerable risk
NEL	no-effect level
NOAEL	no-observed-adverse-effect level
NOEC	no-observed-effect concentration
NOH	*National Reuse of Waste Research Programme*
PEC	predicted environmental concentration
PNEC	predicted no-effect concentration
RA	risk assessment
RIVM	*National Institute of Public Health and Environmental Protection*
S(W)TP	sewage (wastewater) treatment plant
TDI	tolerable daily intake
TETP	terrestrial ecotoxicity potential
USES	*Uniform System for the Evaluation of Substances*
VROM	*Ministry of Housing, Spatial Planning and the Environment*

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