Regional LCA in a global perspective

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Citation

Wegener Sleeswijk, A. (2010, September 2). *Regional LCA in a global perspective*. Uitgeverij BOX Press, Oisterwijk. Retrieved from https://hdl.handle.net/1887/15921

REGIONAL LCA IN A GLOBAL PERSPECTIVE

Colophon

Regional LCA in a global perspective
A basis for spatially differentiated environmental life cycle assessment

PhD thesis Leiden University, The Netherlands

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This work has been made possible by the financial support of Unilever.

ISBN 978-90-8891-187-3

Cover: world map ‘political world’ (Central Intelligence Agency, World Factbook, online version 2010); ‘Earth in a Box’ (iStockphoto); T-O map from the Etymologiae of Isidorus, 1472 (Wikimedia Commons)
Cover design: Anneke Wegener Sleeswijk/ Proefschriftmaken.nl||Printyourthesis.com
Printed by: Proefschriftmaken.nl||Printyourthesis.com
Published by: Uitgeverij BOX Press, Oisterwijk, The Netherlands

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Proefschrift

ter verkrijging van
de graad van Doctor aan de Universiteit Leiden
op gezag van de Rector Magnificus prof. mr. P.F. van der Heijden,
volgens besluit van het College voor Promoties
te verdedigen op donderdag 2 september 2010
klokke 16.15 uur

door

Anneke Wegener Sleeswijk
geboren te Naarden in 1960

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Contents

Preface

When I started writing this PhD thesis I had already been working on LCA for a number of years. I contributed to the development of LCA methodology as well as to a number of LCA case studies. During these years, I got well acquainted with this tool, both with respect to its strengths and with respect to what I considered its limitations.

The strengths of LCA, as I saw them, were in its 'looking behind the obvious' with respect to environmental impacts of products over their entire life cycles, in accounting for the a large spectrum of environmental impacts, in describing the connection between environmental interventions on the one hand and products on the other in an exact manner, in estimating the quantitative relationships between environmental interventions and their impacts, and in preventing dilution from being considered as a solution for pollution. The quantitative aspects of LCA intrigued me: how could we get it right? And what is 'right'?

The limitations that struck me were the points at which I felt we were not yet right in our quantification. These points mainly concerned LCA toxicity assessment: our lack of a measure for 'actual' toxic impacts (beside the potential ones), the fact that metal emissions heavily dominated the toxicity impact scores in LCA, while experts stated this corresponded in no way to their relative environmental harmfulness, and the fact that the assessment of environmental impacts did not account for regional differences, even though the range of processes of a single product life cycle might span the world. These were the three aspects that I felt I should work on to get them right, or at least more right. I was lucky to get the freedom to address all these issues – and one more – in a PhD-project on environmental fate modelling in the context of LCA toxicity assessment.

In 2006, I was involved in a project on LCA normalisation, a subject which I had only had superficial attention for, despite its quantitative character. While working on this project, I discovered an interesting methodological issue, and felt we should adapt our methodology and introduce a new principle, concerning the definition of the reference emissions. Again, I was lucky that there was support for my ideas to include this principle in our normalisation study, and to include the normalisation study in my PhD thesis. With this, I broadened the scope of my thesis from mere LCA toxicity characterisation to life cycle impact assessment as such, be it that the overall focus is still on toxicity assessment. The global character links the different aspects together.

LCA toxicity assessment cannot replace human and environmental risk assessment, not even in a spatially differentiated form. Risk assessment tools are designed for the assessment of ambient concentration dependent effects, which are not part of LCA. With this, risk assessment tools can help assess whether processes in the product life cycle meet environmental standards, and whether they can be considered as environmentally responsible. What LCA toxicity assessment can add is an answer to the question which product alternative is optimal with respect to overall environmental burdening. Spatial differentiation can help to model this as well as possible.

Synopsis

The assessment of the toxic effects of environmental pollution is the key subject of *risk assessment of chemicals (RA)* or *human and environmental risk assessment (HRA and ERA)*, here indicated together as *HERA*. Although basic HERA models for multimedia transport, human exposure and toxic potential form a useful basis for LCIA toxicity modelling, some LCA-specific problems remain to be solved. One of the most criticised aspects of LCA toxicity impact assessment is the concept of *potential impacts* in LCA environmental profiles, as opposed to the *actual impacts* or risks that are estimated with HERA. The contrast between the nature of toxic impacts in LCA and HERA respectively has also been formulated as *general prevention* versus *risk minimisation* and as *less is better* versus *only above threshold*. In this thesis, the possibilities and limitations with respect to the integration of LCA and HERA are explored. It is demonstrated that the functional unit – which is identified as the only fundamental difference between LCA and HERA – makes it impossible to reach a full integration between LCA and HERA, or, more specifically, to assess individual risks with the LCA method. Yet, a method is proposed for the assessment of *risk contributions* of the product life cycle within the context of LCA. Obviously, spatial differentiation of fate and exposure modelling is a condition for this method. Meanwhile, a worldwide coverage of all environmental modelling aspects is a prerequisite for LCA, since the range of product life cycles stretches arbitrarily over the entire world. GLOBOX is a so-called 'multimedia box model' which unites both principles: it is a global model which is spatially differentiated at the level of separate countries, territories*, seas and oceans.

The core of this thesis is the GLOBOX model: a combination of a multimedia model, a human exposure model and an effect model that has been designed specifically for the calculation of LCA characterisation factors for human-toxic and ecotoxic chemicals. GLOBOX differs from existing models by its high level of spatial differentiation, along with a global coverage.

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* These include overseas territories (like Réunion) and uninhabited areas (like Antarctica).

This thesis has five goals:

1. Contributing to an optimal reliability of LCA toxicity assessment by creating a flexible, reasonably detailed system for spatial differentiation of LCA toxicity assessment on a global scale.
2. Enhancing the accuracy of LCA modelling with respect to the behaviour of metals in the environment.
3. The introduction of a method for the assessment of contributions of the product life cycle to toxic risks or *actual impacts*, along with the conventional assessment of *potential impacts*.
4. Analysing the influence of spatial differentiation on LCA characterisation factors for human toxicity and ecotoxity by calculations on a test substance.
5. Creating an updated, global LCA normalisation sytem.

Contrary to existing LCA multimedia fate and exposure models, that often implictly derive their parameters from environmental and exposure data that refer to Europe, the United States or Japan, the GLOBOX model also offers the possibility to make an explicit choice for emissions that occur in areas outside these regions.

Besides the formulation and adaptation of model equations, the collection and construction of background parameters has also played a central role in the research on which this thesis has been based. The GLOBOX model and the underlying parameters (the GLOBACK set of background data) can be found on http://cml.leiden.edu/software/software-globox.html and on http://www.globright.nl. Besides an executable version of the model itself, the following parameter sets are published on these websites:

- GLOBACK 2.0, parts 1 and 2
- supplement to part 1 of GLOBACK 2.0, for the collected subregions of the United States and Canada
- normalisation data

Part 1 of GLOBACK 2.0 contains all spatially differentiated environmental and exposure parameters for the GLOBOX model, including the parameters that determine the spatially differentiated hydrological cycle, and estimates of the food consumption patterns in the individual countries. Part 2 contains the parameters for the air and water flows between the different regions. For a further subdivision of two large countries – the United States and Canada – the GLOBACK part 1 parameters have already been collected as well. After supplementation with the part 2 parameters, these regions can simply be introduced into the GLOBOX model. The normalisation data form a collection of estimates of the emissions to and extractions from the environment for as many chemicals as possible on the global and the European scale, caused by the economic activities in the year 2000. Estimates of different forms of land use have been added as well. Together, these parameter sets form a basis that can be used not only for the GLOBOX model and for LCA normalisation, but also for other environmental models and modelling calculations.

This thesis consists of seven chapters. The chapters 1 and 7 are respectively an introduction and a general discussion on the document as a whole The chapters 2, 3, 5, and 6 have appeared as reviewed papers in international journals, and chapter 4 has appeared as a reviewed book chapter. The chapters 2 and 3 form a theoretical basis. The chapters 4, 5 and 6 together form a practical guide for LCA impact assessment of toxic chemicals, and for LCA normalisation of impact scores for all LCA impact categories. Chapter 5 has been implemented as a software model (GLOBOX), and can as such also be used outside the context of LCA.

Chapter 2: Including sensitivity and threshold information in LCA
In chapter 2, LCA is being considered from two different viewpoints: *general prevention* and *risk minimisation*. The general prevention principle is based on the conviction that environmental pollution is always undesirable an that striving towards a minimisation of pollution is therefore important as such. In some literature, this approach has also been indicated with the term *less is better*. The starting point of the risk minimisation principle is the conviction that minimisation of demonstrable risks should take a central place in the abatement of environmental pollution. Since it is often supposed that many toxic chemicals will only cause effects in concentrations above a certain threshold, this approach has also been called the *only above threshold* approach. As a general trend, the LCA assessment methods incorporated in LCA are assumed to be based on the general prevention principle, while the HERA-related methods are supposed to use the risk minimisation principle as a basis.

The fact that LCA results cannot be related to environmental risks has sometimes been used by critics to dispute the reliability of LCA as such. In this chapter, it is demonstrated that both principles should not necessarily be opposed to each other, because they can very well be united. Within LCA, it is possible to express both principles in combination with each other. To this end, two new variables should be introduced in LCA toxicity modelling: a *sensitivity factor* and a *threshold factor*. Because these variables are region-specific, spatial differentiation is a necessary condition for this approach. The sensitivity factor could indicate to which extent ecosystems in an area are sensitive to a certain chemical, while the threshold factor should be a measure for the fraction of the area where the *no effect level* is already being surpassed. Although it is inherently impossible to calculate risks with LCA, this new approach would render it possible to calculate the contribution of a product to toxic risks in general. For each impact category a two-fold *category indicator result* could be calculated: one according to the traditional method and one on the basis of the new method in the context of risk minimisation. This makes it possible to bring LCA and HERA nearer to each other, meanwhile preserving the characteristic features of LCA.

Chapter 3: LCA versus HERA
In chapter 3, LCA and HERA are compared. In the exisiting literature, some authors regard these two modelling approaches as more or less the same, while others consider them to be completely different. In order to clarify this issue, three levels of comparison are being distinguished.

Level 1 represents the basic equations that describe the environmental behaviour of chemicals and dose-response relationships. With respect to these equations, few differences exist: basically, both tools account for the same environmental processes, make use of the same mathematical equations to relate emissions to environmental concentrations, human intake and effect, and use the same chemical and environmental data.

Level 2 represents the overall model structure of both tools. In relation to HERA, LCA is identified to be characterised by ten specific characteristics: its life cycle perspective, the fact that products instead of substances are the objects of analysis, the large number of economic processes involved, the large number of chemicals and impact categories involved, the broad range of environmental impacts covered by the assessment, the use of characterisation factors, the summation of effects of different chemicals to one overall ‘score’, the independence of time and location, the assessment of separate emission ‘pulses’ instead of continuous fluxes, the use of a functional unit as a basis of the assessment and the relative character of the assessment. Although the modelling structures of LCA and HERA are thus very different, most of these differences are not fundamental in character. A crucial exception is formed, however, by the functional unit. In LCA, the functional unit is responsible for the fact that process emissions are not being assessed in their full extent, but exclusively with respect to their share in a certain amount of a certain ‘functional unit’ of product or service. In contrast, the assessment of processes in their full extent forms the central concept of HERA. It is this last approach that makes it possible to calculate changes in environmental concentrations in a certain area, and subsequently to test them against the prevailing standards.

Level 3 is the level of application, which is directly linked to goals and outputs. The central goal of LCA is giving a quantitative assessment of the environmental impacts of products, for the sake of product improvement or the choice of the least environmentally harmful product alternative. The area of application of HERA is different: HERA is most often applied for keeping toxic risks of chemicals in a certain region below the values of prevailing environmental standards. Here, LCA and HERA are complementary.

Despite the differences described, it is advocated that LCA and HERA should be brought together in a common software model that is designed to generate both types of outcomes. Such a combined model could guarantee an optimal harmonisation of LCA and HERA, especially with respect to the common underlying modelling structures and parameters. Moreover, this effort would result in a broad instrument which could be used by companies for testing their environmental performance in different areas, as a basis for well-considered choices with respect to their environmental management.

Chapter 4: metals in multimedia models

Chapter 4 is dedicated to the inclusion of metals in multimedia modelling. Originally, multimedia models have been designed for modelling the environmental behaviour of organic chemicals. For metals, these models cannot be applied as such because a number of the given model equations do not apply to metals and because some of the substance properties that serve as a modelling basis are not defined for metals. Some authors have, however proposed solutions for these problems by setting a number of parameters to artificial values and by defining ways in which certain equations can be circumvented. By use of these solutions, LCA characterisation factors have been developed for metals in the past. In practice, however, these characterisation factors turned out to be orders of magnitude higher than the characterisation factors for almost all organic chemicals, particularly due to the fact that metals are non-degradable. As a consequence, the reliability of these factors was strongly questioned. In this chapter, it is hypothised that existing characterisation factors for metals are indeed too high, and that this is caused by the fact that a number of metal specific processes, that may play a key role, are either not included in multimedia modes or suffer from shortcomings that especially affect metals. The most important processes are probably speciation and sedimentation in marine environments. The term speciation indicates the fact that metals occur in the environment in different chemical forms that are captured in a dynamic equilibrium. This implies that metals that are emitted to the environment in a certain chemical form will not necessarily remain in this same form. This is important in the context of impact assessment because different forms can largely differ with respect to their biological availability. In this model, it has been presumed that for metals, emitted in inorganic forms, only the fraction that appears as free ions in the environment is biologically available (and thus harmful). An exception is made for metallic mercury and methylmercury, both very harmful, the first especially in its gaseous form and the latter being a well-known environmental conversion product of inorganic mercury species.

For each metal, the free ion fraction in seawater should be introduced individually. For mercury, a separate approach has been designed, because not only the free ionic form, but also the organic and the metallic form are very harmful for human and ecosystem health. Besides speciation, also sedimentation has been subjected to a closer analysis. For a number of well-known metals, the calculation of sedimentation velocities in the upper layer of the ocean has been replaced by measured values in a preliminary version of the GLOBOX model. Although some of these values appear to deviate largely from their modelled equivalents, the most important addition is probably the modelling of two separate oceanic layers: an upper mixed layer, that is considered to be part of the environmental system, and a deeper layer that is not. By distinguishing this deeper layer separately, a sink has been created, which strongly shortens the modelled residence time of metals in the environment. By the introduction of these improvements, the gap between the characterisation factors for organics on the one hand and metals on the other has disappeared, and the toxic effects of metals can be assessed in a more credible way in LCA.

Chapter 5: The GLOBOX model for fate, intake and toxic effect assessment
Chapter 5 forms the core of this thesis. In this chapter, the GLOBOX model is being discussed. GLOBOX is a model for the calculation of spatially differentiated LCA characterisation factor for toxicity. The model distinguishes itself from other models in this field by a strong spatial differentiation, a global coverage and the possibility to calculate the contributions of a product to actual effects or risks, in addition to the more common potential impacts. The model as a whole consists of three submodels or modules: a multimedia fate module, a human intake module and an effect module. The multimedia fate module and the intake module are based on the European EUSES model (version 2.0), which has been designed for the assessment of risks, caused by emissions of organics to the European environment. The adaptations to the multimedia module and the exposure module of EUSES 2.0 largely concern the range of the model and spatial differentiation. Because the product life cycle can stretch arbitrarily over the world, the GLOBOX model has a global coverage. The model is spatially differentiated at the level of countries/territories and seas/oceans. This level of spatial differentiation has been chosen for two reasons: first, the environmental and exposure parameters that the model is based on are strongly location-dependent, and second, the easiest way to locate processes within the life cycle is on a national basis. A total number of 289 regions are distinguished: 239 countries/territories and 50 seas/oceans. Every region is subdivided into a number of environmental compartments, among which air, rivers, fresh and salt lakes and a number of soil and sediment compartments for countries and territories, and air, seawater and sea sediment for seas and oceans. Besides transport between air, water and soil compartments, transport also takes place between equal compartments of different regions, above all by wind, river and sea currents. Transport also exists between rivers and freshwater lakes, and from rivers to seas and oceans. The hydrological cycle – an existing, worldwide water balance – has been regionally differentiated for and integrated into the GLOBOX model, including flows between different seas and oceans. Besides waterflow-related parameters, the regionally differentiated environmental parameters include geographic parameters (*e.g.,* the relative surface areas of fresh and salt lakes, different soil types and land ice in each region), geophysical parameters (*e.g.,* average lake depths), climatologic parameters (*e.g.,* environmental

temperature, wind speed, rainfall and frost periods) and intermedia transfer parameters (for region-dependent multimedia transport).

Many parameters have been collected from literature or calculated from literature data. Where parameters were lacking for certain regions, they were estimated from equivalent parameters for other regions. The parameters that refer to the hydrological cycle have been adapted in such a way that it resulted in a closed water cycle that was in optimal accordance with the overall hydrological cycle. A number of different parameters and equations have been added to the original EUSES multimedia transport module, in particular for three purposes: adding the possibility to introduce metals – besides organics – into the calculations, making a distinction between freshwater lakes, salt lakes and rivers and accounting for temporary or permanent freezing of soil-, ground-, and surface water in cold regions.

The exposure module is spatially differentiated as well. For every country or territory, an estimate has been made of the local food consumption pattern and of the origin and quality of drinking water. Likewise, the average body weight and the share of the population aged below 15 has been estimated and introduced into the model equations.

All spatially differentiated parameters have been collected in a set of two spreadsheets. Part 1 of GLOBACK 2.0 contains all multimedia fate and exposure parameters except air and water flows between the different regions, which are presented in part 2 of this parameter set. The model calculations in the multimedia module eventually result in a system of approximately 3000 equations with the same number of unknown variables, that represent the global multimedia transport and the degradation in each of the 3000 compartments. In the GLOBOX model, these equations are solved simultaneously by matrix inversion. The outcomes consist of the time- and space-integrated concentrations in each of the compartments that result from a standard amount of a chemical that has been emitted to one of the 3000 compartments.

For the calculation of ecotoxicity characterisation factors, the integrated concentrations, that have been caluclated with the multimedia module, are multiplied by the corresponding effect factors, that are the output of the effect module. This results in two characterisation factors: one according to the general prevention principle and one according to the risk minimisation principle. The effect factors referring to the general prevention principle consist of a measure for toxicity only (*e.g.,* the EC_{50}), and will generally be location-independent. The effect factors according to the risk minimisation principle are obtained by multiplication of this same toxicity measure with two supplemental factors: the corresponding sensitivity factor and the corresponding threshold factor, respectively.

For the calculation of human toxicity characterisation factors, the procedure is somewhat more complicated: for this purpose, the integrated concentration has to be multiplied by the intake factor as well. The intake factor indicates the relationship between the concentration in each compartment en the human intake from this compartment by the inhalation of air and the consumption of food and drinking water.

For the implementation of an LCA case study, every emission is multiplied by the corresponding characterisation factors. For every impact category this delivers 3000 partial category indicator results for each emission: one for each compartment. These partial category indicator results can subsequently be summed for all chemicals together to deliver one (total) category indicator result for each impact category, representing the contribution of the product life cycle to the type of toxic impact concerned on a global level. Although spatial differentiation causes a strong enlargement of the number of characterisation factors, the number of eventual category indicator results remains the same. The GLOBOX user should only enter the magnitude of the emissions to the different compartments in each region, together with a limited number of substance properties, to end up with a spatially differentiated assessment of the corresponding toxic impacts of the product life cycle on a global scale, for every toxicity-related impact category.

The model has been tested with nitrobenzene as a test chemical, for emissions to all countries in the world. Spatially differentiated characterisation factors turn out to show wide ranges of variation between countries, especially for releases to inland water and soil compartments. Geographic position, distribution of lakes and rivers and variations in environmental temperature and rain rate are decisive parameters for a number of different characterisation factors. Additionally, population density and dietary intake play a crucial role in the variation of characterisation factors for human toxicity. The countries that show substantial deviations from average values of the characterisation factors represent a significant part of global GDP. It is concluded that spatial differentiation between countries is an important step forward with respect to the improvement of LCA toxicity characterisation.

Chapter 6: LCA normalisation

Chapter 6 concludes with the last, optional step within LCA impact assessment: normalisation. By normalisation, the LCA category indicator results are transformed into relative contributions, a step which assigns a meaning to these previously abstract numbers. Each category indicator result is divided by the category indicator result of the economic system as a whole in a certain reference area and a certain reference year. This can be done on different scales, *e.g.,* on a global scale or on the scale of a certain continent or a certain country. Because a product life cycle will generally span a fairly large geographic range, the scale should preferably not be chosen too small. Normalisation on a global scale is the most natural choice, but when category indicator results have to be evaluated in the context of certain policy goals, the scale is often chosen as to match the policy concerned. In this document, emissions have been collected on two scales: first the global scale, and second the scale of the European Union in 2006, supplemented with Switzerland, Norway and Iceland – the 'EU25+3'. The year 2000 has been chosen as a reference year.

A feature that distinguishes this normalisation study from existing normalisation studies is the fact that not emissions that *took place in* the reference year, but emissions that were *caused by* the economic activities in this year have been used as a starting point for this study. This implies that in this approach, the delay between production and emission is explicitly accounted for, *e.g.,* in the case of CFCs in refrigerators. With this, the normalisation approach has been brought into line with the approach that is commonly used in LCA case studies, as might be expected from a true reference.

Contrary to the preceding chapters, chapter 6 refers not solely to the assessment of toxic substances, but to the entire spectrum of impact categories. The main goal of this normalisation study was the collection of all environmental interventions – that is: the emission data of all substances that are introduced into the environment by mankind, data on the main resource extractions and land use data – on a global scale as well as on the scale of the EU25+3. If emission or extraction data for an important chemical were not available on the demanded level, extra- and interpolation methods were used. In total, data could be collected for 860 environmental intervention types (that is, types of emission, resource depletion and land use together). Only 48 intervention types turned out to be together responsible for 75 percent of all category indicator results for the total of fifteen impact categories considered. All non-toxicity related, emission dependent impacts turned out to be fully dominated by the bulk emissions of only 10 substances or substance groups: carbon dioxide, methane, sulphur dioxide, nitrogen oxides, ammonia, fine dust, non-methane volatile organic chemicals (NMVOCs), and (H)CFC emissions to air and emissions of nitrogen and phosphorous compounds to freshwater. For the toxicity-related emissions (pesticides, organics, metal compounds and some specific inorganics), the availability of information was still very limited, leading to large uncertainty in the corresponding normalisation factors. A better registration of toxic emission seems to be very important, primarily for keeping the environmental impacts of the corresponding substances under control, but also for LCA.

Although this document is meant in the first place as a reference for impact assessment in LCA, it can meanwhile be considered as an LCA study by itself: an analysis that identifies the most important environmental effects of the economic system as a whole. As such, the results of this study emphasise the fact that efficient measures to combat bulk emissions could form an important step forward for the European and global environmental policy.

Conclusion

Although LCA and HERA are complementary tools, the accuracy of LCA can largely be improved by the implementation of a number of elements that are characteristic of human and environmental risk assessment: regional differentiation, and the related distinction between above- and below threshold impacts. Since the range of product life cycles stretches arbitrarily over the entire world, this requires a model with a global range. The GLOBOX model fulfils these conditions. Moreover, the model is provided with a large parameter set, GLOBACK, which is added as a separate module that can also be used as a basis for other models. This parameter set has already been supplemented with a set of parameters for subregions within the United States and Canada. For further completion of the impact assessment, a normalisation model has been added as well. With this, the parameter set of global environmental and exposure parameters has been extended to cover emission and extraction data as well. With the GLOBOX model, specific characterisation factors for toxic chemicals can be calculated for every country, territory or continent and every sea or ocean in the world. Emissions that add to actual impacts or risks are explicitly recognisable in the environmental profile, as part of the potential impacts that constitute conventional LCA practice. With this, the GLOBOX model can add to the usefulness of LCA on a global scale, and to the struggle against environmental pollution, starting with the emissions that cause the highest risks.

1

General introduction: this thesis in the context of the state-of-the-art

1.1 Introduction

One of the most striking features of life cycle impact assessment (LCIA) is its broadness, not only in the spatial sense – in which it should be representative for the world as a whole – but also in the sense of the range of the environmental impact categories to be covered – which aims at giving a complete quantitative representation of anthropogenic influence on the environment. It is not surprising that the pursuit of broadness could not always be combined with profundity in the early days of LCIA development during the nineties of the former century. Now that the foundations of LCIA have been well established, the next mission is the optimisation of its composing parts: the assessment with respect to the individual impact categories. Scientific fields that concern the assessment of singular impact categories can offer a basis for these attempts, but the underlying methods can seldom be copied without modification – largely because of the specific demands that are posed by LCA. Moreover, not all environmental impact categories are equally fit for inclusion in the LCA methodological framework (Udo de Haes, 2006). The toxicity-related impact categories are probably among the most challenging ones These impact categories distinguish themselves from all other LCA impact categories by the fact that so many substances and substance groups are involved, each with their own mechanism with respect to the way in which they interfere with the functioning of organisms. Multimedia transport, multi-pathway exposure and non-linearities in the dose-response relationships, combined with the requirement of a global range of the assessment method, further add to the complexity of toxicity impact assessment.

Within the context of life cycle impact assessment, the design of characterisation factors for the toxicity-related impact categories is probably one of the most complex issues. This complexity is caused by the combination of the large number of chemicals concerned, their diversity in structure and working mechanism, the large influence of local environmental features on the distribution characteristics, the multi-pathway exposure of humans and the lack of a ready-to-use factors from related scientific disciplines. In general, the more advanced LCA characterisation factors for human toxicity are composed of three parts (Heijungs & Wegener Sleeswijk, 1999):

1. The *fate factor*, representing multimedia distribution as well as longitudinal environmental transport, degradation, immobilisation, and outflows to places that are considered to exist outside the environmental system.
2. The *intake factor*, concerning the multimedia human exposure characteristics.
3. The *effect factor*, indicating the toxicity of the chemical under study for humans and for the ecosystems concerned.

In ecotoxicity models, single medium exposure is usually assumed, which implies that the combination of a fate factor and an effect factor is sufficient for the calculation of the ecotoxicity characterisation factor. Fate factors were not yet included in the first characterisation factors for toxicity related impact categories (*e.g.,* Heijungs *et al.*, 1992), but have been introduced in most of the more recent models to enhance the accuracy of the assessment. The minimum requirement for fate modelling consists of a quantitative degradation measure. Most LCA fate models also contain environmental distribution and/or longitudinal transport measures. Multimedia environmental models as introduced by Mackay (1991), in which environmental compartments are assumed to be homogeneously mixed, are often used as a basis. This type of models is also popular in the field of *human and environmental risk assessment* (*HRA* and *ERA*) or *risk assessment of chemicals* (*RA*), here indicated together as *HERA*. The multimedia modelling concept has been introduced into LCA toxicity characterisation in an early stage (*cf.* Guinée & Heijungs, 1993), and has later on been explicitly recommended by the Society of Environmental Toxicology and Chemistry (SETAC) Europe First Working Group on Life-Cycle Impact Assessment (WIA-1) (Hertwich *et al.*, 2002).

The fact that LCA toxicity assessment and HERA make use of the same models gives rise to the question whether both types of assessment could be combined to one common method. However, the functional unit concept in LCA turns out to make this impossible, since it results in the necessity to assess most processes in the product life cycle only partially. Nevertheless, a new concept for LCA toxicity assessment, introduced in the GLOBOX model, makes it possible to distinguish between the *potential impacts* conventionally assessed with LCA toxicity assessment and contributions of the product life cycle to *actual impacts* or risks, thus bringing LCA toxicity assessment nearer to HERA than it has been until now.

Fate, exposure and effect models depend on parameter values that may vary with climate, water flows, food consumption patterns, population densities, ecosystem composition and other spatially diverging qualities. Most existing LCA fate models hardly account for the spatial dependency of these parameters, typically using the

European, the North-American, or the Japanese situation as a standard. Three arguments plea against this lack of spatial differentiation:

1. Leaving out spatial differentiation leads to unknown deviation in modelling results, thus diminishing overall reliability.
2. The use of European, North-American, and Japanese parameters suggests that these models are primarily meant for use in these regions, and makes them less attractive for use in other parts of the world.
3. Without spatial differentiation, it is impossible to distinguish between purely potential impacts and impacts that are expressed as contribution to actual impacts or risks.

For these reasons, the GLOBOX model has been specifically designed for spatial differentiation with respect to fate, exposure and effect modelling. With respect to the model structure and equations, the GLOBOX model is based on the EUSES 2.0 model. Spatially differentiation is defined on the level of countries, territories* and seas/oceans.

Besides spatial differentiation, the GLOBOX model also contains specific adaptations to make it possible to introduce metal emissions into the model, accounting also for speciation in the aquatic compartments. Region-specific fate and exposure parameters – including a global but spatially differentiated hydrological cycle – and emission and extraction estimates for a large number of substances, have been designed specifically for the GLOBOX model. To complete the life cycle impact assessment phase (LCIA), a set of normalisation factors has been added, making it possible to express the results of the assessment in relative, rather than absolute terms.

1.2 Fate

Well-known, general multimedia fate models include ChemCAN (Mackay *et al.*, 1991; Mackay *et al.*, 1996B, CEMC, 2003), CalTOX (McKone, 1993; McKone *et al.*, 2001), SimpleBox (Van de Meent, 1993; Brandes *et al.*, 1996; Den Hollander & Van de Meent, 2004), HAZCHEM (Stringer, 1994), CemoS (Scheil *et al.*, 1995), Globo-POP (Wania & Mackay, 1995), EQC (Mackay *et al.*, 1996A), models of the BETR series (MacLeod *et al.*, 2001, Prevedouros *et al.*, 2004; Toose *et al.*, 2004; MacLeod *et al.*, 2005), G-CIEMS (Suzuki *et al.*, 2004) and WATSON (Bachmann, 2006). The SimpleBox multimedia fate model is included in the combined fate, exposure and effect models USES (RIVM, VROM, WVC, 1994; Linders & Jager, 1997; Linders & Rikken, 1999) and EUSES (ECB, 1997; EC, 2004), that have been developed for HERA-purposes. The CalTOX model is also a combined fate and

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* These include overseas territories (like Réunion) and uninhabited areas (like Antarctica).

exposure model. Most multimedia models are box models that are based on the assumption of instantaneous homogeneous mixing within each (sub)compartment.

Globo-POP, BETR-global and BETR-world are global scale, spatially differentiated fate models. In Globo-POP, the world is divided into nine segments, the boundaries of which are based on climate types for each hemisphere. In BETR-world, the world is divided into 25 parts, roughly consisting of partial continents and oceans, respectively. Both models have been designed primarily as 'pure' fate models for analytical environmental purposes.

A special feature of global multimedia fate models is the fact that polar regions are included in these models. Since frozen soil and water surfaces cause deviations in substance behaviour compared to the behaviour predicted by the conventional equations for substance fate, adapted modelling assumptions are needed for these regions. In Globo-POP, diffusion processes between air and frozen water and soil surfaces are switched off at below zero temperatures.

Models that have been widely used for LCA toxicity assessment include CalTOX and USES. CalTOX is used as a stand-alone LCA toxicity characterisation model (Hertwich *et al.*, 2001) and is also applied for toxicity assessment in the LCA model TRACI (Bare *et al.*, 2002). USES is used as a basis for the adapted model USES-LCA (Huijbregts *et al.*, 2000), which has been used for the calculation of the LCA toxicity characterisation factors that are included in the CML *Handbook on Life Cycle Assessment* (Guinée *et al.*, 2002).

Besides multimedia fate models, the long range air transport model EcoSense (Krewitt *et al.*, 1998A) has been used for LCA as well (Krewitt *et al.*, 1998B). Contrary to the multimedia models, the EcoSense model does not assume homogeneous mixing within the air compartments. The model consists of a combination of two model types: a Gaussian plume model for the short distances and a trajectory model – including a wind rose approach by use of the Wind rose Model Interpreter (WMI) – for the long distance transport. The model – which has a high degree of spatial differentiation on a grid basis – has been implemented for Europe, Asia and the America's, but not for Africa, Oceania, Antarctica and the ocean regions. A similar approach, by use of a combination of the EUTREND Gaussian plume model (Van Jaarsveld & De Leeuw, 1993; Van Jaarsveld, 1995; Van Jaarsveld *et al.*, 1997) and a trajectory model, based on an adapted version of the EcoSense WMI, has been developed by Potting (2000), and subsequently introduced in the EDIP2003 model (Hauschild & Potting, 2005; Potting & Hauschild, 2005). This last model has been implemented for Europe only. With respect to air transport, the long range air transport models are far more accurate than the multimedia box models. Generally they do not, however, account for the mutual exchange between air on the one hand and surface water and soil on the other, or for water flows between different regions. Spatial differentiation is limited to the air compartments.

Some LCIA models contain their own implicit fate models. These models include EDIP (Hauschild & Wenzel, 1998; Hauschild & Potting, 2005; Potting & Hauschild, 2005) and IMPACT 2002 (Jolliet *et al.*, 2003; Pennington *et al.*, 2005). The original EDIP97 toxicity factors (Hauschild & Wenzel, 1998) used to include degradation measures and a simplified approach for multimedia transport. The EDIP2003 model (Hauschild & Potting, 2005; Potting & Hauschild, 2005) is supplemented with a detailed air transport model, as described above. With respect to the updated EDIP2006 factors, available through the internet (LCA Center, 2008), it is briefly mentioned that 'more multimedia transport' has now been included. The IMPACT 2002 model (Jolliet *et al.*, 2003; Pennington *et al.*, 2005) contains its own multimedia fate model, parameterised for Western Europe in two versions: a spatially differentiated and a general, non-differentiated version respectively. Spatial differentiation is based on a grid for air distribution, while for water distribution, it is based on the demarcation of watersheds.

Several authors have introduced spatial differentiation into comprehensive LCA impact assessment models (*cf.* Huijbregts *et al.*, 2003; Hauschild and Potting, 2005; Potting and Hauschild, 2005; Pennington *et al.*, 2005; Rochat *et al.*, 2006; Humbert *et al.*, 2009). In some spatially differentiated multimedia models, a difference is made between an evaluative region (for which emissions can be entered in the model) and a larger, encompassing region of dispersion, in which the emission region is nested. In the USES-LCA model (Huijbregts *et al.*, 2000; Van Zelm *et al.*, 2009), the evaluative region at the continental level (Western Europe) is not spatially differentiated, but the dispersion region (the northern hemisphere) is characterised by its own environmental parameters for three different climate zones. Huijbregts *et al.* (2003) evaluated the influence of spatial differentiation at the continental level by comparing three different versions of the USES-LCA model, with Western Europe, the United States and Australia as three alternative continental levels. Pennington *et al.* (2005) have introduced spatial differentiation in the IMPACT 2002 model at three levels: the level of Western European watersheds (for soil and surface water) and grid cells (for air and sea/ocean), the continental level of Western Europe, and the global level, in which the continental level is nested. Emissions can be entered at the watershed/grid cell or at the continental level. Rochat *et al.* (2006) have applied spatial differentiation at the level of continents to a global version of the IMPACT 2002 model with respect to both emission and dispersion. Another regionally differentiated multimedia model, that has not been designed specifically for LCA, but that has been used in the LCA-context, is BETR-North America (MacLeod *et al.*, 2001). This model comprises North America, differentiated at the level of ecological regions. Humbert *et al.* (2009) recently developed the IMPACT North America model, in which the evaluative region North America – which is nested into a global dispersion level – is differentiated at the level of several hundred zones.

The introduction of metals in multimedia fate models causes some problems, especially in the context of LCA. It has often been remarked that metal speciation models should be included in LCA. Since metals are not degradable, calculated environmental concentrations may become extremely high in closed modelling systems, especially in the surface water compartments where metals tend to end up. As a result, the characterisation factors of metals may become disproportionally large, causing metal emission to dominate environmental profiles in a way that cannot be considered plausible. Critics on these extremely high characterisation factors from the side of metal specialists have been accounted for by LCA specialists, resulting in a common workshop with specialists from both sides in Montréal (Canada) in 2002 (Dubreuil, 2005), commissioned by the UNEP/SETAC Life Cycle Initiative and the International Council on Mining and Metals (ICMM) and a workshop in Apeldoorn (The Netherlands) in 2004, commissioned by ICMM (Aboussouan, 2004). The Apeldoorn workshop resulted in the so-called *Apeldoorn Declaration*, a list of common goals, described in a final report (Heijungs *et al.*, 2004). In the context of these goals, an international cooperation project was started up with CML, the Radboud University in Nijmegen (The Netherlands) and Toronto University (Canada), in order to combine the Canadian TRANSPEC model for the behaviour of metals in surface water (Bhavsar *et al.*, 2004) with LCA toxicity characterisation modelling.

Despite the fact that speciation and complexation have not yet been included in the well-known overall LCA characterisation models, not all models suffer from the problem of extremely high characterisation factors. In the CalTOX model, this problem is avoided by the assumption that the residence time of metals in the surface water compartment is limited to one year (Hertwich *et al.*, 2001). In the EDIP model, sediment is not considered to be part of the environmental system which implies that the sedimentation process is not counterbalanced by resuspension. This causes an effective outflow of metals from the environmental system by sedimentation (Hauschild & Potting, 2005). Besides the TRANSPEC model – an extension of earlier models for the distribution of chemicals in surface water (Diamond *et al.*, 1990, 1992, 1994 and 1999) which is specifically constructed for the behaviour of metals in surface water – another potentially promising model is WATSON (Bachmann, 2006). This last model accounts specifically for the behaviour of metals in soil and surface water in Europe, with a fine-meshed system of spatial differentiation. WATSON is an extension to water and soil of the long range air transport model EcoSense mentioned above (Krewitt *et al.*, 1998A).

As a basis for the GLOBOX model, we have chosen the EUSES 2.0 model of the European Commission (EC, 2004), since this is a well-documented, recently updated model that includes both fate and human exposure modelling and that has a broad public support. The fate model included in EUSES 2.0 is SimpleBox 3.0 (Den Hollander & Van de Meent, 2004). A core characteristic of the GLOBOX model is the extension of the model to the global scale and the introduction of spatial differentiation. The model is also supplemented with three extra compartments: the freshwater is split up into a river and a lake compartment, and both salt lakes and groundwater are distinguished as separate compartments. Furthermore, the model specifically accounts for cold regions, and contains a specific module for the assessment of metals. Many default values for environmental features – *e.g.,* river flows, lake area and depth and residence times in freshwater compartments – have been replaced by regionally specific values that have been collected from literature. For permanently and temporally frozen water and soil surfaces, absorption and volatilisation processes are switched off for the fraction of time that the local average monthly temperature is below 0 °C. For Greenland and Antarctica, the residence time of runoff water is set to the value of a thousand years. For metals, specific equations are added in order to account for speciation that may largely diminish bioavailability. This enhances the reliability of the exposure assessment for metals. Accumulation of metals is prevented by the choice for two different sea compartments: an upper mixed layer (100 m) and a deeper layer. The deeper layer is considered to be located outside the environmental system, thus acting as a sink for poorly degradable substances. Exchange between seawater and sea sediment occurs in the shallow seas, where the total depth does not exceed the mixing depth.

1.3 Human intake

For aquatic and terrestrial ecosystems, environmental exposure is assumed to be directly connected to environmental concentrations within the environmental compartment in which the organisms of each of these ecosystems dwell. In contrast to this single-pathway exposure, human exposure is assumed to result from many different exposure pathways, with many different environmental compartments serving either directly or indirectly as exposure intermediates. This implies that for human exposure, specific exposure modelling is necessary.

Human exposure models are most often part of an integrated fate and exposure model, or of an LCA toxicity model. Human exposure models are included in USES (RIVM, VROM, WVC, 1994; Linders & Jager, 1997; Linders & Rikken, 1999) and EUSES (ECB, 1997; EC, 2004), in CalTOX (McKone, 1993; McKone *et al.*, 2001), in EDIP (Hauschild & Wenzel, 1998; Hauschild & Potting, 2005; Potting & Hauschild, 2005), in IMPACT 2002 (Jolliet *et al.*, 2003; Pennington *et al.*, 2005), and in the CML 'Guide & Backgrounds' (Heijungs *et al.*, 1992) and 'Handbook' (Guinée *et al.*, 2002). Most human exposure models contain estimates of air inhalation, drinking water consumption, of human food consumption and of the contamination of different types of foodstuff as a function of environmental pollution. The IMPACT 2002 model (Jolliet *et al.*, 2003; Pennington *et al.*, 2005) uses food production as a measure for total food consumption. Some models include additional exposure pathways, such as dermal exposure or soil ingestion.

The human exposure model of EUSES 2.0 contains parameters for dietary intake, drinking water purification, drinking water intake, air inhalation and human body weight. The fixed values of these parameters have been replaced by spatially differentiated parameters in the GLOBOX model. Separate parameters have been added in order to account for the fraction of drinking water assumed to be purified and for the distribution of the origins of drinking water between groundwater, river water and lake water, respectively. The original parameter for fish consumption has been split into separate parameter for freshwater fish and marine fish. Food consumption patterns have been estimated for each individual country. The origin of the consumed food has also been accounted for, based on import and export data of different food stuffs. Data on the fraction of the population in each country aged below 15 are used to adapt standard air inhalation rate and drinking water consumption to spatially differentiated values. Population densities are also accounted for in the exposure module - as they are in the original EUSES model. Finally, estimates have been made for the average human body weight in each country, accounting for the relative number of children and the prosperity level in each individual country.

1.4 Effect

With respect to the toxic effect assessment of chemicals, LCA requires a specific approach that differs from the usual risk assessment approach. For LCA, it is important that effect factors reflect the toxicity ratios between chemicals as well as possible. Safety margins, used in case of incomplete data for regulatory purposes, are not suitable for use in LCA effect factors (Pennington *et al.*, 2006).

The effect part of toxicity models is substance-specific. Some models – *e.g.,* USES-LCA (Huijbregts *et al.*, 2000) and IMPACT 2002 (Jolliet *et al.*, 2003; Pennington *et al.*, 2005) – contain a database with toxicity data that are used directly as effect measures, such as EC_{50} or ED_{50} (median Effect Concentration and Dose, respectively) for ecotoxicity and DALY (Disability Adjusted Life Years) for human toxicity. The GLOBOX model does not contain such a database. In contrast to the fate and human intake modules, the effect module is purely conceptual in the current stage. The concept that distinguishes the GLOBOX effect module from most existing effect modules is the explicit introduction of a possibility to assess not only the usual 'potential impacts', but also 'actual impacts' or risk contributions in the context of LCA. To this end, two new, region-specific factors have been introduced: a *sensitivity factor* (SF) and a *threshold factor* (TF). The SF represents the fraction of the local ecosystem that is sensitive to the given substance, while the TF indicates the fraction of the area where the background level reaches or exceeds the *no-effect* concentration of this substance. To obtain region-specific, actual impacts, the effect factor for potential impacts should be multiplied by the SF and the TF. For human toxicity, the sensitivity factor is set to a value of 1 (and can be omitted), assuming equal sensitivity to toxic chemicals for all populations.

The SF and TF can be considered as elaborations of the so called *site factor* (SF) that has been introduced in the EDIP model (Hauschild & Wenzel, 1998; Hauschild & Potting, 2005; Potting & Hauschild, 2005), representing 'spatially determined probability that the full impact will occur'.

With the introduction of the SF and the TF, it has been rendered possible to calculate *contributions* to actual impacts instead of actual impacts in their full extent. This implies that the assessment of actual impacts is made compatible with the functional unit concept. With the introduction of the possibility to make a distinction between characterisation factors for the calculation of the conventional potential impacts (neglecting SF and TF) and actual impacts (applying SF and TF) respectively, a basis has been created for the combination of *risk minimisation* ('only above threshold') and *general prevention* ('less is better').

1.5 LCA characterisation methods

Numerous LCA software models are available for the performance of LCA characterisation (see RIVM, 2007). The number of underlying methods is much more limited, however. The most well-known LCA characterisation methods designed for LCA toxicity assessment and described in international literature include CalTOX (McKone, 1993; McKone *et al.*, 2001), EDIP (Hauschild & Wenzel, 1998; Hauschild & Potting, 2005; Potting & Hauschild, 2005), USES-LCA (Huijbregts *et al.*, 2000; incorporated in the CML *Handbook on LCA* (Guinée *et al.*, 2002)), and IMPACT 2002 (Jolliet *et al.*, 2003; Pennington *et al.*, 2005). The EcoSense model (Krewitt *et al.*, 1998A&B), that has originally been developed for the calculation of the external costs of air pollution, has also been adapted for LCA characterisation purposes. In 2003, a model comparison between CalTOX, EDIP, USES-LCA and IMPACT 2002 was conducted in the context of the European project OMNIITOX (Molander *et al.*, 2004). Subsequently, the UNEP-SETAC Life Cycle Initiative has started up a collaboration between the model developers of the LCA characterisation models CalTOX, EDIP, USES-LCA, IMPACT 2002, EcoSense and the developers of the fate models of the BETR series (MacLeod *et al.*, 2001, Prevedouros *et al.*, 2004; Toose *et al.*, 2004; MacLeod *et al.*, 2005) and the EcoSense-extension WATSON (Bachmann, 2006) to develop a so-called 'consensus model' for LCA toxicity characterisation. This consensus model, called USEtox, has been published in 2008 (Rosenbaum *et al.*, 2008).

The most important difference between USEtox and GLOBOX is probably in their respective starting points: while USEtox is designed from the viewpoint that it should be transparent and parsimonious, GLOBOX is primarily intended to reflect reality as well as possible. As a consequence, GLOBOX is characterised by a high level of spatial differentiation, whereas the designers of USEtox have chosen explicitly to refrain from this complicating subject.

1.6 Normalisation

The interpretation of LCA profiles is not as easy as it seems. Impact scores are expressed in complex units, and reflect environmental impacts in a way that does not correspond directly to perceptible problems or prevailing threats. LCA normalisation aims at providing this 'missing link'. To this end, each impact score is expressed as the relative contribution to a reference situation. This reference situation consists of an environmental profile on a higher scale – that is, the environmental profile of an economic system that the product life cycle is considered to be part of. An example of such reference system is 'the quantified environmental impacts of the European economic system in the year 2000'. The fact that the normalisation results are expressed in the same unit for each impact score makes it easier to make comparisons between impact scores of different impact categories (Norris, 2001).

Existing normalisation studies include studies by Wenzel *et al.* (1997), Breedveld *et al.* (1999), Huijbregts *et al.* (2003), Stranddorf *et al.* (2005A and B), Strauss *et al.* (2006), Bare *et al.* (2006) and Lundie *et al.* (2007). The normalisation study presented here along with the GLOBOX model is characterised by the combination of a relatively large number of impact categories considered (15), large reference areas (Europe and the world), and a large number of environmental interventions (environmental emissions, extractions and land use categories) considered (860). Moreover, the specific choice has been made to aim at the representation of environmental interventions, caused by the economic system in the reference year, rather than the more conventional approach to collect the environmental interventions taking place in this year, thus accounting for the delay between production and emission, *e.g.*, of CFCs in refrigerators. With this, the normalisation approach has been brought into line with the approach that is used in LCA case studies, which makes it suitable as a true reference. Apart from its reference function, this normalisation study can also be considered as an LCA study by itself, with the economic systems in Europe and the world as its respective functional units. As such, it indicates the relative importance of different interventions contributing to environmental problems worldwide.

1.7 Environmental parameters

Many parameters in the fate and exposure part of the GLOBOX model are spatially differentiated. Sometimes, parameters could be based directly on existing data sets – or combined data sets – *e.g.,* the surface areas of different countries and seas and the total lake areas in each country. In many cases, data existed for a number of regions only, making it necessary to estimate the parameter values for the remaining regions. Sometimes, parameters had to be estimated, composed (*e.g.,* the total lake area from the areas of individual lakes, and the 'leaf crop' consumption from the internal use of individual fruits, vegetables and cereals, diminished with estimates of inedible parts (skins and bones) and waste/left-overs) or calculated (*e.g.,* the lengths of sea boundaries from the latitudes and longitudes of their edges). Some parameters were taken over from the Globo-POP model (Wania & Mackay, 1995) and transferred from the meridional zones in the latter model to the individual countries and seas in the GLOBOX model. With respect to the world-wide water balance, existing data had to be adapted and supplemented with estimates in order to get a fitting, closed flow system.

1.8 Goal of this thesis

This thesis has five goals:

1. Contributing to an optimal reliability of LCA toxicity assessment by creating a flexible, reasonably detailed system for spatial differentiation of LCA toxicity assessment on a global scale.
2. Enhancing the accuracy of LCA modelling with respect to the behaviour of metals in the environment.
3. The introduction of a method for the assessment of contributions of the product life cycle to toxic risks or actual impacts, along with the conventional assessment of potential impacts.
4. Analysing the influence of spatial differentiation on LCA characterisation factors for human toxicity and ecotoxity by calculations on a test substance.
5. Creating an updated, global LCA normalisation sytem.

I hope this thesis will be a step forward in LCIA toxicity modelling, and that the GLOBOX model will add to a better understanding of the toxic impacts caused by the variety of substances that are brought into the environment for the sake of products, and that it will not only help to realise the optimisation of product choice and production processes, but that it will also contribute to a more fundamental discussion on the sustainability of present production and consumption.

References

Aboussouan L, Saft, RJ, Schönnenbeck M, Hauschild M, Delbeke K, Struijs J, Russell A, Udo de Haes H, Atherton J, Van Tilborg W, Karman C, Korenromp R, Sap G, Baukloh A, Dubreuil A, Adams W, Heijungs R, Jolliet O, De Koning A, Chapman P, Ligthart T, Van de Meent D, Kuyper J, Van der Loos R, Eikelboom R, Verdonck F (2004) Declaration of Apeldoorn on LCIA of non-ferro metals. *SETAC Globe* **5** (4): 46-47

Bachmann TM (2006) *Hazardous Substances and Human Health: Exposure, Impact and External Cost Assessment at the European Scale.* Trace Metals and other Contaminants in the Environment, 8. Elsevier, Amsterdam, The Netherlands

Bare J, Gloria Th, Norris G (2006) Development of the Method and U.S. Normalization Database for Life Cycle Impact Assessment and Sustainability Metrics. *Environ Sci Technol* **40** (16): 5108-5115

Bare JC, Norris GA, Pennington DW, McKone T (2002) TRACI - The Tool for the Reduction and Assessment of Chemical and Other Environmental Impacts. *J Ind Ecol* **6** (3-4): 49-78

Bhavsar SP, Diamond ML, Gandhi N, Nilsen J(2004) Dynamic coupled metal transport-speciation model: application to assess a zinc-contaminated lake. *Environ Toxicol Chem* **23** (10): 2410-2420

Brandes LJ, Den Hollander H, Van de Meent D (1996) *SimpleBox 2.0: a Nested Multimedia Fate Model for Evaluating the Environmental Fate of Chemicals.* National Institute of Public Health and the Environment (RIVM). Report No. 719101029. Bilthoven, The Netherlands

Breedveld L, Lafleur M, Blonk H (1999) A Framework for Actualising Normalisation Data in LCA: Experiences in the Netherlands. *Int J LCA* **4** (4): 213-220

(CEMC) Canadian Environmental Modelling Centre (2003) *ChemCAN: level III. fugacity model of regional fate of chemicals. Version 6.00.* Canadian Environmental Modelling Centre, Trent University, Peterborough, Ontario, Canada. Available from: http://www.trentu.ca/academic/aminss/envmodel/models/CC600.html

Den Hollander HA, Van de Meent D (2004). *Model parameters and equations used in Simplebox 3.0.* National Institute of Public Health and the Environment (RIVM). Report No. 601200003. Bilthoven, The Netherlands

Diamond ML (1999). Development of a Fugacity/Aquivalence Model of Mercury Dynamics in Lakes. *Water Air Soil Pollution* **111**: 337-357

Diamond ML, Mackay D, Cornett RJ, Chant LA (1990) A Model of the Exchange of Inorganic Chemicals between Water and Sediments. *Environ Sci Technol* **24**: 713-722

Diamond ML, Mackay D, Poulton DJ, Stride FA (1994) Development of a Mass Balance Model of the Fate of 17 Chemicals in the Bay of Quinte. *J Great Lakes Res* **20**: 643-666

Diamond ML, Mackay D, Welbourn PM (1992) Models of Multi-Media Partitioning of Multi-Species Chemicals: the Fugacity/Aquivalence Approach. *Chemospere* **25**: 1907-1921

Dubreuil A (2005) Life-cycle assessment of metals: Issues and research directions. SETAC Press, Pensacola, USA

(EC) European Commission (2004) *European Union System for the Evaluation of Substances 2.0 (EUSES 2.0).* RIVM Report no. 601900005. Prepared for the European Chemicals Bureau by the National Institute of Public Health and the Environment (RIVM), Bilthoven, The Netherlands. Available via the European Chemicals Bureau, http://ecb.jrc.it

ECB (1997) *EUSES, version 1.00. European Union System for the Evaluation of Substances.* Environment Institute, European Chemicals Bureau (ECB), Joint Research Centre European Commission, EUR 17308 EN. Ispra, Italy

Guinée JB, Gorrée M, Heijungs R, Huppes G, Kleijn R, De Koning A, Van Oers L, Wegener Sleeswijk A, Suh S, Udo de Haes HA, De Bruijn H, Van Duin R, Huijbregts MAJ (2002) *Handbook on Life Cycle Assessment. Operational Guide to the ISO Standards.* Kluwer Academic Publishers, Dordrecht [etc.], The Netherlands

Guinée J, Heijungs R (1993) A Proposal for the Classification of Toxic Substances within the Framework of Life Cycle Assessment of Products. *Chemosphere* **26** (10): 1925-1944

Hauschild M, Potting J (2005) *Spatial differentiation in life cycle impact assessment. The EDIP2003 methodology.* Environmental news No. 80 2005. Danish Ministry of the Environment, Copenhagen, Denmark

Hauschild M, Wenzel H (1998) *Environmental assessment of products. Volume 2: Scientific background.* Chapman & Hall, London, United Kingdom

Heijungs R, De Koning A, Ligthart T, Korenromp R (2004) *Improvement of LCA characterization factors and LCA practice for metals.* TNO-report R 2004/347, TNO Environment, Energy and Process Innovation, Apeldoorn, The Netherlands

Heijungs R, Guinée JB, Huppes G, Lankreijer RM, Udo de Haes HA, Wegener Sleeswijk A, Ansems AMM, Eggels PG, Van Duin R, De Goede HP (1992) *Environmental Life Cycle Assessment of Products. Guide & Backgrounds – October 1992.* NOH report 9267. Centre of Environmental Science Leiden University (CML), Leiden, The Netherlands

Heijungs R, Wegener Sleeswijk A (1999) The Structure of Impact Assessment: Mutually Independent Dimensions as a Function of Modifiers. Letters to the Editor: Comments and Reply. Comment. *Int J LCA* **4** (1): 2-3

Hertwich EG, Mateles SF, Pease WS, McKone TE (2001) Human toxicity potentials for life cycle assessment and toxics release inventory risk screening. *Environ Toxicol Chem* **20** (4): 928-939

Hertwich EG, Jolliet O, Pennington DW, Hauschild M, Schulze C, Krewitt W, Huijbregts M (2002) *Fate and Exposure Assessment in the Life-Cycle Impact Assessment of Toxic Chemicals.* In: Udo de Haes HA (Ed.) *Life-Cycle Impact Assessment: Striving towards Best Practice.* Society of Environmental Toxicology and Chemistry (SETAC), Pensacola, Florida and Brussels, Belgium, pp. 101-122

Huijbregts MAJ, Breedveld L, Huppes G, De Koning A, Van Oers L, Suh S (2003) Normalisation Figures for Environmental Life-Cycle Assessment: The Netherlands (1997/1998), Western Europe (1995) and the World (1990 and 1995). *Journal of Cleaner Production* **11** (7): 737-748

Huijbregts MAJ, Thissen UMJ, Guinée JB, Jager T, Kalf D, Van de Meent D, Ragas AMJ, Wegener Sleeswijk A, Reijnders L (2000): Priority Assessment of Toxic Substances in Life Cycle Assessment. Part I: Calculation of Toxicity Potentials for 181 Substances with the Nested Multi-Media Fate, Exposure and Effects Model USES-LCA. *Chemosphere* **41**: 541-573

Humbert S, Manneh R, Shaked S, Wannaz C, Horvath A, Deschênes L, Jolliet O, Margni M (2009) Assessing Regional Intake Fractions in North America. *Sci Total Environ* **407**: 4812-4820

Jolliet O, Margni M, Charles R, Humbert S, Payet J, Rebitzer, Rosenbaum R (2003) IMPACT 2002+: A New Life Cycle Impact Assessment Methodology. *Int J LCA* **8** (6): 324-330

Krewitt W, Mayerhofer P, Friedrich R, Trukenmüller A, Heck T, Greßmann A, Raptis F, Kaspar F, Sachau J, Rennings K, Diekmann J, Praetorius B (1998A) *ExternE – Externalities of Energy.* National Implementation in Germany. IER, Stuttgart, Germany

Krewitt W, Mayerhofer P, Trukenmüller A, Friedrich R (1998B) Application of the Impact Pathway Analysis in the Context of LCA. The Long Way from Burden to Impact. *Int J LCA* **3** (2): 86-94

LCA Center (2008) *LCA data. EDIP factors.* Available at: http://www.lca-center.dk > English pages > LCA data > EDIP factors

Linders JBHJ, Jager DT (eds.) (1997) *USES 2.0, The Uniform System for the Evaluation of Substances, version 2.0; supplement to EUSES.* National Institute of Public Health and the Environment (RIVM). Report No. 679102037. Bilthoven, The Netherlands

Linders JBHJ, Rikken MGJ (eds.) (1999) *Uniform System for the Evaluation of Substances (USES), version 3.0.* RIVM Report No. 601450004. National Institute of Public Health and the Environment (RIVM), Bilthoven, The Netherlands

Lundie S, Huijbregts MAJ, Rowley HV, Mohr NJ, Feitz AJ (2007) Australian Characterisation Factors and Normalisation Figures for Human Toxicity and Ecotoxicity. *Journal of Cleaner Production* **15**: 819-832

Mackay D (1991) *Multimedia Environmental Models. The Fugacity Approach.* Lewish Publishers, Chelsea, Michigan, USA

Mackay D, Di Guardo A, Paterson S, Cowan CE (1996A) Evaluating the Environmental Fate of Chemicals using the EQC Model. *Environ Toxicol Chem* **15** (9): 1627-1637

Mackay D, Di Guardo A, Paterson S, Tam DD (1996B) *ChemCAN 4: Level III fugacity model of regional fate of chemicals. Version 4.95.* University of Toronto, Toronto, Ontario, Canada. Available from:
http://www.trentu.ca/cemc/models/ChemCAN.html

Mackay D, Paterson S, Tam DD (1991) Assessment of chemical fate in Canada. Continued *development of a fugacity model.* Health Canada, Bureau of Chemical Hazards, Ottawa, Ontario, Canada

MacLeod M, Riley WJ, McKone TE (2005) Assessing the Influence of Climate Variability on Atmospheric Concentrations of Polychlorinated Biphenyls using a Global-Scale Mass Balance Model (BETR-global). *Environ Sci Technol* **39** (17): 6749-6756

MacLeod M, Woodfine DG, Mackay D, McKone T, Bennett D, Maddalena R (2001) BETR North America: A regionally segmented multimedia contaminant fate model for North America. *Env Sci Poll Res* **8** (3): 156-163

McKone TE (1993) *CalTOX, a multimedia total exposure model for hazardous-waste sites.* Report UCRL-CR-111456PtI-IV. Lawrence Livermore National Laboratory, Livermore, CA, USA

McKone T, Bennett D, Maddalena R (2001) *CalTOX 4.0 Technical Support Document, Vol. 1.* LBNL - 47254, Lawrence Berkeley National Laboratory, Berkeley, CA., USA

Molander S, Lidholm P, Schowanek D, Recasens M, Fullana P, Palmer I, Christensen F, Guinée JB, Hauschild M, Jolliet O, Carlson R, Pennington DW, Bachmann TM (2004) OMNIITOX – Operational Life-Cycle Impact Assessment Models and Information Tools for Practitioners. *Int J LCA* **9** (5): 282–288

Norris GA (2001) The Requirement for Congruence in Normalisation. *Int J LCA* **6** (2): 85-88

Pennington DW, Margni M, Ammann C, Jolliet O (2005) Multimedia fate and human intake modeling: spatial versus nonspatial insights for chemical emissions in Western Europe. *Env Sci Tech* **39**: 1119-1128

Pennington DW, Margni M, Payet J, Jolliet O (2006) Risk and Regulatory Hazard-Based Toxicological Effect Indicators in Life-Cycle Assessment (LCA). *Hum Ecol Risk Assess* **12** (3): 450-475

Potting JMB (2000) *Spatial Differentiation in Life Cycle Impact Assessment. A Framework, and Site-Dependent Factors to Assess Acidification and Human Exposure.* PhD thesis. Utrecht University, Utrecht, The Netherlands

Potting J, Hauschild M (2005) *Background for spatial differentiation in life cycle impact assessment. The EDIP2003 methodology*. Institute for Product Development. Technical University of Denmark (DTU), Lyngby, Denmark

Prevedouros K, Jones KC, Sweetman AJ(2004) European-Scale Modeling of Concentrations and Distribution of Polybrominated Diphenyl Ethers in the Pentabromodiphenyl Ether Product . *Environ Sci Technol* **38** (22): 5993-6001

RIVM (2007) *Dossier LCA (Life Cycle Assessment)*. National Institute of Public Health and Environmental Protection (RIVM), Bilthoven, The Netherlands. (In Dutch.) Available at: http://www.rivm.nl/milieuportaal/dossier/lca/ > Software > LCA software Algemeen overzicht

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 the Environment (VROM), Ministry of Welfare, Health and Cultural Affairs (WVC). The Hague, Ministry of Housing, Spatial Planning and the Environment. Distribution No. 11144/150. The Netherlands

Rochat D, Margni M, Jolliet O (2006) Continent-specific Intake Fractions and Characterization Factors for Toxic Emissions: Does it make a Difference? *Int J LCA* **11** (Special Issue 1): 55-63

Rosenbaum RK, Bachmann TM, Gold LS, Huijbregts M, Jolliet O, Juraske R, Koehler A, Larsen HF, MacLeod M, Margni M, McKone TE, Payet J, Schuhmacher M, Van de Meent D, Hauschild MZ (2008) USEtox – The UNEP-SETAC toxicity model: recommended characterisation factors for human toxicity and freshwater ecotoxicity in Life Cycle Impact Assessment. *Int J LCA* **13** (7): 532-546

Scheil S, Baumgarten G, Matthies M, Reiter B, Schwartz S, Trapp S, Wagner J-O (1995) An Object-Oriented Software for Fate and Exposure Assessments. *Environ Sci Pollut Res* **2** (4): 238-241

Stranddorf HK, Hoffmann L, Schmidt A (2005A) *Impact categories, normalisation and weighting in LCA. Updated on selected EDIP97-data*. Environmental news No. 78 2005. Danish Ministry of the Environment. Environmental Protection Agency. Copenhagen, Denmark. Downloadable from: http://www2.mst.dk/udgiv/publications/2005/87-7614-574-3/pdf/87-7614-575-1.pdf

Stranddorf HK, Hoffmann L, Schmidt A (2005B) *Update on Impact Categories, Normalisation and Weighting in LCA. Selected EDIP97-data*. Environmental Project Nr. 995 2005. Miljøprojekt. Danish Ministry of the Environment. Environmental Protection Agency. Copenhagen, Denmark. Downloadable from: http://www2.mst.dk/udgiv/Publications/2005/87-7614-570-0/pdf/87-7614-571-9.PDF

Strauss K, Brent A, Hietkamp S (2006) Characterisation and Normalisation Factors for Life Cycle Impact Assessment Mined Abiotic Resources Categories in South Africa: The manufacturing of catalytic converter exhaust systems as a case study. *Int J LCA* **11** (3): 162-171

Stringer DA (ed.) (1994) *HAZCHEM. A Mathematical Model for Use in Risk Assessment of Substances.* Special Report No. 8, ECETOC, Brussels, Belgium

Suzuki N, Murasawa K, Sakurai T, Nansai K, Matsuhashi K, Moriguchi Y, Tanabe K, Nakasugi O, Morita M (2004) Geo-referenced multimedia environmental fate model (G-CIEMS): model formulation and comparison to the generic model an monitoring approaches. *Environ Sci Technol* **38**: 5682-5693

Toose L, Woodfine DG, MacLeod M, Mackay D, Gouin J (2004) BETR-World: A geographically explicit model of chemical fate: application to transport of a-HCH to the Arctic. *Env Poll* **128**: 223-240

Udo de Haes HA (2006) How to approach land use in LCIA or, how to avoid the Cinderella effect? *International Journal of Life-Cycle* Assessment **11** (4): 219-221

Van de Meent D (1993) *SIMPLEBOX: a Generic Multimedia Fate Evaluation Model.* RIVM Report No. 672720001. National Institute of Public Health and Environmental Protection (RIVM), Bilthoven, The Netherlands

Van Jaarsveld JA (1995) *Modelling the long-term atmospheric behaviour of pollutants on various spatial scales.* PhD thesis. Utrecht University, Utrecht, The Netherlands

Van Jaarsveld JA, Van Pul WAJ, De Leeuw FAAM (1997) Modelling transport and deposition of persistent organic pollutants in the European region. *Atmospheric Environment* **31**: 1011-1024

Van Jaarsveld JA, De Leeuw FAAM (1993) OPS: An operational atmospheric transport model for priority substances. *Environmental Software* **8**: 91-100

Wania F, Mackay D (1995): A Global Distribution Model for Persistent Organic Chemicals. *Sci Total Environ* **160/161**: 211-232

Wenzel H, Hauschild M, Alting L (1997) Environmental assessment of products. Volume 1: Methodology, tools and case studies in product development. Chapman, Hall, London, United Kingdom

2

General prevention and risk minimization in LCA: a combined approach*

Abstract

Methods for life cycle assessment of products (LCA) are most often based on the general prevention principle, as opposed to the risk minimization principle. Here, the desirability and feasibility of a combined approach are discussed, along with the conditions for elaboration in the framework of LCA methodology, and the consequences for LCA practice. A combined approach provides a separate assessment of above and below threshold pollution, offering the possibility to combat above threshold impacts with priority. Spatial differentiation in fate, exposure, and effect modelling is identified to play a central role in the implementation. The collection of region-specific data turns out to be the most elaborate requirement for the implementation in both methodology and practice. A methodological framework for the construction of characterisation factors is provided. Along with spatial differentiation of existing parameters, two newly introduced spatial parameters play a key role: the sensitivity factor and the threshold factor. The practicability of the proposed procedure is illustrated by an example of its application. Providing a reasonable data availability, the development of separate LCA characterisation factors for the respective assessment of pollution levels above and below environmental threshold values seems to be a feasible task that may add to LCA credibility.

Keywords

above threshold values, below threshold values, effects, exposure, fate, general prevention, LCA, life cycle assessment (LCA), multimedia models, risk minimization, spatial differentiation, threshold values

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* This chapter has been published as: Wegener Sleeswijk A (2001) General prevention and risk minimization in LCA: a combined approach. *Environmental Science & Pollution Research* **8**: 1-9.

2.1 Introduction

The question whether the emission-related environmental assessment of products using *life cycle assessment* (LCA) should be based on pollution levels (*general prevention*; 'less is better') or on expected effects (*risk minimization*; 'only above threshold') has been discussed since years. The question whether it is possible to combine both approaches in a practical sense, however, has hardly been addressed. In this chapter, a methodological framework for such a combined approach is proposed.

According to the original document in which the terms 'less is better' and 'only above threshold' were introduced (White *et al.* 1995) the 'only above threshold' approach is not compatible with the functional unit concept, and therefore not applicable in LCA. This statement has been outdated by the application of this principle in practicable LCA methodologies for the assessment of above threshold impacts (*cf.* Hogan *et al.* 1996, Potting *et al.* 1998).

(Barnthouse *et al.* 1997) distinguish two extreme principles with respect to the question of what should be the basis of the assessment of environmental harm. With respect to emissions, these extreme principles are described with the terms *general prevention* and *risk minimization*. While general prevention is considered as the principle behind the 'less is better' approach, risk minimization seems to be the driving force behind 'only above threshold' methods. In our view, it is very well possible to combine general prevention with risk minimization. In other words: the 'less is better' approach can very well be combined with a prioritisation of 'above threshold' impacts.

A combination of both principles could not only enrich existing LCA methodology, but may also be interesting in the context of other environmental assessment methods, especially where these methods have largely focussed on above threshold effects until now.

As Potting *et al.* (1999) pointed out already, the procedure is extremely simple in theory: for each chemical and each impact category, areas where the environmental threshold is exceeded should be kept apart from areas where this is not the case. Concentrations of a chemical in both types of areas should be assessed separately. Despite the simplicity of the procedure, its practical elaboration is not as easy as it may seem.

The goal of this chapter is threefold:

1. Discussing the desirability and feasibility of combining the principles of general prevention ('less is better') and risk minimization ('only above threshold') in LCA.
2. Elaborating the underlying reasons for the above-mentioned discrepancy between theoretical simplicity and practical complexity of combining these principles.

3. Proposing a generally applicable methodological framework for the separate assessment of above- and below-threshold pollution in LCA.

The following three sections pertain, respectively, to each of these goals. Simultaneously, the first two of these sections serve as a theoretical background for the third one.

2.2 Risk minimization and general prevention in the context of LCA

2.2.1 Background information

Two LCA concepts play a central role in this chapter: the *functional unit* and the *characterisation factor*. The *functional unit* is the assessment basis in LCA. To compare product alternatives which differ in lifetime and functional capacity, products are assessed on a functional basis, *e.g.* '1000 tonnes of cargo transport over 1000 kilometres' for the comparative assessment of different types of trucks.

The *characterisation factor* represents the relative potential harmfulness of a standard amount (*e.g.* 1 kg) of a chemical in the context of a certain impact category, compared to other chemicals. It is based not only on effect information (*e.g.* relative toxicity), but also fate (*e.g.* degradability) and exposure related information (*e.g.* uptake by crops). Fate, exposure and effect can be represented by separate, composing factors. Multiplication of an emission in the product life cycle with the corresponding characterisation factor delivers a quantitative effect score: the *category indicator result* (ISO 2000). Category indicator results of different chemicals can be summed over the impact category to which they belong.

Spatial differentiation has an influence on the number of characterisation factors, since the area where a chemical is emitted matters for the magnitude of its eventual effect: every area has its own characterisation factors. Since results can eventually be summed, however, spatial differentiation does not necessarily influence the number of category indicator results.

2.2.2 Risk and LCA

Usage of the term 'risk minimization' in the context of LCA suggests that LCA can be used for the assessment of risks. It may even suggest that LCA might be a special form of risk assessment. To a certain extent, this can perhaps be justified. Yet, it should be kept in mind that the risks, assessed with LCA, differ in nature from the risks that are usually assessed with (other forms of) risk assessment (Udo de Haes and Owens 1998). This difference is caused by the nature of the functional unit.

An important quality of emissions, caused by the life cycle of a product, is the fact that they are delimited in terms of time: they are only emitted during the time that they support the production or use of one functional unit – not a continuous production or use process. Consequently, their contribution to environmental concentrations – and therewith to environmental risks – is also delimited in terms of time (Heijungs and Guinée 1994). And even during this delimited time period, a functional unit will seldom be responsible for any environmental risk in its full extent. In the first place, many risks are caused by a number of different processes together. In the second place, many processes in a life cycle will not exist exclusively for the performance of the function, represented by the functional unit. Processes like electricity production support a great many product functions simultaneously. It is not easy to describe the direct relationships between the environmental risks, associated with such processes, and the functions supported. As a consequence, the category indicator results in LCA are inevitably rather abstract figures, that cannot be translated directly to easily imaginable or directly measurable environmental risks (Figure 2.1). Risk in LCA will always remain a rather abstract concept.

2.2.3 LCA and risk minimization

The most important difference between risk minimization and general prevention is the way in which pollution below certain environmental thresholds is treated. Below such thresholds, risks are generally considered to be negligible, or not observable. From the viewpoint of risk minimization, this pollution should be neglected, since its contribution to actual risk cannot be quantified, and is considered to be near to zero. The advantages of a separate assessment of 'above threshold' impacts in LCA are obvious: since these impacts are clearly more severe, they deserve prioritisation.

Spatial differentiation is thus an important requirement for the use of the risk minimization principle in LCA. The fact that this principle has hardly been applied until now is largely caused by inability, rather than by choice, since methods for handling spatial differentiation in LCA are not easily available.

2.2.4 LCA and general prevention

The general prevention principle is defined as the conviction that 'any perturbation in natural systems is likely to have some adverse effects and should be justified' (Barnthouse *et al.* 1997). In the context of LCA, this principle can be practically elaborated in its pure form for those emission-related impact categories for which concentrations below a certain threshold level are considered to cause no or no appreciable risk. Impact categories in this framework include *human toxicity*, *ecotoxicity*, *acidification*, and *eutrophication* (*cf.* Udo de Haes *et al.* 1999).

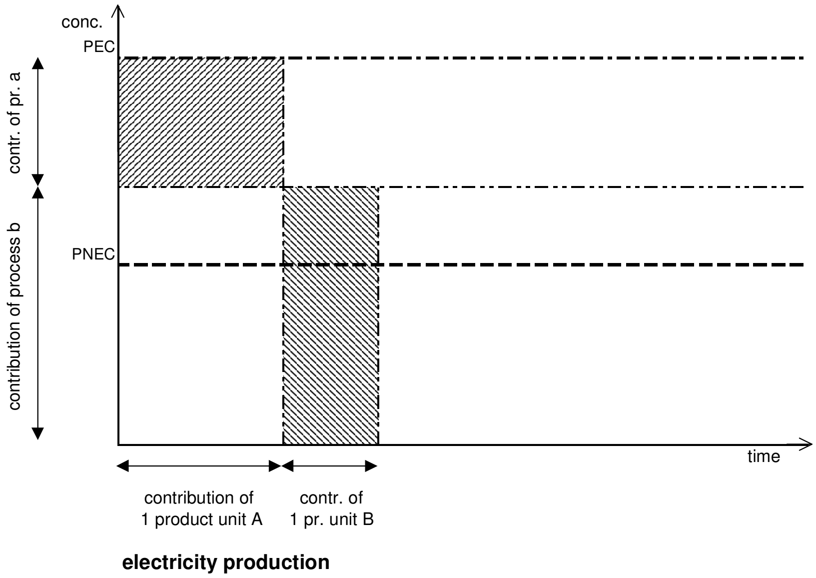

Figure 2.1 Contributions of products A and B to the environmental presence of a chemical emitted by an electric power station in terms of concentration (vertical axis) and time (horizontal axis). While B contributes more in terms of concentration (caused by its production process b), A contributes more in terms of time (caused by its production time). Their contributions to time-integrated concentrations (shaded) are almost equal.

The fact that in LCA the general prevention principle can only be applied in the context of impact categories is an important feature. It implies that it is possible that two different principles apply to one and the same environmental amount of chemical, in the context of two different impact categories to which this chemical potentially adds. For instance, sulphur dioxide is a substance that is considered hazardous in the framework of both acidification and human toxicity. Threshold values are not necessarily equal. It is therefore possible that for a certain environmental amount of sulphur dioxide, the risk minimization principle prevails in the context of *acidification*, while for *human toxicity*, the background concentration remains below the threshold, and the general prevention principle is the only principle that delivers a non-zero result.

2.2.5 The significance of general prevention

Barnthouse *et al.* (1997) mention two possible types of considerations behind the general prevention principle of 'knowledge limitations' and of 'religious/philosophical conviction'. From a scientific point of view, the first type is the most interesting one. Threshold values are usually concentrations below which effects are either not observed or considered negligible. It is commonly accepted that the fact that no effects are observed does not mean that effects do not occur at all, or will not occur in the future. This is especially important for those types of effects for which a care is felt for any effect, whether observed or not. The *human toxicity* impact category is probably the best example of a collection or such effect types: there is a common tendency to avoid unnecessary exposure to potentially hazardous chemicals, even in doses below the reference doses that are believed to be safe.

Knowledge limitations play an important role. More scientifically interesting types of considerations, however, may be distinguished. In the context of the LCA impact categories *ecotoxicity*, *eutrophication*, and *acidification*, at least three additional types may be considered. First, care may be felt when environmental effects are not yet manifest, but are believed to be imminent, *e.g.* when environmental buffers tend to be filled up. Second, a potentially eutrophying substance may occur in relatively high concentrations without causing any effect when it is not the limiting factor. Third, there is a fairly common conviction that it is undesirable that potentially ecotoxic chemicals should occur in the environment in concentrations that exceed natural background levels. In each of these situations, it will probably be commonly accepted that general prevention is useful.

What remains are concentrations of ecotoxics in amounts that do not cause natural background levels to be exceeded (*e.g.* small-scale emissions of heavy metals to the sea), and concentrations of potentially acidifying or eutrophying substances in insensitive areas. In our opinion, these emissions do not need to be assessed at all in LCA, not even in the context of general prevention.

A complicating factor in the application of the general prevention principle is the fact that the optimal environmental concentration of naturally occurring, potentially hazardous substances does not always equal zero. When background levels are below these optimal levels, anthropogenic emissions may be beneficial. Examples are emissions of potentially eutrophying substances to desert areas, and emissions of minerals (*e.g.* zinc, copper) in areas where concentrations of these minerals are sub-optimal for human health. Such emissions should not be assessed as hazardous in the context of the corresponding impact categories, and might even get a positive assessment.

2.2.6 The boundary between general prevention and risk minimization

In some cases, it will be hard to say which of the principles of general prevention and risk minimization applies. This may specifically occur in highly anthropogenic areas, where the prevailing circumstances largely deviate from the natural situation. In such areas, it can be difficult to establish threshold values. A severely polluted river – for instance – may be virtually lifeless. Natural ecosystems have disappeared. Additional effects are hardly possible. In such cases, it is not easy to establish an objective, scientific method to determine the threshold value. Should an emission to this river be considered to cause no risk? Or should the 'natural' threshold value of the river, as it was before pollution started, be applied?

Personally, I think the best solution in such situations is to take the prevailing circumstances as a starting point. After all, it does make a difference whether a chemical is emitted to an already heavily polluted area or to one of the few remaining pieces of unspoilt nature. The fact that we tend to prefer the protection of these virgin areas should be reflected in the assessment, that is, in the category indicator. This implies that threshold values in already polluted areas will have to be considered to be relatively high. This pragmatic solution should not be interpreted as a denial of the importance of combating existing pollution. In polluted areas, these artificial threshold values are just a device that has no meaning outside the context of LCA.

2.3 Combining general prevention with risk minimization

2.3.1 Starting basis

In the former section, the principles of general prevention and risk minimization have been discussed separately. In this section, it will be shown how these principles can be combined. The core of the approach is that pollution levels in above and below threshold areas are kept apart from each other, and are assessed separately. It has been mentioned already that spatial differentiation is a requirement for this approach. The bottleneck for the development of generally applicable methods for spatial differentiation is the enormous amount of information they require. Since product life cycles as a whole will seldom be limited to a particular part of the world, spatial information on fate, exposure and effect characteristics should preferably have a global coverage. The implications for each of these three fields, and the practical consequences for LCA methodology as a whole, are discussed in this section.

2.3.2 Fate modelling

In order to cover all impact categories on a global scale, LCA needs a worldwide multimedia fate model. The most convenient candidates are probably the Mackay type multimedia box models (Mackay 1991). These models account for degradation, immobilisation, intermedia transport, and transport within one medium between different boxes. They are often used for large-scale screening purposes in the context of risk assessment. Two main model variants can be distinguished: the steady state variant ('level 3') and the dynamic variant ('level 4'). In principle, the dynamic variant would be the most appropriate to handle the non-continuous type of emissions that are typical for LCA. The outcome of such models is a concentration course for each environmental compartment. Environmental concentrations can thus be determined at any point of time. What we need in LCA, however, is the time- and space integrated value of the entire concentration curve. Deriving this value would require some modest model adaptations. But a simpler solution is also available. It can be proven that the outcome of the time integration mentioned is numerically identical to the steady-state concentration, caused by an emission flux (kg/year) that is numerically identical to the emission pulse (kg) to be evaluated (Heijungs 1995). Since mixing is assumed to be homogeneous, integration over space can be performed by simply multiplying this value with the magnitude of the distribution volume. Thus, steady state modelling can be used as an expedient for the calculation of the time-integrated environmental amounts (kg·s) that form the assessment basis for emissions in LCA. This is already common practice (*cf.* Guinée *et al.* 1996, Huijbregts *et al.* 2000). In order to keep it clear that the results of the operation should not be interpreted as steady-state concentrations, I would suggest to adapt some terms, to replace *PEC* (predicted environmental concentration) by *PEA* (predicted environmental amount), or *EEC* (expected environmental concentration) by *EEA* (expected environmental amount).

For proper fate modelling, spatial differentiation is a condition, since variables such as temperature, rainfall, wind speed, and ratios between land and water coverage play a central role in multimedia models. In its turn, a spatially differentiated fate model is a condition for making an adequate distinction between above and below threshold exposure, since many chemicals are easily transported from the original emission location to other areas.

2.3.3 Exposure modelling

For water and soil ecosystems, concentration and exposure are sometimes almost used as synonyms. For species for which the direct exposure to the medium in which they dwell is the dominant exposure route, concentration and exposure will indeed be more or less proportional, at least per environmental volume unit. For the assessment of environmental impact on human health, however, additional exposure modelling is indispensable. Inhalation of contaminated air and ingestion of contaminated food are probably the most important routes for human exposure. The spatial aspect is important with respect to regional differences in food consumption patterns, and – above all – with respect to the enormous differences in population densities that exist on a global scale.

2.3.4 Effect modelling

Effect parameters differ per chemical and per impact category. They serve three different purposes:

- to distinguish between sensitive and insensitive areas
- to distinguish between above and below threshold areas
- to establish the relative harmfulness of substances compared to each other.

It is difficult to determine which parameters are the best indicators for the harmfulness of a substance in a general sense, that is, independent of its background concentration. Currently, the most widely used parameters are probably the *no observed effect concentration* (NOEC) for ecotoxicity and the *acceptable daily intake* (ADI) for human toxicity assessment. Regarding the large uncertainties that are associated with the NOEC (*cf.* Chapman *et al.* 1996), it can be considered whether EC_{50} values could serve as a more confident assessment basis for ecotoxicity. With respect to human toxicity, an expert panel has recommended the use of direct toxicity measures, rather than ADI values or similar safety limits (ILSI 1996).

2.3.5 Practical consequences

The necessity of a comprehensive spatial differentiation is probably the most important reason why a general method for the separate assessment of above and below threshold pollution in LCA is not yet available. The construction of such a method would require a vast amount of data. The differentiation level should be low enough to keep a global multimedia model manageable, but high enough to make sense in the context of reliability.

A methodological consequence of spatial differentiation is the necessity to collect fate, exposure and effect parameters on the required level. On the basis of fate and exposure parameters, a global fate and exposure model should be constructed. The effect parameters could be added in separate effect modules for the different impact categories. With the fate and exposure model, it will be possible to produce the time-integrated environmental amounts in every area for all environmental compartments, as well as the time-integrated human exposure in every area, caused by a standard emission of a chemical. With the effect module, it will be possible to distinguish between exposure amounts in sensitive and non-sensitive areas and in above and below threshold areas, respectively, and to weight the severity of standard emissions of different chemicals against each other, for every separate impact category. The result will be an extensive list of characterisation factors for all emission areas distinguished.

Probably one of the most convenient levels to locate processes in LCA is the level of individual countries and oceans. For modelling parameters, this is also a level at which a lot of information is generally available. A disadvantage of the use of countries and oceans as a basic level for spatial differentiation is their incongruity and freakishness. For large countries and oceans, the assumption of homogeneity with respect to concentrations, landscape, climate and population density will be far beside reality. It may be necessary to split up these countries and oceans.

One of the constraints on the applicability of spatial differentiation is the fact that the exact locations of emissions in LCA are often unknown, or even indeterminate. Indeterminacy occurs when the research question is of a general character, *e.g.* 'What is environmentally preferable: paper or plastic wrappings?' Sometimes, it occurs for single processes within a product life cycle, *e.g.* when required aluminium is bought on the world market. In such cases, the best solution is probably to use a probabilistic approach for locating industrial processes artificially, rather than working with global average values for fate, exposure and effect parameters.

Apart from the methodological level, spatial differentiation has also consequences on the level of application. In the LCA *inventory analysis*, it will not be sufficient to collect unit process emission data as such: all emission data should be specified with respect to location on the required level (*e.g.* countries and oceans). This implies that existing LCA databases that lack such information can no longer be used as such. Moreover, the magnitude of the inventory table will be manifold, since different emissions of the same chemical to the same environmental medium can no longer be summed, unless they are emitted in the same area. In the LCA *impact assessment*, all these separate emissions have to be multiplied by the corresponding characterisation factor. The eventual result, however, will be comparable in size and transparency with the existing situation. Instead of one *category indicator result* per impact category, there will be two for some impact categories: one for above, and one for below threshold pollution.

2.4 A methodological framework

2.4.1 Procedure

A basic requirement for the application of the theory sketched in the former sections is an automated, spatially differentiated, flexible fate and exposure model that accounts for environmental transport between different areas in both directions for every environmental medium, and for direct and indirect human exposure via these media. Based on theory discussed in the former sections, separate above and below threshold LCA characterisation factors can be calculated with such by the application of a nine-step procedure.

According to Heijungs and Wegener Sleeswijk (1999), LCA characterisation factors are composed of three separate constituting factors: the fate, exposure and effect factor, respectively. Spatial differentiation refers to each of these constituting factors. When both the fraction of area that is sensitive in the context of each impact category and the fraction of area where the environmental threshold is exceeded are taken into account, this results in two extra factors: the sensitivity factor and the threshold factor. The sensitivity factor indicates the fraction of area that is sensitive to a certain impact category, *e.g.* the fraction of area covered by acidification- sensitive ecosystem, while the threshold factor indicates the fraction of sensitive area where a threshold (*e.g.* the *critical load* for acidification) is exceeded.

In the procedure described below, the resulting five factors will be worked out separately before being combined into two overall characterisation factors for above and below threshold situations, respectively.

1. Collect substance data as required by the model used

Substance data cover physicochemical properties, half-life times in different media, and bio-concentration factors. The exact data required may slightly differ per model, depending on the level of detail covered.

2. Divide up the world into a number of areas, on the basis of differences with respect to fate, collect the area-specific parameters required by the fate and exposure model, and introduce the areas with the corresponding parameters into the fate and exposure model

Since fate is the only aspect that covers all emission-related impact categories, it is the most convenient basis for the distinction between different areas. Differences in fate per area may be caused by climatological or geographical differences. The total number of compartments to be distinguished depends on the level of detail intended. For fate modelling, it is necessary to distinguish at least a number of different climate zones. Since the ratio between land and water coverage can have an important influence the fate of a chemical, it may be desirable to distinguish on this basis between a number of different geographic areas as well. For human exposure modelling, it is important to distinguish between areas that differ with respect to population density. Differences in consumption patterns are another influencing factor.

3. Evaluate the fate factors: calculate the relative distribution of every substance over all environmental compartments, for a standard emission to each of the emission compartments, and multiply the resulting time-integrated concentrations by the corresponding compartmental volumes.

Application of the spatially differentiated multimedia fate model to a standard emission amount of 1 kilogram yields a number of time-integrated concentrations (in $kg{\cdot}m^{-3}{\cdot}kg^{-1}{\cdot}s$): one for each compartment to which an emission can be transported from it either directly or indirectly from the original emission compartment. Multiplication of these values with the volumes of the corresponding compartments delivers the LCA fate factors (in s).

4. Evaluate the exposure factors: calculate the 'standard' exposure to each compartment by multiplying the population magnitude in every area by the corresponding average individual exposure magnitude (based on inhalation and food consumption) for each separate compartment, for a standard time-integrated amount of substance present in that compartment

Contrary to fate factors, exposure factors are more or less impact category specific. Commonly, exposure as such is only taken into account for the impact category 'human toxicity'. It is determined by the direct and indirect exposure to different environmental compartments – largely via inhalation and food and drinking water consumption – and by population magnitude.

Reference doses for human exposure are often expressed per kilogram body weight. In order to combine these values with population magnitudes, it is necessary to convert these doses to doses per individual.

5. Evaluate the sensitivity factors: the fraction of each area that is considered to be sensitive to every separate impact category

6. Evaluate the threshold factors: the fraction of each sensitive part of an area in which the threshold is exceeded, and the fraction in which it is not exceeded, for each individual substance in the context of every separate impact category

7. Determine for each area the effect parameters: an average relative effect measure for each individual substance in the context of every separate impact category, for every exposure route

These parameters aim to set values to determine the relative harmfulness of different substances, in proportion to each other, in the context of every separate impact category. Effect parameters should not include any fate or exposure-related aspects.

8. Evaluate the effect factors: calculate a measure for the average expected effect within each compartment (or: caused by exposure to this compartment) for every impact category

Effect factors should be proportional to the expected effect. Sometimes, inverse effect measures can be used directly as effect factors. Effect measures for different compartments should, however, be expressed in the same dimension for the same impact category. For the human toxicity impact category, this implies that air quality measures in terms of concentrations should be converted to doses, in order to make the effect factors for air, water, and soil mutually compatible. Moreover, effect factors should be compatible with the corresponding exposure factors. For human toxicity, this implies that doses per kilogram bodyweight should be converted to doses per individual. When the average body weight per country is assumed to differ per country, this is an extra source of spatial differentiation.

9. Evaluate the characterisation factors: multiply fate factor, exposure factor, sensitivity factor, threshold factor, and effect factor and aggregate the resulting exposure factors per substance and per impact category for above and below threshold situations by summation

In formula:

$$Q_i^{jn} = \sum_m F_i^{nm} \times X_i^{mj} \times S^{mj} \times T_i^{mj} \times E_i^{mj}$$

where

Q_i^{jn} = characterisation factor for substance *i* in impact category *j*

F_i^{nm} = fate factor that accounts for transport of substance *i* from compartment *n* to compartment *m* and for degradation in compartment *n*

X_i^{mj} = exposure factor that accounts for the average exposure to substance *i* from compartment *m* by the target, corresponding to impact category *j*

S^{mj} = sensitivity factor that accounts for the fraction of compartment *m* that is sensitive for impact category *j*

T_i^{mj} = threshold factor that accounts for the fraction of compartment *m* in which the environmental threshold is either exceeded (for above-threshold calculations) or not exceeded (for below threshold calculations)

E_i^{mj} = effect factor that accounts for the average environmental sensitivity in compartment *m* with respect to impact category *j* for the exposure to substance *i*.

The resulting characterisation factors are part of the LCA method. These factors can be applied in individual case studies by the multiplication of every emission in the product life cycle with the corresponding characterisation factor. The resulting category indicator results are summed per impact category for above and below-threshold situations. Together, these summed category indicator results from the environmental profile of the product under study.

2.4.2 Exemplification

The author of this chapter is currently working on a global fate and exposure model called GLOBOX that meets the requirements mentioned in the former subsection. The model will be spatially differentiated on the level of separate countries and oceans. Since it is not yet operational, it is not possible to calculate fate and exposure factors with it. The fate and exposure factors for this example could therefore not yet be calculated, and have been left out. The same applies to the characterisation factors. Other area-related parameters should be considered as preliminary values that may be changed in the final model.

With respect to environmental transport and degradation equations, the GLOBOX model is largely based on the Dutch model USES 2.0. The parameter requirements of this last model will be used as a basis in this example. The example refers to three emissions: an emission of sulphur dioxide (SO_2) to air, an emission of toluene to water, and an emission of pentachlorophenol (PCP) to soil. These emissions are evaluated in the context of two impact categories: *human toxicity* and *acidification*. The world is divided into countries and oceans. The example is limited to two countries: Norway and Sweden. Only spatially differentiated parameters are mentioned in the table. For the other parameters, default values are assumed to be included in the model. The goal of this example is to give an overview of the parameters to be collected in practice (see Step 1-9):

Step 1: Substance parameters

parameters	sulphur dioxide	toluene	PCP
molecular weight [g·mole^{-1}]	64.07	92.13	266.4
melting point [K]	200	178	462
vapour pressure [Pa]	3.3E+5	2.93E+3	0.013
log K_{ow}	–	2.79	4.8
water solubility [g·m^{-3}]	1.16E+5	5.15E+02	0.14
half-life for photodegradation in air [h]	16.8	31	–
half-life for biodegradation in freshwater [h]	–	120	24
half-life for biodegradation in soil	–	27	1080

Step 2: Areas for spatial differentiation, with the corresponding fate and exposure parameters

areas for spatial differentiation	Norway	Sweden
area [km^2]	324,220	449,964
fraction of area covered by water [–]	0.05	0.09
fraction of area covered by agricultural soil [–]	0.03	0.08
population [individuals]	4,481,162	8,873,052
intake of freshwater fish [g·ind.$^{-1}$·d^{-1}]	10	3
intake of marine fish [g·ind.$^{-1}$·d^{-1}]	40	22
intake of leaf crops [g·ind.$^{-1}$·d^{-1}]	512	481
intake of root crops [g·ind.$^{-1}$·d^{-1}]	125	100
intake of meat [g·ind.$^{-1}$·d^{-1}]	87	68
intake of dairy [g·ind.$^{-1}$·d^{-1}]	615	747

Step 3: Fate factors

distribution compartment	fate factor for emission of substance (…) to emission compartment (…)					
	SO_2 air Norway	toluene fresh w. Norway	PCP agr. soil Norway	SO_2 air Sweden	toluene fresh w. Sweden	PCP agr. soil Sweden
air Norway	…	…	…	…	…	…
freshwater Norway	…	…	…	…	…	…
agr. soil Norway	…	…	…	…	…	…
air Sweden	…	…	…	…	…	…
freshwater Sweden	…	…	…	…	…	…
agr. soil Sweden	…	…	…	…	…	…

Step 4: Exposure factors

human exposure factor of substance (…) to emission compartment (…)					
SO_2 air Norway	toluene fresh w. Norway	PCP agr. soil Norway	SO_2 air. Sweden	toluene fresh w. Sweden	PCP agr. soil Sweden
…	…	…	…	…	…

Step 5: Sensitivity factors

fraction of area that is sensitive to acidification	
Norway	Sweden
0.683	0.862

Step 6: Threshold factors

impact categories	fraction of sensitive area where threshold is exceeded					
	Norway			Sweden		
	SO_2	toluene	PCP	SO_2	toluene	PCP
human toxicity	0	0	0	0	0	0
acidification	0.26	–	–	0.15	–	–

Step 7: Effect parameters

human toxicity	effect measure human toxicity		
	SO_2	toluene	PCP
threshold value for inhalation [$\mu g \cdot m^3$]	50	3000	–
threshold value for ingestion [$\mu g \cdot kg$ b.w.$^{-1} \cdot d^{-1}$]	–	430	30

acidification	effect measure acidification		
	SO_2	toluene	PCP
acidifying potential [kg SO_2 -equivalents]	1.0	–	–

Step 8: Effect factors

human toxicity	effect factors human toxicity		
	SO_2	toluene	PCP
oral exposure [$s \cdot kg^{-1}$]	–	2.3E+9	4.1E+10
inhalatory exposure [$s \cdot kg^{-1}$]	8.6E+10	2.3E+9	4.1E+10

acidification	effect factors acidification		
	SO_2	toluene	PCP
air distribution [kg SO_2 -equivalents]	1	–	–

Step 9: Characterisation factors

emission compartment	characterisation factor for impact category (…) of substance (…)			
	human toxicity			acidification
	SO_2	toluene	PCP	SO_2
air Norway	…	…	…	…
freshwater Norway	…	…	…	…
agr. soil Norway	…	…	…	…
other soil Norway	…	…	…	…
air Sweden	…	…	…	…
freshwater Sweden	…	…	…	…
agr. soil Sweden	…	…	…	…
other soil Sweden	…	…	…	…

2.5 Conclusion

Above and below-threshold pollution are both important environmental issues that are worth being taken into account in LCA. Preferably, however, they should be assessed separately. Above-threshold pollution is directly connected to risk, and should therefore be combated with priority.

Spatial differentiation is a condition for the distinction of above and below-threshold conditions. Because of the global character of LCA, and the indeterminacy of exact unit process locations that is typical of LCA, the level of spatial resolution cannot be too high. Differentiation on the level of individual countries is probably the most convenient option.

The choice for a separate assessment of above and below-threshold pollution in LCA will have consequences for both methodology and practice. The recommended methodological adaptations require that existing fate, exposure, and effect parameters are replaced by spatially differentiated parameters. Effect parameters should include two new elements: the sensitivity factor and the threshold factor. For LCA practice, consequences are largely limited to the need to collect spatially-differentiated emission data.

It has been shown that separate assessment of above and below-threshold pollution in LCA is theoretically feasible. Practical feasibility depends on data availability, but does not seem to be fully out of the question. A methodological implementation of the proposed procedure will bring LCA nearer to risk assessment, without losing track of the specific characteristics of life cycle impact assessment.

Acknowledgement

The author would like to thank Helias A. Udo de Haes for his valuable comments. The author is grateful to Unilever for financing her PhD project, in the context of which this chapter has been written.

References

Barnthouse L, Fava J , Humphreys K, Hunt R, Laibson L, Noesen S, Owens J, Todd J, Vigon B, Weitz K, Young J (eds.) (1997) *Life-Cycle Impact Assessment: The State-of-the-Art.* SETAC, Pensacola, Florida, USA

Chapman PM, Caldwell RS, Chapman PF (1996) Warning: NOECs are Inappropriate for Regulatory Use. Letter to the Editor. *Environ Toxicol Chem* **15**: 77-79

Guinée J, Heijungs R, Van Oers L, Wegener Sleeswijk A, Van de Meent D, Vermeire T, Rikken M (1996) USES, Uniform System for the Evaluation of Substances. Inclusion of Fate in LCA Characterisation of Toxic Releases Applying USES 1.0. *Int J LCA* **1**: 133-138

Heijungs R (1995) Harmonization of Methods for Impact Assessment. *Environ Sci Pollut Res* **2**: 217-224

Heijungs R, Guinée JB (1994) The Flux-Pulse Problem in LCA. *LCA News* **4**: 6-7

Huijbregts MAJ, Thissen UMJ, Guinée JB, Jager T, Kalf D, Van de Meent D, Ragas AMJ, Wegener Sleeswijk A, Reijnders L (2000) Priority Assessment of Toxic Substances in Life Cycle Assessment. Part I: Calculation of Toxicity Potentials for 181 Substances with the Nested Multi-Media Fate, Exposure and Effects Model USES-LCA. *Chemosphere* **41**: 541-573

ILSI (1996) *Human Health Impact Assessment in Life Cycle Assessment: Analysis by an Expert Panel.* ILSI Health and Environmental Science Institute, Washington DC, USA

ISO (2000) *Environmental Management – Life Cycle Assessment – Life Cycle Impact Assessment. ISO/FDIS 14042:(E).* First edition 2000-03-01. ISO 14042: 2000, Geneva, Switzerland

Mackay D (1991) *Multimedia Environmental Models. The Fugacity Approach.* Lewis Publishers, Chelsea, Michigan, USA

Potting J, Hauschild M, Wenzel H (1999) "Less is Better" and "Only Above Threshold": Two Incompatible Paradigms for Human Toxicity in Life Cycle Assessment? *Int J LCA* **4**: 16-24

Potting J, Schöpp, W, Blok K, Hauschild M (1998) Site-Dependent Life-Cycle Impact Assessment of Acidification. *J Ind Ecol* **2**: 63-87

Udo de Haes HA, Jolliet O, Finnveden G, Hauschild M, Krewitt W, Mueller-Wenk R (1999) Best Available Practice Regarding Impact Categories and Category Indicators in Life Cycle Impact Assessment. Background Document for the Second Working Group on Life Cycle Impact Assessment of SETAC-Europe (WIA-2). *Int J LCA* **4**: 66-74 and 167-174

Udo de Haes HA, Owens JW (1998) *Evolution and Development of the Conceptual Framework and Methodology of Life-Cycle Impact Assessment.* Society of Environmental Toxicology and Chemistry, Pensacola, Florida, USA

Wania F, Mackay D (1995) A Global Distribution Model for Persistent Organic Chemicals. *Sci Total Environ* **160/161**: 211-232

Wegener Sleeswijk A (1997) *Product versus Process in Impact Assessment.* Proceedings, Eco Informa'97, München, pp. 192-197

White P, De Smet BB, Udo de Haes HA, Heijungs R (1995) LCA Back on Track. But is it One Track or Two? *LCA News* **5**: 2-4

3

Similarities, differences and synergisms between HERA and LCA – an analysis at three levels[*]

Abstract

Linkages between Human and Environmental Risk Assessment (HERA) and Life Cycle Assessment (LCA) can be analysed at three levels: the basic equations to describe environmental behavior and dose-response relationships of chemicals; the overall model structure of these tools; and the applications of the tools. At level 1 few differences exist: both tools use essentially the same fate and effect models, including their coefficients and data. At level 2 distinctive differences emerge: regional or life cycle perspective, emission pulses or fluxes, scope of chemicals and types of impacts, use of characterisation factors, spatial and temporal detail, aggregation of effects, and the functional unit as basis of the assessment. Although the two tools typically differ in all these aspects, only the functional unit issue renders the tools fundamentally different, expressing itself also in some main characteristics of the modeling structure. This impedes full integration, which is underpinned in mathematical terms. At level 3 the aims of the tools are complementary: quantified risk estimates of chemicals for HERA versus quantified product assessment for LCA. Here, beneficial synergism is possible between the two tools, as illustrated by some cases. These also illustrate that where full integration is suggested, in practice this is not achieved, thus in fact supporting the conclusions.

Keywords

HERA, LCA, functional unit, toolbox, combined approach

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[*] This chapter has been published as: Udo de Haes HA, Wegener Sleeswijk A, Heijungs R (2006) Similarities, Differences and Synergisms between HERA and LCA – An Analysis at Three Levels. *Human and Ecological Risk Assessment* **12** (3): 431-449.

3.1 Introduction

Human and Environmental Risk Assessment (HERA) and Life Cycle Assessment (LCA) are often associated with each other. We observe that the comparison between the two types of tools in the course of the development of LCA has become increasingly accurate and detailed. At the same time still quite some 'wrestling' takes place with the topic. Where are the two types of tools the same, where do they differ, and which differences are fundamental?

Let us start with a short description of the two tools. HERA is seen here as a tool, analyzing the risks for human health and for the environment associated with the regular release of chemicals. In the Organization for Economic Co-operation and Development's (OECD 1995) framework, it consists of four steps: hazard identification, where the capacity of a chemical to cause adverse effects is investigated; exposure assessment, where the emission volume of and the degree of exposure to a chemical is determined; hazard assessment, where the dose-response relationship for the chemical is determined; and risk characterisation, in which the results of exposure assessment and effect assessment are compared to one another, often in the form of the ratio of the predicted environmental concentration (PEC) to the predicted no-effect concentration (PNEC). In contrast, LCA is a tool for the analysis of environmental impacts associated with products (including services) over their whole Life Cycle (*i.e.*, product systems); it consists of four main 'phases' (as called in the ISO 14040 series on LCA), that is: Goal and Scope Definition, Inventory Analysis, in which the processes composing a product system are analysed, Impact Assessment, in which the environmental impacts associated with these processes are analysed, and Interpretation, in which the results are compared with the goals set in the Goal and Scope Definition phase. It is the Life Cycle Impact Assessment phase (or LCIA), including impacts both on humans and on the environment, which bears resemblance with a large part of HERA; therefore this chapter will mainly focus on this phase of LCA. In particular, it is the characterisation step of LCIA where models and concepts akin to those of HERA are used to quantify the contributions of releases of chemicals in terms of impacts to humans and ecosystems.

In the first main reports on LCA in general and LCIA in particular, particularly from Heijungs *et al.* (1992), Fava *et al.* (1993), and Lindfors *et al.* (1995), no operational connection to HERA has been made; LCA largely stands by itself. The same holds true for the International Organization for Standardization (ISO) standards on LCA (ISO 1997, 2000). Any reference to risk assessment approaches is missing. A first implementation of the use of Risk Assessment models in LCIA is discussed by Guinée and Heijungs (1993), focusing on toxic impacts. Later, White *et al.* (1995) discuss the position of the tools in relation to each other in a more general sense, distinguishing between an 'only above threshold approach,' like in HERA, and a 'less-is-better-approach,' like particularly in LCA, using a functional unit as reference. In line with this, but much more precise, Barnthouse *et al.* (1997) distinguish between two types of techniques. They summarise the difference as follows: 'LCIA focuses on relative, marginal comparisons of systems using a functional unit approach'; and, in contrast: 'environmental ... risk assessment work(s) with absolute measures such as actual concentrations' (p. 5).

In this context the concept of the 'functional unit' in LCA needs clarification. LCA aims to compare different products 'from cradle-to-grave' (*i.e.*, product systems) with respect to their environmental impacts. Such a comparison only makes sense, if the two products do fulfill the same function, qualitatively and quantitatively. Thus, not one milk bottle and one milk carton should be compared, but for instance 40 bottles and 1,000 cartons, both capable of the packaging of 1,000 liters of milk. The latter is the functional unit. It is an arbitrarily chosen unit of function, aiming to achieve comparability between the product systems at stake. Other examples include: one square meter painted for a period of 10 years; or: one passenger transport between Amsterdam and London.

Owens (1997) proposes to use HERA as a more detailed and site-specific analysis after an LCA has been carried out; Assies (1998) goes one step further and offers a method to include background levels to incorporate elements of HERA into LCA. In Wrisberg *et al.* (2002), LCA and HERA are systematically compared on a much larger number of issues, including among others the relationship to a functional unit. Cowell *et al.* (2002) mention this as a core aspect in their comparison of LCA and HERA.

Recently, more in depth investigations have been carried out where the two types of tools are the same and where they do differ, again focusing on a broad number of issues. By doing so, Olsen *et al.* (2001) identify a number of harmonies and discrepancies between the two types of tools, focusing on Risk Characterisation of chemicals and Life Cycle Impact Characterisation of chemicals. They conclude that the relative character of LCA due to the use of the functional unit is a very important feature of LCA, in contrast to the absolute character of RA. They also conclude that there are overlaps between the tools and that they can complement each other in an overall environmental effort. Wegener Sleeswijk *et al.* (2003) go one step further and conclude that although LCIA and HERA are not fundamentally different on most investigated topics, the functional unit approach in LCA remains as a central, fundamentally different point of distinction. Interestingly enough, the authors still make a plea for integration of both tools. This plea for integration of the two tools is more explicitly the aim of a recent study by the Swedish Environmental Protection Agency (Flemström *et al.* 2004).

In summary, the following picture arises. The two tools, HERA and LCIA, have much in common; they also differ in a number of aspects, the use or not-use of the functional unit being a, or even the main point of difference; the question to which extent the two tools can be integrated needs further investigation, together with the need for clarification about what in fact is meant by 'integration'; and in their application the two tools can complement each other.

In this chapter, we build on this arising picture. In order to achieve more clarity on the harmonies and discrepancies and on the potentials of 'integration' of the two tools, we will distinguish between three levels of analysis: (1) the level of the basic equations to describe the environmental behavior and dose-response relationships of chemicals as used in Risk Characterisation and in Life Cycle Impact Characterisation; (2) the level of the overall model structure of these analytical tools; and (3) the level of their applications. At all three levels, the focus will be on the impact of toxic substances, being the main focus of HERA, and therefore the main field of attention.

The first level, dealing with the basic equations on the fate and effect of chemicals, the inclusion in the two tools, will shortly be discussed. The second level, dealing with the overall modeling structure, will be investigated in more depth where the differences between HERA and LCIA are indeed fundamental in character. This will be achieved using both a conceptual approach, focusing on various characteristics, and a mathematical underpinning of the differences. And at the third level a number of case studies will be discussed of combined use in practice. As a result, a picture is to emerge as to what the common basis of Risk Characterisation and Life Cycle Impact Characterisation is, what the fundamental differences are, and where there can be beneficial synergism.

3.2 Level 1: basic equations

The first level of analysis concerns the basic ingredients of the tools. These are:

- the environmental processes and other phenomena that are to be incorporated (such as biodegradation of chemicals, infiltration in soil, ingestion of chemicals incorporated in food);
- the mathematical relationships postulated for each of these phenomena (such as the principle of mass conservation, the approximation of first-order kinetic chemistry, the lognormal approximation to the distribution of species sensitivity);
- the chemical and environmental data needed in these relationships (such as the octanol water partition coefficient, bio-concentration factors, the ambient temperature).

Both LCIA and HERA in principle use the same relationships and data from environmental chemistry, ecology, and human and eco-toxicology to model the behavior and impacts from chemicals released to the environment.

There may be some differences in practice, though. A specific HERA study is usually restricted to one single substance, whereas a specific LCA study deals with many hundreds of chemicals. Therefore, HERA can use more sophisticated models to cover more specialised phenomena. An example concerns the use of the biotic ligand model (BLM) (DiToro *et al.* 2001; Niyogi and Wood 2004), which may be used for HERA for copper and silver and a few other chemicals; in LCIA its usefulness is as yet limited, because it does not enable an equal approach for all chemicals to be included. Likewise, one HERA study is usually restricted to a particular site, but it can also extend to the level of a country or region; in contrast, a typical LCA study spans the entire globe. As a consequence, in HERA, more site-specific conditions can be handled than in LCIA. Thus, LCIA will in general cover fewer environmental processes, and the processes that are covered will in general be dealt with in a more simplified or generic way. Further, we can observe that HERA more often uses stochastic models and data than does LCA (Cooke and Bedford 2001). Nevertheless, HERA and LCIA use essentially the same chemical, toxicological and ecological processes, relationships, and data.

Another difference is that HERA will and should in general be used in a more conservative way than LCA. HERA often focuses on regulating the admission of chemicals in a safe way, thus requiring the use of safe levels and safety factors for less-known chemicals. As indicated in the introduction, LCA is not used for admission, but for comparison. This requires that most-realistic data are used instead of (realistic) worst-case values. In line with this, HERA typically focuses on fifth percentile values (like in HC_5, LD_5, or ED_5), whereas LCIA focuses on the 50-percentile values (HC_{50}, etc.) (*cf.* Payet and Jolliet 2005). Still, the same data sources are shared between LCIA and HERA.

These theoretical considerations on the similarities between LCIA and HERA are also reflected by the development of these tools in practice. For instance, important parts of the USES (Uniform System for the Evaluation of Substances) model for HERA (Jager and Visser 1994) has been used within LCIA by Guinée *et al.* (1996) and by Huijbregts *et al.* (2000), as the CalTox model for HERA (Maddalena *et al.* 1995) has been used in LCA by Hertwich *et al.* (2001). More recently, developments within the use of species-sensitivity distributions (SSDs) within HERA (Posthuma *et al.* 2002) have been taken up in LCA by Huijbregts *et al.* (2002) and Udo de Haes *et al.* (2002).

3.3 Level 2: overall model structure

3.3.1 Fundamental versus secondary differences

The second level of analysis concerns that of the overall model structure of the tools with respect to the general concepts applied and the mathematical framework. As this section deals with this overall model structure, HERA will not be compared with LCIA only, but also with LCA as a whole. The model structure of a tool reflects its function in two main respects: (1) main goal (2) scope.

Different overviews have been published to illuminate the similarities and differences between HERA and LCA in each of these respects (*cf.* Olsen *et al.* 2001; Udo de Haes *et al.* 2002; Sonnemann *et al.* 2004;Wegener Sleeswijk *et al.* 2003; Flemström *et al.* 2004; Pennington *et al.* 2004). As a general conclusion, we state that fundamental differences are related to the main goal of the tools, whereas scope and areas of application give rise to secondary differences of a more incidental character. In this section, we shall underpin this central statement by providing a stepwise description of the various differences (conceptual analysis). This description is underpinned in symbolic terms (mathematical analysis) presented in an annex to this chapter. Together these constitute a basis for the next section on combining both tools in practice.

3.3.2 Conceptual Analysis

According to Wegener Sleeswijk *et al.* (2003), the following main characteristics of LCIA can be identified as compared to HERA:

a. Life cycle perspective

b. Product as object of analysis

c. Number of processes, chemicals, and impact categories involved

d. Range of impacts covered

e. Use of characterisation factors

f. Summation of effects of different chemicals

g. Independence of time and location

h. Emission pulses instead of fluxes

i. Functional unit as a basis of assessment

And we add to this:

j. Relative and absolute character of the assessment

We will now discuss to what extent these differences are fundamental or only secondary.

a. Life cycle perspective

Despite the term 'life cycle assessment,' assessment from a life cycle perspective is not restricted to LCA. Application of the Life cycle perspective as such is sometimes defined as *life cycle thinking* (Fava 2002). Likewise, Life Cycle Management (or LCM) can build on more tools than LCA alone (*cf.* Wrisberg *et al.* 2002). The introduction of life cycle thinking in HERA implies that the purpose of risk management no longer remains restricted to one central process, but that upstream and downstream processes are accounted for as well, either in a qualitative or in a quantitative form. In this way, risk assessment can be performed in a life cycle framework. This is particularly clear from the EUSES (European Union System for the Evaluation of new and existing Substances) model, where risks are evaluated at every stage of a chemical's life cycle, and multiple sources of exposures to a single substance are considered (ECB 1997). This is implemented by calculating concentrations and exposures on an average basis for the entire region in which the different processes composing the life cycle take place. It can be concluded that not only for LCA, but also for HERA, an aggregation of releases across the life cycle may take place.

b. Product as object of analysis

In LCA, not chemicals as such, but products (including services) – as the cause of the emission of chemicals – form the object of the analysis; or more precisely, product systems, that is, all processes related to a product in its full life cycle. As mentioned before, some products are in fact chemical substances or preparations. Accordingly, the product as the object of analysis is not necessarily exclusive for LCA. However, the way in which a product is investigated in the two tools does differ, which will be investigated with respect to the following topics.

c. Large number of processes, chemicals, and impact categories involved

The large number of (industrial) processes, emitted chemicals to be assessed, and impact categories involved in this assessment, is quite specific for LCA. LCA tries to give an overall image of all quantifiable effects that are directly or indirectly caused by a product, including problem shifting to other chemicals, other impact categories or other stages of the product life cycle. HERA life cycles are typically restricted to one chemical and usually include fewer industrial processes, while only one or two impact categories are addressed. Although it may often not be feasible to perform a risk assessment on the same level as LCA in these respects, it is not impossible, at least in a theoretical sense. The number of processes, chemicals, and impact categories involved is therefore not a fundamental difference between LCA and HERA.

d. Range of impacts covered

HERA typically focuses on toxicity-related impacts, with respect to both human and ecosystem health. LCA has much broader ambitions, and typically includes in addition climate change, stratospheric ozone depletion, acidification, eutrophication, and even aims to include impacts related to land use and the depletion of resources (like minerals, fossil fuels, fish, and timber). Even though Cowell *et al.* (2002) consider the coverage of resources by LCA as 'the only aspect of the two approaches that is completely different,' we do not consider this as a fundamental difference. There is, by the way, a tendency to broaden the scope of HERA to include eutrophying impacts and impacts of desiccation (Latour *et al.* 1994).

e. Use of characterisation factors
Characterisation factors, which enable aggregation of the potential impacts of different chemicals, are very specific for LCA. In the end, however, they are not more than a technical aid. For human toxicity and ecotoxicity, characterisation factors form an intermediate step in the calculation of category indicator results, based on (time-integrated) doses and predicted exposures or environmental concentrations, respectively. It is very well possible to calculate these category indicator results directly, without the use of characterisation factors. Reversely, it is also very well possible to use characterisation factors in HERA for the calculation of risk characterisation ratios (RCRs), as will be shown in the next section.

f. Summation of effects of different chemicals
In the LCIA phase, the impacts of different chemicals that contribute to one impact category are summed up to one score for that category. Examples concern climate change, stratospheric ozone depletion, eutrophication, acidification, and a number of human and ecotoxicity categories. The procedure for this is as much as possible science based and used to be seen as a specific feature of LCIA. The reason behind it is based on practicality, rather than strict necessity. Without summation, a typical LCA study would deliver tens to hundreds of results, particularly for the human toxicity and ecotoxicity categories. For a contribution analysis (see, *e.g.*, Guinée *et al.* 2002) between different chemicals, this is indeed how LCA proceeds. For the comparison of product alternatives, however, it is more practical to end up with a limited number of results, consisting of an impact score of the product alternatives for each impact category as such. As mentioned before, recent developments include the construction of species sensitivity distributions (SSDs) for entire ecosystems (Udo de Haes *et al.* 2002; Posthuma *et al.* 2002). With this development, summation of chemicals is also getting within the reach of HERA (Traas *et al.* 2002), thus causing the summation of effects of different chemicals to be no longer specific for LCA.

g. Independence of time and location
In LCA, spatial and temporal characteristics were originally not accounted for. In Guinée *et al.* (2002), two spatial scales are distinguished for toxicological impact assessment with respect to environmental fate. This type of spatial differentiation is in accordance with the spatial differentiation in the EUSES model, the follow-up of the earlier USES model of RIVM (ECB 1997). Potting (2000) has even used a relatively very high grade of spatial differentiation by calculating characterisation factors for acidifying and some toxic chemicals for Europe on the basis of a 100× 100 km grid. Similar work has been done by Pennington *et al.* (2005), again for Europe. The influence of spatial variation of parameters on LCIA results is assessed by Huijbregts *et al.* (2003). Current LCA developments include the development of a global fate and exposure model (GLOBOX) that is differentiated at the level of separate countries, being the first impact assessment methodology that accounts for this type of differentiation (Wegener Sleeswijk 2003). At the same

time that we can observe increasing spatial detail in LCIA, we see that HERA is also performed at higher scale levels. As mentioned earlier, EUSES already includes the level of world regions. Similarly, MacLeod *et al.* (2001) present the regionally segmented BETR model for North America, Toose *et al.* (2004) extend this to cover the entire globe, and Wania and Mackay (1995) present another model covering the earth. Thus LCIA, starting at a global level, and HERA, starting at a local level, have met each other at the national/regional level. Temporal differentiation is sometimes accounted for in the inventory analysis of LCA (the LCI phase). No impact assessment methodology that accounts for this type of differentiation has been developed until now. In HERA, such as for instance in the EUSES model, however, temporal differentiation is not accounted for either. Hence, LCA also includes higher spatial resolution, and independence of time is thus not specific for LCA.

In relation to types of impacts, LCA looks both at medium and long-term time horizons, whereas HERA focuses on the short and the medium term. This largely depends on the types of substances involved, and is not a fundamental difference.

h. Emission pulses instead of fluxes

The production of a certain amount of a product corresponds to certain quantities of raw materials needed, and corresponding quantities of chemicals emitted to the environment (in kg). Such quantities (pulses) are usually assessed directly in LCIA, without accounting for the production capacities – and the connected emission characteristics – of the processes involved (in kg per year). In HERA, these production capacities and concomitant emission characteristics (fluxes) form the basis of the assessment. Although a bit unusual, it is possible to take the production flow of products (in functional units *per year*) – and the connected emission fluxes – as a starting point in LCA, instead of the products as such. Thus, even the alleged incompatibility between models based on emission fluxes (as in HERA) and models based on emission pulses (as in LCIA), already being resolved mathematically (Heijungs 1995), does not pose a fundamental difference between LCA and HERA.

i. Functional unit as a basis of assessment

This point has already been indicated in the introduction. The functional unit is the assessment basis of LCA, enabling comparison between different products that provide the same function. The products to be assessed thus are quantitatively characterised in terms of this function, for example '1 square meter of painted surface area during 10 years' in an LCA of paint. This makes it possible to account for differences in product lifetime or durability (one paint may last longer than the other) and efficiency (one paint may have greater covering power than the other). Processes throughout the product life cycle are quantitatively related to each other on the basis of their relative contribution to the defined functional unit. This implies that most processes – and the related emissions – are only partially included in the analysis: so much electricity for this given functional unit, and not the electricity from one whole plant (Udo de Haes *et al.* 2002) in this context make a distinction between full mode of analysis (as in HERA) and attribution mode of analysis (as in LCA); see further in the Appendix. Both Olsen *et al.* (2001) and Wegener Sleeswijk *et al.* (2003) conclude that the functional unit can be considered as a key feature by which LCA fundamentally differs from RA.

j. Relative and absolute character of the assessment
Use of the functional unit as a basis for the modeling also determines another key characteristic of LCIA, that is, the relative character compared with the absolute character of HERA. As indicated in the introduction, Barnthouse *et al.* (1997) were the first to put this sharply. A functional unit usually is arbitrary in size; we could as well take 100 square meters to be painted, or 10,000 liters of milk to be packed, as long as it is the same size for all products to be compared. Instead, in HERA a fixed flow is taken as a starting point, usually the production volume of the chemical. This is transformed into environmental flows and concentrations, usually compared with given acceptable threshold flows or levels. HERA is therefore described as an absolute, 'only-above-threshold' approach. In contrast, LCA is in this context described as relative, 'less-is-better,' indicating the desirability of any decrease of hazardous substances, rather linking with prevention than with control.

We conclude that the latter two points, the use of the functional unit in contrast to actual flows, linked with the distinction between a relative versus an absolute modeling structure, fundamentally distinguish between LCIA and HERA. The other eight points are seen as secondary differences that in practice may occur to a greater or lesser degree. Besides these ten points, the literature mentioned earlier identifies a number of procedural differences as well. Among these are reporting formats, reviewing requirements, and the role in legislation. These type of differences have nothing to do with the model structure itself, and are therefore not discussed in this chapter.

3.3.3 Mathematical Analysis

Another way to analyse the differences between the tools is by means of symbolic language. In order to analyse mathematically to which extent observed differences are fundamental or not, it is first of all needed to phrase the tools in terms that are as much as possible similar. For instance, when it is said that LCA uses characterisation factors whereas HERA does not, it is necessary to investigate whether the tools do so for reasons that are primarily historical or practical, or for fundamental reasons. In the Appendix, we will show how the rephrasing of HERA-practice with characterisation factors helps to understand which differences between LCA and HERA indeed are fundamental and which are not.

Four differences are investigated mathematically: the use of a functional unit, the mode of analysis, the area, and the aggregation of impacts. The 'mode of analysis' is a new concept, introduced by Udo de Haes *et al.* (2000). It indicates the difference between full mode, where only processes in their full size are taken into account as in HERA, and attribution mode, where processes are taken into account only as far as they are related to a given reference as in LCIA. It is concluded that the first two are fundamental differences, the latter two secondary differences depending on the scope of the study.

3.3.4 In conclusion

Taking the results of the conceptual and the mathematical analysis together, we come to the following conclusion. The only fundamental difference between HERA and LCA is the use of flows of actual (or absolute) size in HERA and the use of the functional unit concept in LCA. In practice, this goes together with a difference between an absolute character of the analysis in HERA and a relative character in LCA. And in mathematical terms, this expresses itself in a difference between a full mode modeling structure in HERA and an attribution model modeling structure in LCA.

3.4 Level 3: applications

The third level deals with the application of the tools. If it is true, as concluded earlier, that the two tools cannot be fully integrated, this does not prevent combined use. On the contrary, it is the idea of a toolbox that a given decision can be supported by more types of information. Such a plea is for instance made by Wrisberg *et al.* (2002), Hofstetter and Hammitt (2002), Cowell *et al.* (2002), and Udo de Haes *et al.* (2004).

There are some clear examples of efforts to combine both tools. This can take different shapes. A first example of combines use concerns the study of Sonnemann *et al.* (2004). These authors compare two situations regarding the combustion of coal: situation 1 with the plant close to the mining site, in a very populated region, and situation 2 with the same plant farther away, in a less densely populated region, but in need of more transport. The results of the LCA study indicate that situation 1 is to be preferred, due to the lower energy demands for transport; whereas the results of the HERA study indicate that situation 2 is to be preferred due to the lower exposure of people to the plant emissions. The authors appear to be concerned about the differing results obtained with the two tools.

A second example concerns a study on insulation by Nishioka *et al.* (2002). The authors make a cost-benefit analysis to compare the current situation with respect to insulation of homes in the United States with a situation in which the complete housing supply would be heat insulated, according to a certain standard. For this purpose, they have constructed 'a model framework that allows for the evaluation of benefits combining risk assessment and LCA,' presented as 'an analytical framework that can incorporate Life Cycle impacts using a risk assessment framework' (p. 1004). Results are formulated in terms of energy savings, emission and risk reductions. No separate results are presented for the risk assessment and the LCA part: apparently, both tools have merged into a new analytical instrument.

A third example that underlines the usefulness of a toolbox approach, combining the application of both LCA and HERA, is provided by Saouter and Feijtel (2000), describing a case study comparing different detergent products from Procter and Gamble, in which a parallel ERA study and an LCA study are performed. These gave contradictory results; that is, of two products, the LCA study showed that for most of the impact categories product A had a lower score, whereas the HERA study showed that product B was to be preferred. But correctly, the authors argue that this illustrates the need to use complementary tools in the context of environmental management of chemical products. In fact, for the authors it is not astonishing that the results can differ, as the LCA study analysed the products from cradle-to-grave, and the HERA study focused on the waste management process only.

Recently, a follow-up of this study has taken place in the framework of the EU OMNIITOX project on the improvement of both LCA and HERA methodology (Pant *et al.* 2004). It concerns a new case study on detergents by Procter and Gamble, analyzing different outcomes of various LCIA models and an ERA model. Observing that the results of the different tools vary a great deal, the authors conclude: 'This puts a challenge to the OMNIITOX project to develop a method that finds common ground regarding fate and exposure as well as the effect side to overcome this situation of diverging results and to reflect realistic conditions as far as possible' (p. 281). So apart from the justified plea for a common ground at level 1, and despite the findings of their precedents, the authors of the secondary study seem to worry about the differing results of the HERA and LCA studies.

3.5 Discussion

So far, our findings can be summarised as follows. At level 1, the level of the basic equations, LCA and HERA show many similarities. The basic equations are essentially the same for both tools, be it that sometimes the spatial or temporal resolution will be different. The data on chemical properties and on environmental conditions are also essentially the same, although some differences are introduced, again due to differences in spatial or temporal resolution, and due to a difference in use (worst case vs. realistic case). At level 2, the level of the overall model structure, the two tools differ fundamentally on one point: the use of a functional unit in LCA in contrast to the use of processes in their full size in HERA. This goes together with the difference between a relative or an absolute approach, and a difference between an attribution and a full mode of analysis. This difference renders, at the level of the models underlying the tools as a whole, full integration of the two tools impossible. At level 3, the use of the two tools can be well combined in practice in the form of a toolbox.

This in fact is a rather simple message. But it is by no means supported by all authors in the field. Interestingly enough, in the example given on the integrated approach by Sonnemann *et al.* (2004) comparing two locations for one coal plant, the authors present the following interpretation of their result. They say that the result 'clearly demonstrates the need for a more integrated approach that does not so easily allow two environmental impact analysis tools to provide such contradictory and inconsistent results.' We do not agree with this interpretation; to put it in somewhat more challenging terms, we argue that only if two tools do produce independent, and thus possibly differing results, it is worthwhile to combine their use in a toolbox. Still, it is interesting to know whether Sonnemann *et al.* (2004) indeed achieved an integration of the two tools, a further aim of their study. Do they manage in this respect?

The procedure chosen by the authors is to make a distinction between impact categories at different spatial scales. Thus, impacts with a global reach such a climate change, are investigated by current LCA at a global level. In contrast, categories at a local level, such as human toxicity, are investigated at a lower level with a higher spatial resolution. This in itself is an interesting approach, compromising between the global and local requirements. However, we do not agree that this would imply an integration of LCA and HERA. The local analysis may be inspired by HERA due to its local focus, but the structure of the model is still straightforward LCA with its clear link to a functional unit as reference.

As to the example of the case study on insulation by Nishioka *et al.* (2002), the fact that these authors end up with a common, unambiguous result for their combined HERA/LCA study brings up the same question we asked earlier: Do these authors indeed achieve an integration of HERA and LCA?

Closer investigation of the study reveals that the authors have abandoned the usual functional unit concept. What they have done seems to boil down to the introduction of the life cycle concept in a combined *Risk Analy*sis/cost-benefit analysis context. The approach clearly differs from, for instance, the life cycle perspective in EUSES: not a chemical as such, neither a product, but a societal scenario (insulation of all homes) forms the object of the analysis. Although the study is quite limited in character from a conventional LCA point of view with respect to the number of life cycle processes actually involved, the number of emissions accounted for, and the refrain from the use of characterisation factors, it is interesting to see how near HERA and LCA could conceptually approach each other if applied to scenario analysis. The results are, however, presented in the form of risks. The absence of the functional unit makes it impossible to introduce this approach in the common LCA practice of general product assessment, and thus, to aggregate effects over the life cycle. Therefore, this study should in our opinion be considered as a modified form of risk assessment.

Yet another approach is followed in the case study on detergents by Pant *et al.* (2004). For the LCA part in this study, the system boundaries are limited to such an extent that they become the same as those for the HERA part. For both types of analysis only emissions to water during waste management are investigated. By doing this, we are not any more at the level of the models as a whole but just at the level of the basic equations. And at that level we fully agree that 'common ground regarding fate, exposure and effect modelling' should be achieved. And it is precisely at this level that the OMNIITOX project is due to produce very relevant results.

A last remaining question to be solved is, whether level 1 is indeed the limit for the integration of the two tools: Is the use of equal basic equations and equal input data the nearest point to which HERA and LCA could approach each other? If this were indeed the case, we might conclude that we are not far off from the maximum realisation of bringing HERA and LCA together. As stated earlier: HERA and LCA focus already on essentially the same chemical, toxicological, and ecological processes, and use the same relationships and data. Current LCA fate, exposure, and effect models are already being based on existing HERA concepts, also at level 1 of the basic equations and data. Is there nothing left to be possibly achieved?

We believe there is. The current problem with the discrepancy between LCA and HERA does not so much regard their structural difference, as discussed at level 2, but rather their lack of applicability as a combined tool. In principle, it is possible to apply both HERA and LCA to the same case, as becomes clear from some of the examples elaborated earlier. In practice, however, the implementation of such a combined case study requires a careful study process at all three levels. At level 1, it is not enough that the same equations and data can be used, but these must be used. At level 2, very specific methodological choices are required, aiming at a balance between the two tools. As we have seen earlier, these choices may easily cause one of the two tools to become subordinate to the other, or even to lose one or more of its essential features. And at level 3, yet another problem arises: the interpretation of seemingly conflicting results. Even to the experienced user in the field of either HERA or LCA it may be confusing if the outcomes of the studies suggest opposite solutions for the environmentally preferred choice. It may become fully unclear how to proceed, and the credibility of both tools among practitioners may be endangered. This situation should be avoided.

In their plea for a partial integration of LCA and HERA, Wegener Sleeswijk *et al.* (2003) propose 'that RA and LCA are to be incorporated in a common modeling tool, containing a common database. Such an overall modeling tool would deliver both risks of individual chemicals and impact scores for all LCA impact categories as outputs' (p. 86). In our view, the development of what we would like to call a 'combined software tool,' providing a harmonisation of equations and data where possible, and including the equations for the two tools in a balanced way, would probably be the best conceivable option to overcome the problems mentioned. In practice, the user of such a combined software tool could choose between two modes: either HERA or LCA, but within the same user-interface. If desired, the modes could be implemented both in consecutive steps, and the results could be compared in a scheme. The difference between the use of this common tool and the use of harmonised, but separate tools, would have implications for each of the three levels. At level 1, entry of chemical data by the user, and entry of model equations by the modeler, would be needed only one time, instead of two times as is the case nowadays. At level 2, differences would be pre-programmed as a number of consistent, but mutually exclusive options, whereas at level 3, the context in which the results are to be compared would be included as well.

In a combined software tool, the position of HERA and LCA in relation to each other may well be visualised as two cross-sections through the same apple: one may reveal a different rotten section than the other.

3.6 Conclusions

Although an increasingly clear picture was already arising on the links between HERA and LCA, a number of questions are in need of further clarification. What do the tools share, how far are they compatible, can they be integrated, and how is their relationship in applications? We addressed these questions by making a distinction between three levels of analysis: (1) the level of the basic equations to describe the environmental behavior and dose-response relationships of chemicals; (2) the level of the overall model structure of these analytical tools; and (3) the level of the applications of the tools.

Our findings can be summarised as follows. At level 1, LCA and HERA can make use of each other. The basic equations are in principle the same for both tools, be it that the spatial or temporal resolution may be different, and that there may be a difference between worst-case and realistic-case assumptions. At level 2, the two tools typically differ on many aspects, but the issue of the functional unit makes the tools fundamentally different, thus impeding full integration. This also expresses itself in a difference between an absolute versus a relative approach, and between a full-mode versus an attribution mode of analysis, as has been underpinned in mathematical terms. At level 3, the use of the two tools can be well combined in practice in the form of a toolbox. Even better would be the construction of a combined software tool, in which both models would be accommodated. With such a tool, it could become common practice to combine HERA and LCA, which could enable decision makers to weight the results against each other.

A number of recent cases seem to contradict these outcomes. In particular, some studies indicate the possibility of full integration of the tools as a whole, a conjecture that is contradicted by the present authors. With closer inspection of the given cases, however, we either observe that the suggested integration fully takes place in the framework of one of the two tools, or that it takes place at level 1 of the basic equations. In this way, the investigated cases in fact support the conclusions arrived at in the present contribution.

References

Assies JA (1998) A risk-based approach to life-cycle impact assessment. *J Haz Mat* **61**: 23-29

Barnthouse L, Fava J, Humphreys K, Hunt R, Laibson L, Noesen S, Owens J, Todd J, Vigon B, Weitz K, Young J (eds.) (1997) *Life-Cycle Impact Assessment: The State-of-the-Art.* SETAC, Pensacola, FL, USA

Cooke T, Bedford R (2001) *Probabilistic Risk Assessment: Foundations and Methods.* Cambridge University Press, Cambridge, UK

Cowell SJ, Fairman R, Lofstedt RE (2002) Use of risk assessment and life cycle assessment in decision making: a common policy research agenda. *Risk Anal* **22** (5): 879-894

DiToro DM, Allen HE, Bergman HL, Meyer JS, Paquin PR, Santore RC (2001) Biotic ligand model of the acute toxicity of metals. 1. Technical basis. *Environ Toxicol Chem* **20** (10): 2383-2396

ECB (1997) *EUSES, version 1.00. European Union System for the Evaluation of Substances.* Environment Institute, European Chemicals Bureau (ECB), Joint Research Centre European Commission, EUR 17308 EN. Ispra, Italy

Fava J, Consoli, F, Denison R, Dickson K, Mohin T, Vigon B (1993) *A Conceptual Framework for Life-Cycle Impact Assessment.* SETAC, Pensacola, FL, USA

Fava JA (2002) Life Cycle Initiative: A joint UNEP/SETAC partnership to advance the life-cycle economy. *Int J LCA* **7**: 196-198

Flemström K, Carlson R, Erixon M (2004. *Relationships between Life Cycle Assessment and Risk Assessment – Potentials and Obstacles.* Naturvardsverket , 071-SNV Rapport 5379. The Swedish Environmental Protection Agency, Stockholm, Sweden

Guinée J and Heijungs R (1993) A proposal for the classification of toxic substances within the framework of life cycle assessment of products. *Chemosphere* **26** (10): 1925-1944

Guinée J, Heijungs R, Van Oers L, Wegener Sleeswijk A, Van de Meent D, Vermeire T, Rikken M (1996) USES - Uniform System for the Evaluation of Substances. Inclusion of fate in LCA characterisation of toxic releases applying USES 1.0. *Int J LCA* **1** (3): 133-138

Guinée JB, Gorrée M, Heijungs R, Huppes G, Kleijn R, De Koning A, Van Oers L, Wegener Sleeswijk A, Suh S, Udo de Haes HA, De Bruijn H, Van Duin R, Huijbregts MAJ (2002) *Handbook on Life Cycle Assessment. Operational Guide to the ISO Standards.* Kluwer Academic Publishers, Dordrecht, The Netherlands

Heijungs R 1995. Harmonization of methods for impact assessment. *Environ Sci Pollut Res* **2** (4): 217-224

Heijungs R (2001) *A Theory of the Environment and Economic Systems. A Unified Framework for Ecological Economics and Decision-support.* Edward Elgar, Cheltenham, UK

Heijungs R, Guinée JB, Huppes G, Lankreijer RM, Udo de Haes HA, Wegener Sleeswijk A, Ansems AMM, Eggels PG, Van Duin R, De Goede HP (1992) *Environmental Life Cycle Assessment of Products. Guide & Backgrounds – October 1992.* NOH report 9267. Centre of Environmental Science Leiden University (CML), Leiden, The Netherlands

Hertwich EG, Mateles SF, Pease WS, McKone TE (2001) Human toxicity potentials for life cycle assessment and toxics release inventory risk screening. *Environ Toxicol Chem* **20** (4): 928-939

Hofstetter P, Hammitt JK (2002) Selecting Human health metrics for environmental decision-support tools. *Risk Anal* **22** (5): 965-983

Huijbregts MAJ, Thissen UMJ, Guinée JB, Jager T, Kalf D, Van de Meent D, Ragas AMJ, Wegener Sleeswijk A, Reijnders L (2000): Priority Assessment of Toxic Substances in Life Cycle Assessment. Part I: Calculation of Toxicity Potentials for 181 Substances with the Nested Multi-Media Fate, Exposure and Effects Model USES-LCA. *Chemosphere* **41**: 541-573

Huijbregts M, Van de Meent D, Goedkoop M, Spriensma R (2002) *Ecotoxicological impacts in life cycle assessment.* In: Posthuma L, Suter GW II, Traas TP (eds.) *Species Sensitivity Distributions in Ecotoxicology*, pp 421-33. Lewis Publishers, Boca Raton, FL, USA

Huijbregts MAJ, Lundi S, McKone TE, Van de Meent D (2003) Geographical scenario uncertainty in generic fate and exposure factors of toxic pollutants for life-cycle impact assessment. *Chemosphere* **51**: 501-508

ISO (1997) *Environmental Management – Life Cycle Assessment – Principles and framework.* First edition 1997-06-15. ISO 14040: 1997, Geneva, Switzerland

ISO (2000) *Environmental Management – Life Cycle Assessment – Life Cycle Impact Assessment.* First edition 2000-03-01. ISO 14042: 2000(E), Geneva, Switzerland

Jager DT, Visser CJM (1994) *Uniform System for the Evaluation of Substances (USES), Version 1.0.* Ministry of Housing Spatial Planning and the Environment, The Hague, Netherlands

Latour JB, Reiling R, Slooff W (1994) Ecological standards for eutrophication and desiccation: Perspectives for risk assessment. *Water Air Soil Pollut* **78** (3-4): 265-278

Lindfors L-G, Christiansen K, Hoffmann L, Virtanen Y, Jutilla V, Hanssen O-J, Rønning A, Ekvall T, Finnveden G (1995) *LCA-Nordic. Technical Report No 10. Impact Assessment.* TemaNord 1995: 503. Nordic Council of Ministers, Copenhagen, Denmark

Mackay D (2001) *Multimedia Environmental Models: The Fugacity Approach.* Second Edition. Lewis Publishers, Boca Raton, FL, USA

MacLeod M, Woodfine DG, Mackay D, McKone T, Bennett D, Maddalena R (2001) BETR North America: A regionally segmented multimedia contaminant fate model for North America. *Env Sci Poll Res* **8** (3): 156-163

Maddalena RL, McKone TE, Laytonz DW, Hsieh DPH (1995) Comparison of multi-media transport and transformation models: Regional fugacity model vs. CalTOX. *Chemosphere* **30** (5): 869-889

Nishioka Y, Levy JI, Norris GA, Wilson A, Hofstetter P, Spengler JD (2002) Integrating risk assessment and life cycle assessment: a case study of insulation. *Risk Anal* **22** (5): 1003-1017

Niyogi S, Wood CM (2004) Biotic Ligand Model, a Flexible Tool for Developing Site-Specific Water Quality Guidelines for Metals. *Environ Sci Tech* **38**: 6177-6189

OECD (1995) *Report of the OECD workshop on environmental hazard/risk assessment.* OECD, Paris, France

Olsen SI, Christensen FM, Hauschild M, Pedersen F, Larsen HF, Tørsløv J (2001) Life cycle impact assessment and risk assessment of chemicals – a methodological comparison. *Environ Imp Assess Rev* **21**: 385-404

Owens JW (1997) Life-cycle assessment in relation to risk assessment: An evolving perspective. *Risk Anal* **17** (3): 359-365

Pant R, Van Hoof G, Schowanek D, Feijtel TCJ, De Koning A, Hauschild M, Pennington DW, Olsen SI, Rosenbaum R (2004) Comparison between three different LCIA methods for aquatic ecotoxicity and a product environmental risk assessment: Insights from a detergent case study within OMNIITOX. *Int J LCA* **9** (5): 281-342

Payet J, Jolliet O (2005) *Comparative assessment of the toxic impact of metals on aquatic ecosystems: The AMI method.* In: Dubreuil A (Ed) *Life Cycle Assessment of Metals: Issues and Research Directions.* SETAC, Pensacola, FL, USA

Pennington DW, Potting J, Finnveden G, Lindeijer E, Jolliet O, Rydberg T, Rebitzer G (2004) Life cycle assessment. Part 2: Current impact assessment practice. *Env Int* **30**: 721-739

Pennington DW, Margni M, Ammann C, Jolliet O (2005) Multimedia fate and human intake modeling: spatial versus nonspatial insights for chemical emissions in Western Europe. *Env Sci Tech* **39**: 1119-1128.

Posthuma L, Suter II GW, Traas TP (2002) *Species Sensitivity Distributions in Ecotoxicology.* Lewis Publishers, Boca Raton, FL, USA

Potting J (2000) *Spatial Differentiation in Life Cycle Impact Assessment. A Framework, and Site-dependent Factors to Assess Acidification and Human Exposure.* PhD thesis Universiteit Utrecht

Saouter E, Feijtel T (2000) *Use of life cycle analysis and environmental risk assessment in an integrated product assessment.* In: Hauschild M, Olsen S, Poll C, Bro-Rasmussen F (eds.) *Risk Assessment and Life Cycle Assessment*, pp 81-97. TemaNord 2000: 545, Nordic Council of Ministers, Copenhagen, Denmark

Sonnemann GW, Castells F, Schuhmacher M (2004) *Integrated Life-Cycle and Risk Assessment for Industrial Processes.* Lewis Publishers, Boca Raton, FL, USA

Toose L, Woodfine DG, MacLeod M, Mackay D, Gouin J (2004) BETR-World: A geographically explicit model of chemical fate: application to transport of a-HCH to the Arctic. *Env Poll* **128**: 223-240

Traas TP, Van de Meent D, Posthuma L, Hamers T, Kater, BJ, De Zwart D, Aldenberg T (2002) *The potentially affected fraction as a measure of ecological risk.* In: Posthuma L, Suter GW II, Traas TP (eds.) *Species Sensitivity Distributions in Ecotoxicology*, pp 315-344. Lewis Publishers, Boca Raton, FL, USA

Tukker A (2002) *Risk Analy*sis, life cycle assessment – The common challenge of dealing with the precautionary frame (Based on the toxicity controversy in Sweden and the Netherlands). *Risk Anal* **22** (5): 821-832

Udo de Haes HA, Heijungs R, Huppes G, Van der Voet E, Hettelingh J-P (2000) Full mode and attribution mode in environmental analysis. *J Ind Ecol* **4** (1): 45-56

Udo de Haes HA, Finnveden G, Goedkoop M, Hauschild M, Hertwich EG, Hofstetter P, Jolliet O, Klöpffer W, Krewitt W, Lindeijer E, Müller-Wenk R, Olsen SI, Pennington DW, Potting J, Steen B (2002) *Life-Cycle Impact Assessment: Striving Towards Best Practice.* SETAC Press, Pensacola, FL, USA

Udo de Haes HA, Heijungs R, Suh S, Huppes G (2004) Three strategies to overcome the limitations of Life-Cycle Assessment. *J Ind Ecol* **8** (3): 19-32

Wegener Sleeswijk A, Heijungs R, Erler ST (2003) Risk assessment and life-cycle assessment: Fundamentally different yet reconcilable. *Greener Management International* **41**: 77-87

Wania F, Mackay D (1995) A global distribution model for persistent organic chemicals. *Sci Total Environ* **160/161**: 211-232

White P, De Smet B, Udo de Haes HA, Heijungs R (1995) LCA back on track. But is it one track or two? *LCA News* **5** (3): 2-4

Wrisberg N, Udo de Haes HA, Triebswetter U, Eder P, Clift R (2002) *Analytical Tools for Environmental Design and Management in a Systems Perspective: The Combined Use of Analytical Tools.* Kluwer Academic Publishers, Dordrecht, The Netherlands

Appendix: Mathematical analysis of HERA and LCA

In this annex a mathematical analysis will made of both HERA and LCA, identifying which differences between the two tools are fundamental, and which differences are only secondary depending on the scope of the given study. HERA and LCA can both be regarded as dealing with a phase of release assessment or inventory analysis, and with a phase of impact assessment. Let us start with HERA. In a given region, all activities that emit a specified substances (index s) to a specified compartment (index c) are taken into consideration. Assuming a continuous flow and a steady-state release, each process or activity (index p) can be specified as emitting an amount $\Phi_{s,c,p}$. The total mass flow or emission flux ($\Phi_{s,c}$; in kg/yr) is thus given by

$$\Phi_{s,c} = \sum_{p \in region} \Phi_{s,c,p}$$

Multi-media fate models, and in particular Type III multi-media models (Mackay 2001), possibly combined with exposure models, calculate a steady-state concentration in a number of target compartments or organisms (index t) from this. A usual and convenient simplification is that the relation between emission flux and steady-state concentration is linear, neglecting second- and higher-order kinetics. The proportionality factor for fate and exposure that connects for a specified substance release compartment c and target compartment or organism t, can be written as $F_{s,c,t}$, and the resulting steady-state concentration is

$$C_{s,t} = \sum_{c} F_{s,c,t} \Phi_{s,c}$$

Effect models translate this concentration into a response indicator on target compartment or organism t. An often-used method is to construct a risk characterisation ratio (RCR) as

$$RCR_{s,t} = E_{s,t} C_{s,t}$$

where $E_{s,t}$ measures the sensitivity of target t for substance s. A convenient choice is the reciprocal of the predicted no-effect concentration (PNEC):

$$E_{s,t} = \frac{1}{PNEC_{s,t}}$$

but indicators on the basis of species sensitivity distribution are becoming increasingly popular (Huijbregts *et al.* 2002). The combination of the fate/exposure and effect assessment can be written as

$$RCR_{s,t} = \sum_{c} E_{s,t} F_{s,c,t} \Phi_{s,c}$$

Then comes the LCA. The inventory analysis yields an inventory table, a list of quantified emissions (in mass terms: m) of specified substances (index s) to specified compartments (index c); hence $m_{s,c}$. Each entry of this list is an aggregation of the mass of substance s emitted to compartment c of each of the processes that are included in the product system. The mass emitted by each process is specified as

$$m_{s,c} = \sum_{p \in world} \Phi_{s,c,p} T_p \left(fu \right)$$

where T_p is the time that process p is active for the functional unit (fu) under study. In the characterisation step of the impact assessment, each mass release is multiplied by the appropriate characterisation factor $CF_{s,c,t}$ that connects substance s emitted to compartment c to target category indicator t. Furthermore, an aggregation over release compartments and substances is performed. Thus,

$$CIR_t = \sum_{s} \sum_{c} CF_{s,c,t} m_{s,c}$$

where CIR_t denotes the impact category indicator result for target organism or impact category t. For the purpose of comparison, we need to specify how a particular characterisation factor is constructed from a fate/exposure and effect model. In fact, this is the same model as that used for HERA, but with a unit release as input:

$$CF_{s,c,t} = E_{s,t} F_{s,c,t} 1$$

Entering this into the previous formula yields

$$CIR_t = \sum_{s} \sum_{c} E_{s,t} F_{s,c,t} m_{s,c}$$

Let us juxtapose the two equations for release and impact assessment of HERA

$$RCR_{s,t} = \sum_{c} CF_{s,c,t} \sum_{p \in region} \Phi_{s,c,p} \tag{3.1}$$

and for inventory and impact assessment of LCA:

$$CIR_t = \sum_s \sum_c CF_{s,c,t} \sum_{p \in world} \Phi_{s,c,p} T_p \left(fu \right) \tag{3.2}$$

We see the following similarities (*cf.* Tukker 2002):

- characterisation factor: HERA and LCA can use the same methodology for deriving characterisation factors (CF), and probably even the same lists;
- aggregation: HERA and LCA both aggregate over initial release compartments in calculating indicators.

We can also list the differences:

- area: HERA is often restricted to one region, LCA covers the whole world;
- mode of analysis, *i.e.* the difference between a full mode and an attribution mode* (Udo de Haes *et al.* 2000): HERA takes all activities in this region fully into account, LCA takes activities into account as far as they are needed for the functional unit
- aggregation: the result of the HERA is an indicator (RCR) per target compartment (*t*) per substance (*s*), the result of LCA is an indicator (CIR) per target compartment (*t*), but aggregated across substances;
- units: the time factor (*T*) included in the LCA-formula makes the difference in units between the result of HERA and that of LCA.

Of the four differences identified above, the mode of analysis and the functional units are fundamental differences that arise from differences in goal, while the area and the aggregation are secondary differences, arising from differences in scope. Both fundamental differences are directly related to the functional unit concept.

It has been noted that the choice of a certain region for HERA is usual, but not mandatory. In principle, one may choose the world as the region here, in which case this difference disappears. As to the aggregation, measures of toxic pressure as the result of a number of chemicals is increasingly becoming available (Traas *et*

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* The dichotomy introduced here between including a process in its full extent and including it only for a part has been described at various places under various names. Udo de Haes *et al.* (2000) approach it from the technical side and use the terms full-mode and attribution-mode. Heijungs (2001) speaks of commodity-flow accounting and activity-level analysis. Barnthouse *et al.* (1997) approach this dichotomy from the consequence side and uses the terms absolute and relative to indicate these two modes. Likewise, Olsen *et al.* (2001) employ the terms absolute and comparative. Below, we will further use the terms of Barnthouse *et al.*, absolute and relative, relative meaning in relation to a functional unit.

al. 2002). Supposing both aspects would change, the basic equation for HERA would become

$$RCR_t = \sum_s \sum_c CF_{s,c,t} \sum_{p \in world} \Phi_{s,c,p} \qquad (3.1')$$

and the only difference with the basic equation for LCA, Equation (2) is the presence of the factor $T_p(fu)$, expressing the relation with the functional unit. See also Table 3.1.

Table 3.1 Overview of differences between the model structure of LCA and HERA at the conceptual and mathematical level.

conceptual analysis		mathematical analysis	
#	aspect	LCA (Eq. (3.2))	HERA (Eq. (3.1) and (3.1'))
a)	life cycle perspective	$\sum_p$	$\sum_p$
b)	product as object of analysis	–	–
c)	number of processes, chemicals, and impact categories involved	–	–
d)	range of impacts covered	–	–
e)	use of characterisation factors	CF	CF
f)	independence of time and location	–	–
g)	summation of effects of different chemicals	$\sum_s$	– and $\sum_s$
h)	emission pulses instead of fluxes	T_p	–
i)	functional unit as a basis of assessment	fu	–

In conclusion: what rests from this mathematical analysis as fundamental difference is the use of the functional unit and the mode of analysis (*i.e.*, the difference between a full mode and an attribution mode). Obviously, the two are related: the presence of the time factor (T_p) in the LCA-formula marks the difference in unit. And in its turn, the time factor has been introduced to be able to connect activities and emissions to products by means of the functional unit. Thus, the ultimate difference between the overall model structure of LCA and HERA concerns the use of a functional unit in LCA (*cf.* Olsen *et al.* 2001, Wegener Sleeswijk *et al.* 2003), and in line with that the use of the attribution mode of analysis mode of analysis (Udo de Haes *et al.* 2000).

4

Metals in the ocean: an adapted LCA fate and exposure model[*]

4.1 Introduction

One of the main output categories of human economic activity is generally characterised as products. The fact that we produce and consume products is the major cause of most anthropogenic environmental impacts. Every product may thus be held responsible for a certain amount of environmental damage. This damage is generally not only caused by the product as such or by its direct use, but also by processes, linked to production and waste management. In order to control or assess the overall environmental damage for which a product is responsible, the entire product life cycle should be accounted for.

Individual processes within the product life cycle may be controlled by operating with environmental constraints, and also by environmental monitoring, combined with the use of RA techniques. These techniques may be very specifically attuned to individual process circumstances and may give a detailed image of what is going on at a specific location.

Although environmental control of individual processes is necessary for minimising the environmental effects of each of these processes, it is generally not best for minimising the overall environmental burden of a product. Individual processes may be optimised, but it is difficult to use RA to account for the effects of substituting an entire process by another process, taking place at a different location (*e.g.* when metal parts of the product are replaced by plastic parts), let alone for the trade-off effects of such choices (*e.g.* on product durability, and thus on long-range material use and waste production). For this type of questions, product LCA is a more suitable tool.

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[*] This chapter has been published as: Wegener Sleeswijk A (2005) *Metals in the Ocean. An adapted LCA Fate and Exposure Model.* In: Dubreuil A (ed.) *Life-Cycle Assessment of Metals: Issues and Research Directions.* Society of Environmental Toxicology and Chemistry (SETAC), Pensacola (FL), USA. pp. 205-213.

While RA is thus used for control in the context of individual (production) processes, LCA is generally the preferred instrument for overall product assessment. Product assessment may be necessary for the environmental optimisation of a certain product, but also for the choice between product alternatives. In this last case, process locations are often undetermined by definition. Questions on environmental comparisons between product alternatives – for example between glass and plastic bottles, or between paper and cotton nappies – often apply to a national or even international context, thus going beyond the level of individual processes at individual locations.

The life cycle of a product may easily cover tens of processes, causing hundreds of emissions, spread over a large part of the world. In order to keep the assessment manageable and feasible, these large numbers of emissions and emission locations make it necessary to use more simplified methods for LCA than the more constrained RA methods that are usually applied for the assessment of chemicals emitted from a particular process. RA looks in detail at toxic chemical impacts, for example.

For the abovementioned reasons, LCA is by necessity a less specific instrument than RA, producing results that apply to a more general context.

One of the core parts of LCA is LCIA. In LCIA, the emissions and subtractions, caused by the product to be assessed, are quantified in the context of a number of environmental impact categories, such as resource depletion, global warming, ozone layer depletion, acidification, eutrophication, ecotoxicity and human toxicity. The toxicity-related impact categories – to which metal emissions contribute – are considered to be the most complex ones, and the preliminary attempts to tackle them belong to the most criticised parts of LCA.

One of the central characteristics of LCA is the fact that it produces results in the form of 1 quantified environmental impact score for each of the environmental impacts assessed and for each product alternative involved in the assessment. This implies that the effects of different substances not only should be quantified, but also should be added up somehow. This is accomplished by ascribing different characterisation factors to individual substances. that serve as weighting factors for the eventual relative harm in the context of each impact category, caused by the emission of a standard amount of substance. In these characterisation factors, not only environmental hazard but also the environmental residence time and exposure characteristics are discounted. Very different effect types of different substances are quantified in such a way that they become comparable.

Generally applicable models are needed in order to handle large numbers of substances in an equivalent manner. It is common practice in LCIA to make use of Mackay-type multimedia models to account for substance fate. Although these models have originally been designed for organic chemicals, Diamond *et al.* (1990, 1994) applied and validated their use for metals in an early stage. Later on, this type of application was officially recommended in the EC Technical Guidance Documents (EC 1996). The LCA characterisation factors for metals in the Handbook on Life Cycle Assessment (Guinée 2002) are based on the work of Huijbregts *et al.* (2000). These authors used the suggestions of Crommentuijn *et al.* (1997) on how to handle metals in the SimpleBox model (Brandes *et al.* 1996) underlying the fate part of their model USES-LCA. Metal-specific elimination processes in the marine environment and metal-specific exposure characteristics were not accounted for, however. This may have lead to important deviations in modelling results, causing the relative effects of metals to be possibly overestimated by orders of magnitude.

The fact that metals are relatively sensitive to such over-estimations seems to be largely caused by two facts. In the first place, metals are non-degradable, and thus remain in the environment for a relatively long time, thereby spending a relatively large part of their environmental lifetime in the ocean compartment. In the second place, metal speciation in the marine environment reduces their availability to marine organisms. The first priority for the improvement of LCIA for metals is therefore to refine the LCA fate and exposure models with respect to the behaviour of metals in the ocean. The goal of this chapter is to set a modest and tentative first step in this direction, in order to investigate possible directions for improvement within the existing context of global-scale multimedia modelling.

4.2 The GLOBOX model

The adaptations described in this model have been introduced in the GLOBOX fate and exposure model for LCA. GLOBOX is a model under construction for the calculation of spatially differentiated LCA characterisation factors on a global scale (Wegener Sleeswijk *in prep.*). GLOBOX consists of 3 main modules: an impact-category independent fate module, a human-exposure module applicable to all impact categories that are related to human exposure to chemicals, and an effect module, which contains effect-related parameters for every separate impact category. The fate and exposure modules are differentiated on the level of separate countries and oceans, which means that there are about 250 regions. Each country or ocean has its own set of homogeneous compartments, and all countries and oceans are interconnected by atmospheric and aquatic flows. Oceanic water bodies are handled as a 2-compartment system: the surface mixed layer and the deep ocean. Multimedia transport and degradation equations are taken from the European Union System for the Evaluation of Substances (EUSES) multimedia model SimpleBox 2.0 (Brandes *et al.* 1996; ECB 1997), supplemented by specific equations to account for advective air and water transport between different countries or oceans. Distribution parameters for multimedia transport are differentiated per country or ocean with respect to climatic features, water coverage, and land use. All distribution equations are solved simultaneously by matrix inversion (matrix dimension 3000×3000), allowing for the calculation of global-scale multimedia transport. Human exposure calculations are based on intake by food and drinking water consumption and inhalation of the exposed population. Exposure parameters are differentiated per country with respect to population density, estimated mean body weight, consumption pattern, fraction of drinking water derived from surface water and groundwater, respectively, and fraction of drinking water that has been purified. GLOBOX requires only substance-specific input of physico-chemical and toxicity data to calculate specific human and ecological toxicity characterisation factors for unit emissions to any compartment in any country of the world.

4.3 Adaptations

In order to adapt the GLOBOX model for metals, a small number of adaptations has been introduced. The adaptations that have been introduced so far cover the following subjects:

- speciation (with specific attention for Hg)
- adsorption to suspended particles, and
- sedimentation and vertical mixing.

Moreover, the model-dependency on parameters that make no sense in the context of metals, such as octanol-water partition coefficient, water solubility, and vapour pressure, has been eliminated.

4.3.1 Speciation

One of the most well-known metal-specific processes is speciation. Ratios between the different species depend on regional environmental properties such as temperature, acidity, the presence of complexing agents, and the medium considered.

Speciation influences both fate and exposure. With respect to fate as such, Diamond *et al.* (1992) developed an approach to account for species interconversion between species by use of specific rate constants. As they state, however: 'The practical difficulty is that the rate constants for species interconversion … are rarely known'. We therefore accounted for the influence of speciation on fate only in an implicit way, by using overall environmental transport rates for individual metals, as will be elaborated in section 4.3.4. With respect to exposure, however, we tried to account for speciation in a more explicit way.

Mainly due to the presence of complexing agents in marine waters, speciation tends to differ largely between fresh and marine waters. Because most of these complexing agents are not present in artificial test media, this factor is generally not accounted for by marine toxicity data. In order to get a good picture of the relative toxicity of metals in marine surface waters, it should be accounted for separately.

Different metal species differ with respect to their chemical and toxic properties. The bio-availability of metals is believed to be largely determined by the free ion activity, rather than by the total aqueous concentration of a metal (Morel 1983).

In the GLOBOX model, only the fraction of free ions is considered to be potentially toxic, except for Hg, for which the (highly bioavailable) organic species are taken into account separately. Relative concentrations of free ions in seawater were derived from Byrne *et al.* (1988). These values refer the ocean as a whole. Specific values for the relative amount of free ions in the mixing layer of the ocean could only be found for Cd and Zn (Nolting *et al.* 1999). Although the difference between relative free ion concentrations in the ocean as a whole on the one side and in the surface layer on the other side can be enormous – mainly due to complexation by dissolved organic ligands in the surface layer – we applied the overall values to the oceanic surface layer as well for all other metals, for lack of better data. In the test medium, we assumed the relative free ion concentrations to equal the values reported by McGloskey (1996). An overview of all values is given in Table 4.1. For the calculation of the relative bioavailability of metal ions in seawater, we used the quotient of the relative concentration seawater (surface layer if available) and test medium, respectively.

Table 4.1 Relative concentrations of free ions in seawater (derived from Byrne *et al.* at T = 5°C and pH = 8.2) in the surface layer of the ocean (Nolting *et al.* 1999), and as assumed in the test medium (McGloskey 1996).

metal	free ions in seawater (%)	free ions in surface layer (%)	free ions in test medium (%)
Cd	3.2	0.8	71
Cr	0.0011		91
Cu	12		76
Pb	5		40
Ni	68		77
Zn	73	0.9	80

4.3.2 Mercury speciation

Mercury takes a special place among metals, first because of the volatile character of its elemental species, and second because of the environmentally important role of organometalic forms (largely methylmercury). Mackay *et al.* (1995) and Diamond (1999) use a 'three species model' for Hg, in which they make a distinction between elemental, inorganic, and organic mercury. For each of these groups of species, they present partition coefficients as well as concentration fractions in each environmental medium. In order to deal with temperature dependency, Mackay *et al.* (1995) present values for the enthalpy of phase change (ΔH) along with the partition coefficients. Thus, partition coefficients (*K*) can be deduced at any desired temperature (*T*) expressed in absolute degree as

$$\mathrm{d}(\ln K)\,/\,\mathrm{d}T = \Delta H^0\,/\,RT^2 \tag{4.1}$$

where *R* is the gas constant (Van 't Hoff equation).

For inorganic Hg (and other metals), partition coefficients (among which are specific values for marine waters) are provided by Crommentuijn *et al.* (1997). For elemental and organic Hg species, we calculated partition coefficients on the basis of the values provided by Mackay *et al.* (1995). To correct for the environmental temperature of 282° K, we used the Van 't Hoff equation. The partition coefficients for partitioning between wet sediment and water, and between wet suspended matter and water, were calculated from the respective solid-water partition coefficients by assuming the volume ratio between water and solids to be 4 for sediment and 9 for suspended matter. The solid-water partition coefficient for soil was assumed to equal the corresponding sediment value. The volume ratio between solids and water was assumed to be 1 for soil, allowing for the calculation of separate soil-water partition coefficients. The aerosol-air partition coefficients were calculated from the ratio between aerosol-water and air-water partition coefficients. The fraction of the chemical associated with aerosols ($\mathrm{Fass_{aer}}$) was calculated from these values to be 1.0 for each of the 3 Hg species.

In order to make it possible to introduce Hg into the GLOBOX model without changing the model as such more than strictly necessary, a weighted mean of the partition coefficients for the three separate species was calculated for each relevant phase change. As weighting factors, the ratios in which the 3 species occur in the 'departure medium' were used.

4.3.3 Adsorption to suspended particles

Most substances in the water compartment will be adsorbed to a greater or lesser extent to suspended particles. For aquatic toxicity assessment, we leave the adsorbed fraction out of consideration in our model. The ratio between adsorbed and dissolved species of metal ions in seawater depends on the concentration and nature of suspended particles, on the mutual forces between these particles on the one hand and each individual metal on the other, and on qualities of the solvent (*e.g.* fresh or salt water). Crommentuijn *et al.* (1997) gives an overview of empirical partition coefficients between suspended matter and seawater, established for a number of metals in water of the North Sea and Wadden Sea. We have used these values as best available estimates.

4.3.4 Sedimentation and vertical mixing

In this chapter, the term 'sedimentation' is understood to refer to the gravitation-driven sinking of particles and adsorbed substances, whether or not these particles and substances eventually reach the sediment. Sedimentation in the surface mixed ocean layer thus refers to particle transport to the deep ocean layer, and not necessarily to the ocean sediment.

In the EUSES model, the sedimentation rate of organics is modelled as a function of the suspended matter-water partition coefficient, the sedimentation rate of these particles as such, and the concentration of suspended particles. For metal sedimentation in the surface mixed ocean layer, we developed a specific approach.

For metals sedimentation in the surface mixed ocean layer is a key process. The sedimentation rate of metals in the surface mixed ocean layer thus largely determines the residence times of metals in the environmental system, and therewith eventually their relative environmental impacts as assessed by LCA.

Deriving sedimentation rates from the combination of particle sedimentation rates and suspended matter-water partition coefficients – the standard procedure for organics in the EUSES model – is not satisfactory for the purpose of modelling sedimentation of metals in the surface layer of the ocean. Suspended matter is a heterogeneous mixture of particles that largely differ in size and content, and therefore also in sedimentation rate and metal adhesion. Partition coefficients are average values that do not reflect the specific adsorption of a metal to a specific kind of suspended matter. The particle sedimentation rate in the EUSES model is an average value that does not reflect the specific sedimentation rate of different kinds of particles. Combining these average values may cause deviations between the calculated and actual sedimentation rates that – if applied to the ocean surface mixed layer – may eventually produce unrealistic LCA results for metals. If possible, the use of empirical, metal-specific residence times of metals in the surface mixed layer for the estimation of sedimentation rates would be largely preferable.

Bruland (1980) gives an overview of mean residence times with respect to particulate removal of metals in a 80 m surface mixed layer of the North Pacific, estimated from measured concentrations and inputs by atmospheric fluxes and vertical mixing (Table 4.2). Other sources of in- and output, such as eddy diffusion (or convection), and horizontal advection and diffusion, are stated to play a minor role within this oceanic region, and have been left out of consideration. We adapted these residence times for a 100 m surface mixed layer, assuming a constant mean net deposition rate, and used these adapted residence times for the calculation of advective flows from the surface mixed layer to the deep ocean.

Table 4.2 Estimated atmospheric fluxes, net vertical mixing input fluxes, and mean residence times in surface mixed layer (80 m) with respect to particular removal of metals in the North Pacific (Bruland 1980).

metal	atmospheric input (nmol×cm^{-2}×y^{-1})	net vertical mixing input fluxes (nmol×cm^{-2}×y^{-1})	mean residence time (part. removal) (y)
Cd	0.0018	0.14	0.1
Cu	0.16	0.21	10
Pb	0.18	-0.01	3
Ni	0.043	0.8	20
Zn	0.40	0.15	1.0

4.4 Results and discussion

In current LCIA models, the characterisation factors for metals – used to quantify their relative environmental harmfulness – are very high in comparison to characterisation factors for organic pollutants. This phenomenon is largely caused by the fact that metals are nondegradable. According to commonly used multimedia models (*e.g.*, the EUSES model), the only ways by which metals can leave the environmental system are sedimentation and sediment burial. This makes their residence times in the environmental system – especially in the world oceans – comparatively high. Because characterisation factors are not only proportional to toxicity measures and concentrations but also to environmental residence times, the relative harmfulness of metals according to these factors may easily go against intuition.

It may be questioned whether the magnitude of the differences between present characterisation factors for metals on the one hand and organic pollutants on the other are not too high. By taking some metal-specific processes into account we have tried to set a first step towards the improvement of metal-specific LCA characterisation factors.

In Table 4.3, the results of the application of a preliminary version of our metal-adapted GLOBOX model (Wegener Sleeswijk *in prep.*) are compared to the corresponding results of the USES-LCA model (Guinée 2002). In order to avoid the biasing influence of differences in toxicity, which we will not discuss here, we focussed on exposure as such. Table 4.3 therefore lists (relative) exposure magnitudes, not characterisation factors. (The characterisation factors have been divided by their composing EFs.) It should be remarked that the comparison between GLOBOX and USES-LCA should be handled with care, first because GLOBOX and USES-LCA are different models, and second because we could only use a very preliminary version of GLOBOX in this stage. In order to make results of both models comparable, we normalised both to toluene as a reference.

Table 4.3 Relative exposure magnitudes of human population and marine ecosystems to metals, compared to toluene, caused by equally large standard emissions to the ocean compartment.

metal	relative human exposure		relative marine ecosystem exposure	
	GLOBOX	USES-LCA	GLOBOX	USES-LCA
Cd	1.88E–04	1.13E+01	7.63E+00	1.64E+04
Cr	4.80E–08	5.48E+00	1.95E–03	7.49E+03
Cu	6.57E–04	9.00E+01	2.73E+01	4.43E+04
Pb	4.97E–04	3.13E+01	2.03E+01	3.25E+03
Hg	4.15E–03	3.66E+03	1.69E+02	2.93E+04
Ni	3.67E–03	3.99E+02	1.50E+02	2.80E+05
Zn	4.63E–05	1.04E+02	1.89E+00	1.95E+04
geometric means	1.54E–04	8.27E+01	6.31E+00	2.24E+04
toluene	1.00E+00	1.00E+00	1.00E+00	1.00E+00

It appears that the metal-specific adaptations, mad in the GLOBOX model, result in a complete reversal of the original image: For human exposure, the relative exposure magnitudes are now lower for all metals than for toluene, while for marine ecosystem exposure, they are in the same order of magnitude as toluene on average. For some metals, a difference with toluene of 1 or 2 orders of magnitude remains. For human toxicity we see a difference of 5 orders of magnitude, while for marine ecotoxicity, a difference of 4 orders of magnitude shows up between GLOBOX and USES-LCA results. Although the adaptations in this preliminary version of GLOBOX are only a very first step towards adequate LCA modelling of metal-specific processes in the marine environment, these results may be considered an indication that the present chasm between LCA characterisation factors for metals and organic pollutants will most probably largely diminish if metal-specific processes are introduced into current LCA models.

In order to get a more reliable image of the relative harmfulness of metals, further research and model development are needed. A large number of possibilities to extend current LCA fate and exposure models with respect to metals remain to be explored, among which are the following:

- a more detailed and specific quantitative elaboration of the processes that we tried to cover here: metal speciation, adsorption to suspended particles, sedimentation, and vertical mixing;
- accounting for the specific organic ligand complexation in the upper mixed ocean layer for all metals;
- accounting for the kinetic aspects of metal speciation;
- accounting for the toxic aspects of complexed metals and particle-adsorbed chemicals;
- accounting for geochemical effects on environmental residence times of chemicals; and

- distinguishing between the open ocean and coastal zones as separate modelling regions.

Despite all efforts that have been made and that may be made in the future, we expect that metal emissions will still easily dominate LCA emission profiles, while this may be against intuition and knowledge of the actual relative damage caused by these substances. This phenomenon raises the question of whether the LCA approach to assess the anthropogenic environmental presence of substances merely on the basis of amounts, independently of the environmental concentrations caused by these amounts, always makes sense. It may be argued that as long as total anthropogenic emission levels of a substance do not considerably add to the natural background in a certain compartment, or alternatively, as long as concentrations remain far below environmental no effect levels, direct or indirect emissions to this compartment could be left out of consideration. Although this seems to be an attractive and sensible option, it should, in practice, be handled with great care. Multimedia models presume homogeneous concentrations and instantaneous dilution of emitted substances. Increased concentrations around emission sources remain invisible, and even increased concentrations in large areas may be averaged out by lower concentrations elsewhere in the same compartment. The fact that a certain environmental threshold is not surpassed on an average basis, as pointed out by the result of multimedia modelling application, does not imply that this threshold is not surpassed on a local level. Considerable effects may occur without being recognised by multimedia modelling alone. Further research is needed in order to enable a more specific approach that leaves out those emissions that cause no harm at all, but that maintains – possibly in an adapted form – the assessment of emissions that cause local effects.

Acknowledgement

I thank Miriam Diamond for giving many valuable comments and suggestions. This work is part of a PhD project at Leiden University, financed by Unilever.

References

Brandes LJ, Den Hollander H, Van de Meent D (1996) *SimpleBox 2.0: a Nested Multimedia Fate Model for Evaluating the Environmental Fate of Chemicals. National Institute of Public Health and the Environment (RIVM).* Report No. 719101029. Bilthoven, The Netherlands

Bruland KW (1980) Oceanographic Distributions of Cadmium, Zinc, Nickel, and Copper in the North Pacific. *Earth and Planetary Science Letters* **47**: 176-198

Byrne RH, Kump LR, Cantrell KJ (1988) The Influence Of Temperature and pH on Trace Metal Speciation in seawater. *Marine Chemistry* **25**: 163-181

Crommentuijn T, MD Polder, Van der Plassche EJ (1997) *Maximum Permissible Concentrations and Negligible Concentrations for Metals, taking Background Concentrations into Account.* National Institute of Public Health and the Environment (RIVM). Report No. 601501001. Bilthoven, The Netherlands

Diamond ML (1999). Development of a Fugacity/Aquivalence Model of Mercury Dynamics in Lakes. *Water Air Soil Pollution* **111**: 337-357

Diamond ML, Mackay D, Cornett RJ, Chant LA (1990) A Model of the Exchange of Inorganic Chemicals between Water and Sediments. *Environ Sci Technol* **24**: 713-722

Diamond ML, Mackay D, Poulton DJ, Stride FA (1994) Development of a Mass Balance Model of the Fate of 17 Chemicals in the Bay of Quinte. *J Great Lakes Res* **20**: 643-666

Diamond ML, Mackay D, Welbourn PM (1992) Models of Multi-Media Partitioning of Multi-Species Chemicals: the Fugacity/Aquivalence Approach. *Chemospere* **25**: 1907-1921

EC (1996) *Technical Guidance Documents in Support of Commission Directive 93/67/EEC on Risk Assessment for New Notified Substances and Commission Regulation (EC) No. 1488/94 on Risk Assessment for Existing Substances. Part II: Environmental Risk Assessment. EC catalogue number 002-EN-C.* European Commission (EC), Office for Official Publications of the European Community, Luxembourg

ECB (1997) *EUSES, version 1.00. European Union System for the Evaluation of Substances.* Environment Institute, European Chemicals Bureau (ECB), Joint Research Centre European Commission, EUR 17308 EN. Ispra, Italy

Guinée JB, Gorrée M, Heijungs R, Huppes G, Kleijn R, De Koning A, Van Oers L, Wegener Sleeswijk A, Suh S, Udo de Haes HA, De Bruijn H, Van Duin R, Huijbregts MAJ (2002) *Handbook on Life Cycle Assessment. Operational Guide to the ISO Standards.* Kluwer Academic Publishers, Dordrecht, The Netherlands

Huijbregsts, MAJ, Thissen UMJ, Guinée JB, Jager T, Kalf D, Van de Meent D, Ragas AMJ, Wegener Sleeswijk A, Reijnders L (2000) Priority Assessment of Toxic Substances in Life Cycle Assessment. Part I: Calculation of Toxicity Potentials for 181 Substances with the Nested Multi-Media Fate, Exposure and Effects Model USES-LCA. *Chemosphere* **41**: 541-573

Mackay D, Wania F, Schroeder WH (1995) Prospects for Modeling the Behavior and Fate of Mercury, Globally and in Aquatic Systems. *Water, Air, and Soil Pollution* **80**: 941-950

McCloskey JT, Newman MC, Clark SB(1996) Predicting the Relative Toxicity of Metal Ions Using Ion Characteristics: Microtox® Bioluminescence Assay. *Environ Toxicol Chem* **15**: 1730-1737

Morel FMM (1983) *Principles of Aquatic Chemistry*. Wiley-Interscience, NY, USA

Nolting RF, De Baar HJW, Timmermans KR, Bakker K (1999) Chemical Fractionation of Zinc versus Cadmium Among Other Metals Nickel, Copper and Lead in the Northern North Sea. *Marine Chemistry* **67**: 267-287

Wegener Sleeswijk A (*in prep.*) GLOBOX: a Spatially Differentiated Global Fate and Exposure Model.

Wegener Sleeswijk A, Kleijn R, Karman C, Bernhard R, Van der Vlies L (2003) REIMSEA: an LCA Toxicity Characterization Model for the North Sea. Supplement to 'REIM: LCA-based Ranking of Environmental Models' Including Toxicity Characterization Factors for 12 Organics and 7 Metals. CML Report 159. Centre of Environmental Science, Leiden University. Leiden, The Netherlands

5

GLOBOX: a spatially differentiated global fate, intake and effect model for toxicity assessment in LCA*

Abstract

GLOBOX is a model for the calculation of spatially differentiated LCA toxicity characterisation factors on a global scale. It can also be used for human and environmental risk assessment. The GLOBOX model contains equations for the calculation of fate, intake and effect factors, and equations for the calculation of LCA characterisation factors for human toxicity and ecotoxicity. The model is differentiated on the level of 239 countries/territories and 50 seas/oceans. Each region has its own set of homogeneous compartments, and the regions are interconnected by atmospheric and aquatic flows. Multimedia transport and degradation calculations are largely based on the EUSES 2.0 multimedia model, and are supplemented by specific equations to account for the advective air and water transport between different countries and/or seas. Metal-specific equations are added to account for speciation in fresh and marine surface water. Distribution parameters for multimedia transport equations are differentiated per country or sea with respect to geographic features, hydrology, and climate. The model has been tested with nitrobenzene as a test chemical, for emissions to all countries in the world. Spatially differentiated characterisation factors turn out to show wide ranges of variation between countries, especially for releases to inland water and soil compartments. Geographic position, distribution of lakes and rivers and variations in environmental temperature and rain rate are decisive parameters for a number of different characterisation factors. Population density and dietary intake play central

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* This chapter has been published as: Wegener Sleeswijk A, Heijungs R (2010) GLOBOX: a spatially differentiated global fate, intake and effect model for toxicity assessment in LCA. *Science of the Total Environment* **408**: 2817-2832.

roles in the variation of characterisation factors for human toxicity. Among the countries that show substantial deviations from average values of the characterisation factors are not only small and remote islands, but also countries with a significant economic production rate, as indicated by their GDPs. It is concluded that spatial differentiation between countries is an important step forward with respect to the improvement of LCA toxicity characterisation factors.

Keywords

LCA, spatial differentiation, toxicity assessment, multimedia model, global model, actual impacts

5.1 Introduction

The life cycles of products 'from cradle to grave' comprise large numbers of economic processes, including mining activities, agricultural and industrial processes, product use activities, and waste processing. A product life cycle may consist of tens to hundreds of processes, taking place in many different parts of the world. In product life cycle assessment (LCA), the environmental effects of all these processes can be quantified, resulting in an environmental profile. This profile comprises different categories of environmental impacts (the so-called 'impact category indicators'), ranging from global warming to more regional and local effects like acidification and local toxicity-related impacts. A formalised framework for LCA has been defined by the International Organization for Standardization, in the 14040 series (ISO, 2006a,b). This framework offers guidelines for the overall structure and terminology of LCA methods. With respect to toxicity assessment, Pennington *et al.* (2006) contrast risk assessment for regulatory purposes, in which worst-case situations and safety factors are import elements, with comparative risk assessment and LCA, in which a more realistic and fair comparison is the aim. This chapter builds on the comparative paradigm.

Much progress has been made during the past ten years by the introduction of the multimedia modelling concept into LCA toxicity characterisation (*cf.* Guinée and Heijungs, 1993), which has been explicitly recommended by the Society of Environmental Toxicology and Chemistry (SETAC) Europe First Working Group on Life-Cycle Impact Assessment (WIA-1) (Hertwich *et al.*, 2002). Spatial differentiation of these models on a global scale can be considered as a natural next step.

Multimedia environmental models – as first proposed by Mackay (1991) are widely used for toxicity characterisation in LCA. Commonly used models include USES-LCA (Huijbregts *et al.*, 2000; Van Zelm *et al.*, 2009), CalTOX (Hertwich *et al.*, 2001), IMPACT 2002 (Pennington *et al.*, 2005) and USEtox (Rosenbaum *et al.*, 2008). In environmental risk assessment – for which most multimedia models have originally been designed – the spatial scope of the fate and intake model is generally linked to the magnitude of the region for which it is to be applied, and its direct surroundings. Product life cycles, however, usually include processes from all over the world. For this reason, the spatial scope of regional models should be expanded for use in LCA. This implies that the ranges of model parameters, such as environmental temperature or meat consumption, will largely increase, which brings up the question whether spatial differentiation may be inescapable for fate and intake assessment in LCA.

The subject of spatial differentiation in LCA has been pioneered by Potting (2000) with practical applications for acidification (Potting *et al.*, 1998) and for human exposure to air emissions. Other early studies on the subject include those by Hertwich *et al.* (2001), McKone *et al.* (2000), Nigge (2000), Krewitt *et al.* (2001) and Schulze (2001).

Several authors have introduced spatial differentiation into comprehensive LCA impact assessment models (*cf.* Huijbregts *et al.*, 2003; Hauschild and Potting, 2005; Potting and Hauschild, 2005; Pennington *et al.*, 2005; Rochat *et al.*, 2006; Humbert *et al.*, 2009). In some spatially differentiated multimedia models, a difference is made between an evaluative region (for which emissions can be entered in the model) and a larger, encompassing region of dispersion, in which the emission region is nested. In the USES-LCA model (Huijbregts *et al.*, 2000; Van Zelm *et al.*, 2009), the evaluative region at the continental level (Western Europe) is not spatially differentiated, but the dispersion region (the northern hemisphere) is characterised by its own environmental parameters for three different climate zones. Huijbregts *et al.* (2003) evaluated the influence of spatial differentiation at the continental level by comparing three different versions of the USES-LCA model, with Western Europe, the United States and Australia as three alternative continental levels. Pennington *et al.* (2005) have introduced spatial differentiation in the IMPACT 2002 model at three levels: the level of Western European watersheds (for soil and surface water) and grid cells (for air and sea/ocean), the continental level of Western Europe, and the global level, in which the continental level is nested. Emissions can be entered at the watershed/grid cell or at the continental level. Rochat *et al.* (2006) have applied spatial differentiation at the level of continents to a global version of the IMPACT 2002 model with respect to both emission and dispersion. Another regionally differentiated multimedia model, that has not been designed specifically for LCA, but that has been used in the LCA-context, is BETR-North America (MacLeod *et al.*, 2001). This model comprises North America, differentiated at the level of ecological regions. Humbert *et al.* (2009) recently developed the IMPACT North America model, in which the evaluative region North America – which is nested into a global dispersion level – is differentiated at the level of several hundred zones.

Global, spatially differentiated fate models that are not specifically designed for LCA include Globo-POP (Wania and Mackay, 1995), BETR-World (Toose *et al.*,

2004) and BETR-Global (MacLeod *et al.*, 2005). These models are primarily designed for the analysis of the global distribution of persistent organic pollutants (POPs), *i.e.* the 'global fractionation' phenomenon. In principle, these models could also form a useful basis for LCA-directed global fate modelling.

The GLOBOX model for LCA toxicity assessment comprises the entire world. With respect to the basis of spatial differentiation, four types of possibilities had to be considered:

1. Differentiation on the basis of ecozones (*e.g.* Webster *et al.*, 2004). This type of regionalisation defines the region according to homogeneous ecological conditions. It is basically an effect-oriented differentiation.
2. Differentiation on the basis of watersheds (*e.g.* Pennington *et al.*, 2005). Here the regions are defined according to distribution-oriented features, with emphasis on the distribution of chemicals in the aquatic compartment.
3. Differentiation on the basis of grid cells (*e.g.* Prevedouros *et al.*, 2004). This method of defining regions easily connects with GIS-available data, *e.g.*, on vegetation, population, and wind.
4. Differentiation on the basis of political boundaries, *e.g.* continents and oceans or countries and seas. This is primarily an inventory-driven approach, for instance it connects with country-specific emission databases, like ecoinvent or the TRI. But of course, there are also intake-related parameters (like food consumption patterns) which are available at this level.

Since LCA studies often have to deal with large numbers of emissions to different environmental compartments, an inventory-driven approach is specifically interesting in the context of LCA. For this reason, spatial differentiation in the GLOBOX model is based on political boundaries. In order to account for the large differences in human intake characteristics that exist within continents, the level of countries and seas was chosen as the basis of differentiation. GLOBOX is a level 3 (or steady state) multimedia model (Mackay, 1991), based on the European Union model EUSES 2.0 (EC, 2004), and can be considered as an extended and more refined elaboration of this model.

The main goals of the GLOBOX model are:

1. Accounting for spatial variation in fate, intake and effect parameters at the level of countries/territories and seas/oceans.
2. Accounting for the global range of life cycles.
3. Accounting for life cycle processes outside the Euro-American and Japan regions.

The idea behind the model is that LCA requires region-specific characterisation factors (CFs) for releases of any toxic chemical at any location in the world. These factors should account for the summed impacts of such an emission in all countries/territories (further referred to as 'countries') and seas/oceans (further referred to as 'seas') over which it is dispersed during its lifetime.

GLOBOX basically consists of three related parts. First, it is a mathematical model for fate, intake and effect. Second, the mathematical equations contain many regionalised parameters, such as temperature, lake depth and leaf crop consumption. This chapter describes some of the estimation routines. The regionalised parameters themselves are available as the GLOBACK data set. Third, the model equations and an interface with the GLOBACK data set have been implemented in software. The GLOBOX software program, a full list of model equations, and the GLOBACK parameter set are downloadable from cml.leiden.edu.

5.2 The GLOBOX model

5.2.1 Model structure

GLOBOX is based on the EUSES 2.0 model (EC, 2004). Apart from a higher level of spatial differentiation, the main difference between GLOBOX and EUSES 2.0 is a difference in model structure: while the EUSES 2.0 unit world consists of a number of scales that are nested into each other, the GLOBOX environmental assessment system consists of a series of interconnected regions at the same modelling level.

Like most general purpose fate-exposure-effect models (Rosenbaum *et al.*, 2007), the GLOBOX model consists of three main modules: an impact category independent fate module, a human intake module, applicable to all impact categories that are related to human intake of chemicals, and an effect module, in which effect-related parameters can be introduced for every separate impact category. The effect module is the only module that focuses on impact category specific processes and data. Both other modules are impact category independent. The impact category specific character of the characterisation factor – which is the product of fate-, intake and effect factor – is thus determined by the effect factor only.

A specific parameter set – GLOBACK – contains estimates on fate and intake-related parameters for each separate country and sea. All data can be overruled by the user's own estimates if desired. The model requires only substance-specific input of physico-chemical and toxicity data to calculate specific human and ecological toxicity characterisation factors for unit emissions to any compartment in any country of the world. The principal characteristics of the GLOBOX model are listed in Table 5.1.

Table 5.1 Summary table of principal characteristics of the GLOBOX model.

model quality	elaboration
basics	multimedia model based on EUSES 2.0
impact categories (toxicity related)	human toxicity (carcinogenic and non-carcinogenic) and ecotoxicity (aquatic (separate for river, lake and salt lake) and terrestrial)
fate, intake and effect	all included
emissions compartments	air; rivers, freshwater lakes, salt lakes; seawater; natural soil, agricultural soil; urban soil
distribution compartments	air, rivers, freshwater lakes, salt lakes, groundwater, seawater, freshwater lake sediment, salt lake sediment, sea sediment, natural soil, agricultural soil, urban soil
chemicals considered	organic chemicals and metals
spatial variation	distinction between 239 different countries and 50 different seas (global scale)
intake routes considered	air, drinking water, leaf crops, root crops, meat, dairy, freshwater fish, sea fish
additional options to basic model	taking into account above- and below-threshold concentrations separately. (Requires additional data input). Risk assessment calculations (steady state), *e.g.* emission scenarios.
chemical input and model parameters	model parameters included in model (can be changed by user); chemical input to be entered by user
distinct features of model	global range of model; high level of spatial differentiation; accounting specifically for cold regions and salt lakes; specific equations for metals in water

The combination of a global range and a high level of spatial differentiation is the central feature that distinguishes the GLOBOX model from other LCA multimedia models. 239 individual countries/territories (CIA, 2004) and 50 individual seas/oceans (IHO, 1986) form the basic level of spatial differentiation in the model.

At the level of effect assessment, the model contains specific equations for the distinction between potential and actual impacts. Two aspects are accounted for in this context: first the difference between sensitive and insensitive areas, and second the difference between areas with prevailing environmental concentrations above and below environmental threshold levels, as we proposed earlier (Wegener Sleeswijk, 2003).

The *Supporting information* provides further details on aspects such as a spatially differentiated version of the global hydrological cycle, constructed for the GLOBOX model, the treatment of cold regions, and metal-specific model features.

5.3 Fate

5.3.1 General

Multimedia transport and degradation calculations are largely based on the multimedia fate model in EUSES 2.0, and are supplemented by specific equations to account for environmental-flow-mediated (advective) air and water transport between different countries and/or seas. All distribution equations are solved simultaneously by matrix inversion, allowing for the calculation of global-scale multimedia transport. The model-internal output of the fate module, applied to a standard emission of a certain substance to a certain compartment, is a list of approximately 3000 fate factors describing the specific spatial distribution of this emission over all environmental boxes. These factors can be considered as the time-integrated amounts of substance in all individual boxes that result from the given standard emission (Heijungs, 1995).

5.3.2 Specific features of the GLOBOX fate module

The fate module is differentiated with respect to geographic, geophysical, climatological, intermedia transfer and water-balance-related parameters. In addition to the subjects covered by the EUSES 2.0 model, a number of fate-related subjects are explicitly addressed in the GLOBOX model:

- cold regions: permanent or temporal ice cover of land and sea areas
- rivers, freshwater lakes and internally drained (endorheic) salt lakes as three separate inland water compartments
- groundwater as a separate compartment
- irrigation of agricultural soil with surface water and groundwater, respectively
- metal-specific equations.

EUSES 2.0 is spatially differentiated on the basis of a limited number of spatially differentiated parameters. The GLOBOX fate module has a wider range of spatial differentiation. In Table 5.2, the spatially differentiated parameters in the fate module of the GLOBOX model are listed, together with the sources from which the values have been extracted or derived. Parameters that have not been spatially differentiated are not included in this table. The values of these last parameters have been set to the corresponding parameter values in the EUSES 2.0 model (*e.g.* 1000 m for the atmospheric mixing height).

Table 5.2 Spatially differentiated fate parameters in the GLOBOX model.

parameter	sources used (direct or for derivation)
area of country lengths of land boundaries[a] lengths of coastlines[a]	CIA (2000, 2004)
fraction natural, agricultural and urban soil	CIA (2000, 2004); UNSD (2007); WRI (2000)
land area, covered by freshwater lakes[b] land area, covered by endorheic salt lakes[a] total depths and mixing depths of lakes[b] water residence time in lakes[b]	Babkin (2003); CIA (2004); ILEC/UNEP (1994, 1995, 1996); LakeNet (2004); Statistics Finland (2004); SWCSMH (2004)
area of lake sediment that is part of the system	follows from assumption on maximum mixing depth
area of sea total depth of sea[b]	Statistics Finland (2004); Van der Leeden *et al.* (1990)
area of sea sediment that is part of the system	follows from assumption on maximum mixing depth
lengths of sea boundaries[a]	calculations, based on latitudes and longitudes at the border edges
permanent ice cover of land (glaciers and ice fields)*	CIA (2004); Statistics Finland (2004)
mixing depth of the natural and urban soil compartments[b] suspended matter concentration in inland waters and seawater[b] fraction of solids in soil runoff[b] fractions of air, water and solids in natural, agricultural and urban soil[b] fraction of organic carbon in soil, lake and sea suspended matter and lake and sea sediments[b] sea temperature[b] fraction of sea area covered by ice[b] deposition rate of aerosol particles[b]	Wania & Mackay (1995); Troll & Paffen (1966)
concentration of hydroxyl radicals in air[b]	Toose *et al.* (2004)
temperature (countries) wind speed (countries) temporal ice cover (lakes)[a]	Nellestijn & Dekker (1995); long year averages (30 years); values, measured at weather station in or near capitals used as approach for country-scale values
rain rate (countries)[b]	FAO (2004); Nellestijn and Dekker (1995); Korzoun *et al.* (1977) (for Antarctica)
rain rate (seas)[b]	Babkin (2003); Korzoun *et al.* (1977); Van der Leeden *et al.* (1990)
river inflows from other countries	FAO (2004)

parameter	sources used (direct or for derivation)
river outflows to other countries	
water runoff from soil	
water flow from soil to groundwater	
water flow from groundwater to river water	
groundwater inflows from other countries	
groundwater outflows to other countries	
use of surface water for sprinkling and irrigation[a]	FAO (2004); WRI (2004)
use of groundwater for sprinkling and irrigation[a]	
water flow from groundwater to sea	
volume of rivers[a]	Shiklomanov & Rodda (2003)
volume of ice shields[a]	
evaporation rate from lakes	climate-dependent assumptions
evaporation rate from salt lakes	
river outflows to sea	FAO (2004); Gleick (1993); balancing items

[a] Not included in EUSES 2.0.

[b] Not differentiated in EUSES 2.0.

5.3.3 Compartments

Twelve distribution compartments are distinguished: air, rivers, freshwater lakes, freshwater lake sediments, salt lakes, salt lake sediments, natural, agricultural and urban soil, groundwater, seawater, and seawater sediments. Compared to EUSES 2.0, salt lakes, salt lake sediments, and groundwater are additional compartments. The distinction of river and freshwater lake as two separate freshwater compartments is new as well. Only endorheic salt lakes are accounted for in the salt lake compartment – salt lakes with an open connection to the sea are excluded from the assessment. The separate distinction of endorheic salt lakes (and their sediments) makes it possible to pay attention to the vulnerability of the ecosystems in these compartments, from which pollutants cannot escape by water outflow. Groundwater is distinguished as a separate compartment in order to deal with the influence of groundwater pollution on the quality of drinking water and irrigation water. Finally, the distinction between rivers and lakes as separate freshwater compartments makes it possible to account for the large regional differences in residence time between freshwater compartments in different countries, caused by relative differences in lake volume. Reservoirs are considered to be part of the *freshwater lake* compartments.

5.3.4 Intramedium transport

The *Supporting information* contains further details on the transport of a chemical between the air compartments of adjacent regions, between different types of aquatic compartments within each region, into and between the seas, and into the groundwater. It also provides information on the subdivision of the soil compartment regarding various types of soil use.

5.4 Human intake

5.4.1 General

Human intake characteristics are decisive for the eventual human exposure to pollutants in the environment. In Table 5.3, the spatially differentiated parameters in the human intake module of the GLOBOX model are listed, together with the sources from which their values have been extracted or derived.

Table 5.3 Spatially differentiated human intake parameters in the GLOBOX model.

parameter	sources used (direct or for derivation)
population	CIA (2004)
average human body weight[b]	CIA (2004); World Bank (2000)
air inhalation rate[b]	CIA (2004)
drinking water consumption[b]	CIA (2004)
origin of drinking water (groundwater or surface water)	WRI (2004)
purification of drinking water from surface water (fraction)[b]	UNSD (2004)
food consumption for each food category (leaf crops, root crops, dairy products, meat, freshwater fish, marine fish)[b]	FAO (2000)
food import for each food category[a]	FAO (2000)
food export for each food category[a]	FAO (2000)

[a] Not accounted for in EUSES 2.0.

[b] Not differentiated in EUSES 2.0.

A detailed description on how these parameters have been derived is given in the *Supporting information*.

5.4.2 Intake fraction versus characterisation factor

Although LCIA needs characterisation factors, many authors nowadays concentrate on the intake fraction (iF) in their publications on human toxicity assessment in LCIA (c.f. Pennington *et al.*, 2005; Huijbregts *et al.*, 2005; Rochat *et al.*, 2006; Rosenbaum *et al.*, 2008; Humbert *et al.*, 2009). There is a fundamental reason why we made another choice here. The intake fraction expresses the fraction of a chemical, wherever released, that enters the population, wherever the individuals live (Bennett *et al.*, 2002). The body weight of these individuals is not accounted for in this variable. In the GLOBOX model, values for the human body weight are regionally differentiated, ranging between 30 kg (for four African countries) and 70 kg (for Vatican City), depending on the degree of welfare and the relative number of children. Although it may be questioned whether the introduction of a body weight (with a variation of only a factor 2) makes enough difference to justify the introduction of an extra complication, we like to emphasise the more fundamental side of it in this chapter, in which the relative role of different modelling parameters takes such a central place. It is in that context that we focus on the characterisation factor instead of the intake fraction.

For a related reason, we replaced the production-based approach for determining the intake by humans (Pennington *et al.*, 2006) by a consumption-based approach, accounting for the intake per kilogram of body weight. Thus, if polluted food is consumed by a population, characterised by a relatively low average body weight, the resulting impact will be relatively high, and vice versa. A drawback of this approach is the fact that the modelling of export and import of food requires data and assumptions that may introduce additional uncertainty. Nevertheless, we believe that the principle of using a consumption-based approach in combination with a regionalised body weight is an innovative feature of GLOBOX that deserves a further discussion as to its practical trade-off between accuracy and precision.

5.5 Toxic impacts

5.5.1 General

Region-specific values for toxicity data like EC_{50} and ED_{50} (median Effect Concentration and Dose, respectively) values are not available for most chemicals. This does not imply, however, that it should be impossible to add any region-specific information on toxicity as such. In an earlier publication, we advocated the introduction of the possibility to distinguish between sensitive and non-sensitive areas and between areas with prevailing concentrations above and below a certain environmental threshold (Wegener Sleeswijk, 2003). This distinction is sometimes also referred to as the difference between 'actual' and 'potential' impacts (White *et al.*, 1995). Although LCA traditionally focuses on potential impacts, we have introduced the possibility to choose for an assessment of 'above threshold' effects in the effect module of the GLOBOX model. To this end, two new, both chemical and impact category specific parameters are introduced: the *sensitivity factor* (SF) for ecotoxicity and the *threshold factor* (TF) for both ecotoxicity and human toxicity.

The sensitivity factor reflects the fraction of area that is sensitive to a certain chemical, *e.g.* the fraction of area covered by sensitive ecosystems, while the threshold factor reflects the fraction of sensitive area where a predefined no-effect level for the ecosystem concerned (*e.g.* the *hazardous concentration 5%* (HC_5): the concentration above which 5% of species are adversely affected) is exceeded by the existing background concentration of that chemical. A low value of the sensitivity factor reflects the situation that a large part of a region does not house sensitive species. This may be the case in highly urbanised regions, on bare rocks, where terrestrial ecosystems are almost lacking, or in regions where aquatic or terrestrial ecosystems do occur, but not the species that are sensitive to a specific chemical. A low value of the threshold factor reflects the situation that the background concentration exceeds the threshold value in only a limited part of the region, *e.g.* around a certain factory. Note that SF and TF reflect the presence of actual impacts of a chemical in a region. They do not concern the severity of an impact (Humbert *et al.*, 2009) or the safety margin in case of incomplete data for regulatory purposes (Pennington *et al.*, 2006).

As a default, SF and TF are both set to a value of 1. Available information on (in)sensitive areas or on a distinction between above and below-threshold situations can be added in a simple and consistent way by estimating the SF and/or the TF, reflecting the fraction of the area of each region that is sensitive to a certain chemical, or the fraction of area where a certain threshold is (almost) reached or exceeded.

5.5.2 Characterisation of toxic impacts

The GLOBOX model combines fate-, intake and effect factors for the calculation of region-specific toxicity characterisation factors. The physico-chemical and toxicity-related data, needed as input for the exemplifying calculations in this chapter, were taken from the USES-LCA 1.0 model (Huijbregts *et al.*, 2000), which includes substance-specific data sets. With respect to toxicity, the USES-LCA 1.0 data set lists DALYs (*disability adjusted life years*) for human toxicity and PDFs (*potentially disappeared fractions*) for aquatic and terrestrial ecotoxicity.

Toxicity-data may vary among different sources, not only with respect to their values, but also with respect to toxicity modelling. For use in LCA, it is important that the toxicity data for different chemicals reflect the best estimate of toxicity ratios between different chemicals as well as possible, without uncertainty-dependent safety margins that are sometimes used for risk assessment purposes.

Characterisation factors for the calculation of spatially differentiated potential impacts are calculated as the volume-weighted (for ecotoxicity) or population-weighted (for human toxicity) average RCR-values:

$$IPECRtox_{eco} = \frac{\sum_{j \in L} \left(RCRtox_{eco}(j) \times V_{comp}(j) \right)}{\sum_{j \in L} \left(V_{comp}(j) \right)}$$

for ecotoxicity and

$$IPECRtox_{hum} = \frac{\sum_{j \in L} \left(RCRtox_{hum}(j) \times Npop(j) \right)}{\sum_{j \in L} Npop(j)}$$

for human toxicity, where $IPECRtox_{eco}$ (–) and $IPECRtox_{hum}$ (–) are the *integrated potential effect characterisation ratios* for ecotoxicity (terrestrial, river, freshwater lake, salt lake or seawater) and human toxicity, respectively, $RCRtox_{eco(j)}$ (–) and $RCRtox_{hum(j)}$ (–) are the *risk characterisation ratios* for region j for ecotoxicity and human toxicity, $V_{comp(j)}$ (m^3) refers to the volume of the compartment in region j where the corresponding ecosystem dwells (soil, river, freshwater lake, salt lake or seawater), $N_{pop(j)}$ (–) is the human population in region j and L is the total set of regions. Human toxicity may refer to carcinogenic or to non-carcinogenic toxicity.

Multiplication of the (unweighted) characterisation factors for the potential effect by the sensitivity factor and the threshold factor yields the 'actual' impact score:

$$IAECRtox_{eco} = \frac{\sum_{j \in L} \left(RCRtox_{eco}(j) \times V_{comp} \times SF_{eco}(j) \times TF_{eco}(j) \right)}{\sum_{j \in L} \left(V_{comp}(j) \right)}$$

for ecotoxicity and

$$IAECRtox_{hum} = \frac{\sum_{j \in L} \left(RCRtox_{hum}(j) \times Npop(j) \times TF_{hum}(j) \right)}{\sum_{j \in L} Npop(j)}$$

for human toxicity, where $IAECRtox_{eco}$ (–) and $IAECRtox_{hum}$ (–) are the *integrated actual effect characterisation ratios* for ecotoxicity and human toxicity, $SF_{eco(j)}$ (–) is the sensitivity factor for ecotoxicity and $TF_{terr(j)}$ (–) and $TF_{hum(j)}$ (–) are the threshold factors for ecotoxicity and human toxicity, respectively. The sensitivity factor is not defined for human toxicity because all human populations are assumed to be equally sensitive to the chemicals to be assessed.

It is usual in LCA to define toxicity characterisation factors in relation to the emission of a reference substance to a certain reference compartment:

$$CF_{toxpot}(s) = \frac{IPECRtox(s)}{IPECRtox(ref)}$$

for potential impacts and

$$CF_{toxact}(s) = \frac{IAECRtox(s)}{IAECRtox(ref)}$$

for actual impacts, to be used for ecotoxicity ($CF_{tospoteco}$ (–) and $CF_{toxacteco}$ (–)) and human toxicity ($CF_{tospothum}$ (–) and $CF_{toxacthum}$ (–).

5.6 Results for nitrobenzene

5.6.1 General

In order to test the GLOBOX model, sets of characterisation factors have been calculated for nitrobenzene as a test chemical (see Table 5.4 for the physico-chemical properties and the degradation rate constants of nitrobenzene). Since there are 239 countries with each up to seven possible emission compartments, 50 seas with each two possible emission compartments, and seven toxicity-related impact categories, each set of characterisation factors for a certain chemical consists of up to ((239×7)+(50×2))×7=12411 numbers. In practice, this is somewhat less, since not all compartments exist in every country, and some substances may exert no effect for some impact categories.

Table 5.4 Physico-chemical properties and degradation rate constants of nitrobenzene.

physico-chemical properties			degradation rate constants at 25° C		
parameter	unity	value	parameter	unity	value
molecular weight	g/mol	123	rate constant for degradation in air	s^{-1}	7.00E–08
vapour pressure at 25 °C	Pa	33	rate constant for photolysis in water	s^{-1}	7.74E–08
solubility at 25 °C	mg/l	1 921	rate constant for biodegradation in bulk surface water	s^{-1}	1.56E–07
melting temperature	°C	6	rate constant for biodegradation in aerobic sediment	s^{-1}	1.56E–07
octanol-water partition coefficient (K_{ow})	–	69	rate constant for biodegradation in anaerobic sediment	s^{-1}	1.60E–06
organic carbon-water partition coefficient (K_{oc})	l/kg	156	rate constant for biodegradation in bulk soil	s^{-1}	1.56E–07

Source: Huijbregts *et al.* (2000).

The emission of nitrobenzene to Dutch air was chosen as a reference emission in CF calculations. Different calculations were performed in order to give an indication of the answers to the main research questions, related to spatial differentiation:

- Does spatial differentiation cause substantial differences between LCA toxicity characterisation factors?
- Which environmental parameters are primarily responsible for the spatial variation in characterisation factors?
- How can differences between extreme values of characterisation factors be explained?
- To which extent is spatial differentiation in LCA toxicity assessment necessary with respect to the reliability of LCA outcomes?

- For which countries is spatial differentiation – instead of the use of standard EU CFs – important?

5.6.2 Differences between characterisation factors

Differences between characterisation factors for a certain impact category and a certain chemical, released to a certain compartment, can be analysed and described in many different ways. In this chapter, we have chosen for the interquartile range (IQR), in relation to the median. Abbreviations, used for the emission compartments, are given in Table 5.5.

Table 5.5 Emission compartments and abbreviations, used throughout this chapter.

emission compartment[a]	abbreviation
air	air
agricultural soil	agr
urban soil	urb
river water	riv
fresh lake water	lake
salt lake water	salt

[a] *Natural soil* and *seawater* are also possible emission compartments in the GLOBOX model, but have not been used for the calculations in this chapter.

Since we are primarily interested in CFs that apply to emissions in inhabited countries, we excluded uninhabited territories and sea areas as emission regions (but not as effect regions) from the statistical calculations in this chapter. Greenland was excluded as well, because its extreme environmental circumstances causes CFs for emissions in Greenland to be so extreme that they would fully dominate CF ranges for most impact category/emission compartment combinations, and thus create a distorted image of these ranges, while in global perspective, Greenland is quite unimportant from an emission point of view.

Total ranges, interquartile ranges and median values of the CFs for inhabited countries excluding Greenland are represented in Figure 5.1.

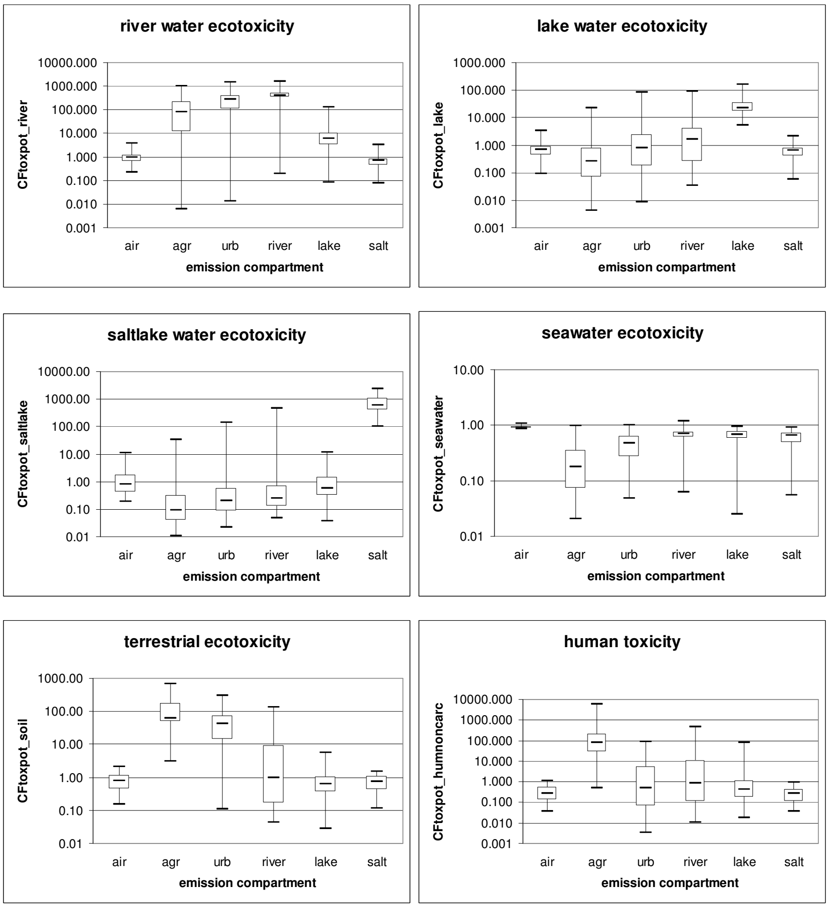

Figure 5.1 Total ranges, interquartile ranges and median values of the GLOBOX characterisation factors (potential impacts) for nitrobenzene for different impact categories and emission compartments.

Total ranges of characterisation factors turn out to vary by orders of magnitude for almost all impact categories and emission compartments. Interquartile ranges are much smaller, but may still be considerable, especially for the human-toxicity related impact categories. This implies that, at least for nitrobenzene emissions, spatial differentiation has a substantial influence on the magnitude of characterisation factors for a large number of countries.

5.6.3 Individual parameters and characterisation factors: a sensitivity analysis

Due to the complexity of the web of equations, embedded in the GLOBOX model, it is difficult to establish the relationship between individual parameters on the one hand and characterisation factors on the other directly from model equations. An analysis of the model outcomes may, however, deliver new insights into the relative importance of individual parameters for the resulting CFs. To evaluate which of the environmental parameters are primarily responsible for the large spatial variation in characterisation factors, a sensitivity analysis was performed. To this end, an alternative version of the GLOBACK parameter set was constructed, with minimal spatial variation, setting all easily adaptable parameters to (weighted) average values.* Full spatial differentiation was first compared to minimal spatial differentiation – with all easily adaptable parameters set to their average values for inhabited countries (except Greenland) and for seas. No average values could be applied to geographic parameters like *total surface area* and *border length*, or to flow parameters like *river inflow* and *river outflow*, since this would disturb the internal coherence of the geographic system and the global water balance, respectively. The total range of the characterisation factors, resulting from 'full differentiation' versus 'minimal differentiation', is represented in Figure 5.2. Relative ranges are especially large if characterisation factors are strongly dependent on emission locations, *e.g.* for river emissions in countries with salt lakes (where rivers may end up in a salt lake) versus river emissions in countries without salt lakes (which usually end up in seas). It is clear from Figure 5.2 that the influence of geographic and flow parameters alone on the range of characterisation factors is substantial for most impact category/emission compartment combinations. The additional range of the fully differentiated version reflects the influence of all other parameters together. Since each individual parameter may cause either an increase or a decrease of the characterisation factor, influences may (partly) balance each other. This implies that the difference in range between *full differentiation* and *minimal differentiation* is not automatically indicative for the influence of individual parameters. A large difference indicates that there should be at least one additional parameter that has a significant influence on the range of the characterisation factor. A small difference indicates either that geographic and flow parameters are dominant or that other influential parameters compensate each other's impact on the range of the characterisation factor.

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* Some parameters had to be slightly adapted in order to have the switch-off of spatial differentiation make sense, *e.g.* in the case of population: equal population densities – not equal populations as such – were applied for the different countries.

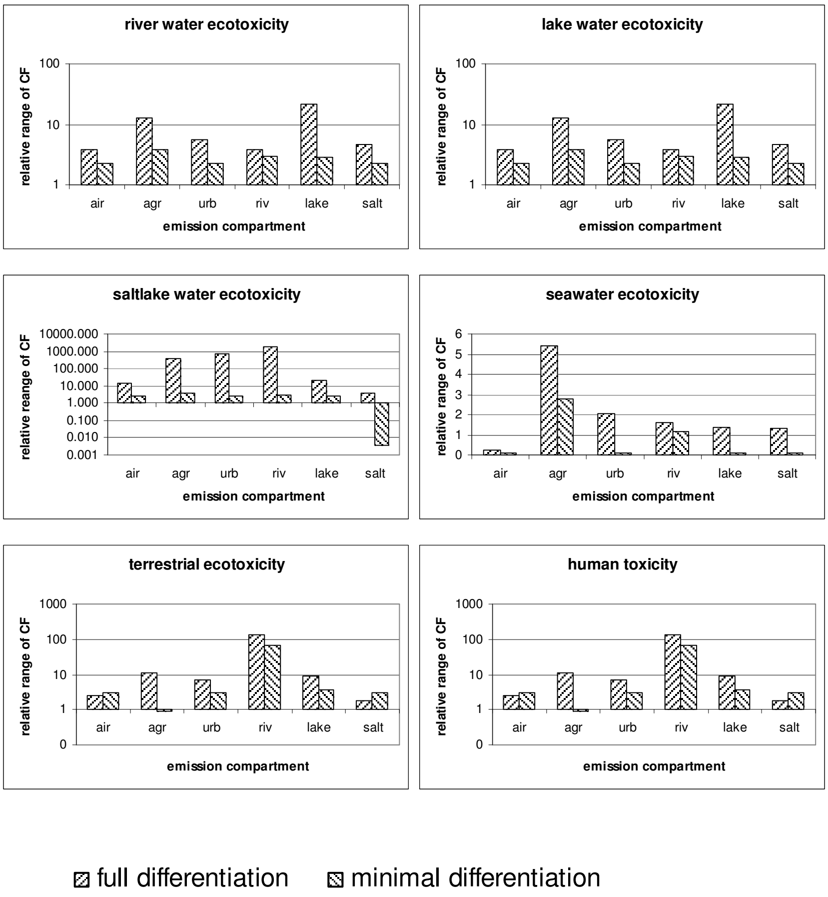

Figure 5.2 Relative range (range divided by mean) of GLOBOX characterisation factors for nitrobenzene, resulting from 'full differentiation' versus 'minimal differentiation'

To evaluate the influence of each single parameter, the entire set of characterisation factors was recalculated for 15 additional variant versions of the GLOBACK parameter set. For each set, minimal spatial variation was applied to all parameters or parameter categories but one. The differences in outcome between the version with minimal spatial variation and each of the variants with one spatially differentiated parameter indicate the relative contribution of this parameter to the total influence of spatial differentiation on the values and ranges of the characterisation factors. In Table 5.6, the parameters that cause a deviation of more than 25% from the median or the interquartile range of the variant with minimal spatial differentiation are indicated for each impact category and emission compartment.

Table 5.6 Parameters that cause a deviation of more than 25% from median nitrobenzene CFs (normal font), inter quartile range (italics) or both (bold), compared to the situation with minimal differentiation.

> 25% influence of parameter differentiation on CF for emission compartment mentioned[1]						
parameter	aquatic ecotoxicity (river)	aquatic ecotoxicity (lake)	aquatic ecotoxicity (salt lake)	aquatic ecotoxicity (seawater)	terrestrial ecotoxicity	human toxicity[5]
area division nat/agr/urb	–	–	–	agr	urb	urb
lake parameters[3]	*riv*, salt	air, agr, urb, riv, lake, *salt*	air, agr, urb, *riv*, *lake*, salt	lake, *salt*	lake, salt	urb, riv, lake, salt
river volume	*air*, *agr*, *urb*, riv, lake, *salt*	*riv*, *urb*	*riv*, *urb*	*riv*	riv	riv
ice cover	–	*lake*	–	*lake*	–	–
area sea sediment	–	–	–	–	–	–
geophysical parameters[4]	–	–	–	–	–	–
temperature	agr, *lake*	agr, urb, *riv*, *lake*	agr, urb, *salt*	*air*, lake, *salt*	agr, *urb*, lake	agr, urb, lake
wind speed	–	*lake*	*salt*	*lake*	–	–
rain rate	–	agr, *lake*	*agr*, *riv*		*air*, *lake*, *salt*	*air*, *salt*
population (density)	n.a.	n.a.	n.a.	n.a.	n.a.	agr, *urb*, *riv*, lake
mean body weight	n.a.	n.a.	n.a.	n.a.	n.a.	–
fraction of population with access to safe drinking water	n.a.	n.a.	n.a.	n.a.	n.a.	–
fraction of drinking water that is groundwater	n.a.	n.a.	n.a.	n.a.	n.a.	–
dietary intake	n.a.	n.a.	n.a.	n.a.	n.a.	air, *agr*, riv, salt
food import/export	n.a.	n.a.	n.a.	n.a.	n.a.	–
sea fish catch per sea	n.a.	n.a.	n.a.	n.a.	n.a.	–

[1] n.a.=not applicable.

[2] Variability of the relative coverage of the area by natural (nat), agricultural (agr) and urban (urb) soil respectively.

[3] Area, depth, mixing depth and sediment area of both freshwater lakes and salt lakes.

[4] Mixing depth of non-agricultural soil compartments, volume fraction of particles in inland water and soil runoff, volume fraction air and water in agricultural and non-agricultural soil compartments, organic carbon content of soil, suspended matter and sediment, deposition rate of aerosols, concentration of hydroxyl radicals in air.

[5] Non-carcinogenic and carcinogenic are taken together here, because of the reference substance nitrobenzene, these impact categories have equal CFs.

It can be concluded from Table 5.6 that most of the parameters that have been differentiated in the GLOBACK parameter set have an important influence on the characterisation factors of nitrobenzene for a number of impact category/emission compartment combinations. For nitrobenzene, spatial differentiation seems to be more important for water and soil emissions than for emissions to air, which may be explained by the fact that air compartments are characterised by a relatively high mixing rate, resulting in a relatively fast convergence of environmental concentrations in air compartments. With respect to human intake, the differentiation of population and dietary intake turns out to play a crucial role.

5.6.4 Individual parameters and characterisation factors: correlations

From the sensitivity analysis elaborated above, a number of important combinations of model parameters and characterisation factors have been selected for correlation analysis. Two types of correlation coefficients have been determined: the Pearson correlation coefficient *r*, indicating the degree of correspondence to a linear function, and the Spearman rank order correlation coefficient, indicating the degree of monotony with respect to rise or descent as such. In Table 5.7, both types of correlation coefficients are reported for the selected parameters and characterisation factors.

Table 5.7 Correlation coefficients for linear correlation (Pearson (*r*)) and rank correlation (Spearman) between model parameters and nitrobenzene CFs for a selection of parameters and CFs.

parameter	CF	emission compartment	Pearson corr. coeff. (*r*)	Spearman rank order corr. coeff.	*N*
relative lake area	aquatic ecotoxicity (lake)	air	0.33	0.35	231
relative lake volume	aquatic ecotoxicity (lake)	air	0.37	0.38	231
relative salt lake area	aquatic ecotoxicity (salt lake)	air	0.55	0.37	231
relative alt lake volume	aquatic ecotoxicity (salt lake)	air	0.42	0.37	231
rain rate	terrestrial ecotoxicity	air	-0.61	-0.62	231
leaf crop consumption	human toxicity	air	0.24	0.27	231
temperature	aquatic ecotoxicity (lake)	agr	-0.38	-0.53	216
temperature	terrestrial ecotoxicity	agr	-0.73	-0.73	216
temperature	human toxicity	agr	-0.11	-0.37	216
population density	human toxicity	agr	0.59	0.65	216
relative urban area	terrestrial ecotoxicity	urb	0.33	0.44	223
relative river volume	aquatic ecotoxicity (river)	riv	0.37	0.42	223
freshwater fish consumption	human toxicity	riv	-0.02	0.20	223
frost period	aquatic ecotoxicity (lake)	lake	0.45	0.38	182
relative lake area	human toxicity	lake	-0.09	-0.40	182
relative lake volume	human toxicity	lake	-0.04	-0.46	182
wind speed	aquatic ecotoxicity (lake)	lake	-0.12	-0.21	182
relative salt lake area	aquatic ecotoxicity (salt lake)	salt	0.32	0.25	33

parameter	CF	emission compartment	Pearson corr. coeff. (*r*)	Spearman rank order corr. coeff.	*N*
relative salt lake volume	aquatic ecotoxicity (salt lake)	salt	0.63	0.63	33

It is clear from Table 5.7 that large correlations exist between most of the selected parameters and the corresponding characterisation factors. From the differences between Pearson and Spearman correlation coefficients it appears that the relationship between parameter and characterisation factor is probably non-linear in at least a number of cases. The strongest relationship ($r = -0.73$), exists between temperature on the one hand and the characterisation factor for terrestrial ecotoxicity in case of emission to agricultural soil on the other, at least for nitrobenzene.

5.6.5 Explanation of the influence of individual parameters

The influence of individual parameters on characterisation factors can be explained in a qualitative way on the basis of the general properties of multimedia distribution and human exposure. The GLOBOX model contains a number of possibilities for a quantitative check of the resulting suppositions. Model outcomes for pairs of countries with distinct values for certain parameters will be used to illustrate the explanations, elaborated in this paragraph. In Table 5.8, an overview of a number of key parameters is given for these countries.

Table 5.8 Key parameters for a selection of countries.

	Afghanistan	New Zealand	Mongolia	Mali
total area [km^2]	647 500	268 680	1 565 000	1 240 000
length of coastline [km]	0	15 134	0	0
area salt lakes [km^2]	2 020	0	5 098	0
average temperature in capital [ºC]	12	14	-2	28
rain rate [mm/year]	327	1 732	241	282
river volume [km^3]	1.6	9.2	0.8	1.6
population density [inhab./km^2]	44	15	2	10
crop consumption per capita [g/day]	434	676	331	463
meat consumption per capita [g/day]	18	146	130	30

The fact that geographic and river flow parameters have a large influence on characterisation factors can be explained by the distribution of released substances between land and sea regions. Chemicals that are released on islands, on peninsulas and in areas with a comparatively long coastline will usually spend a relatively large part of their lifetime in sea areas, where seawater aquatic ecotoxicity is the only toxicity related impact category to which they contribute. This influence will be largest for emissions to isolated areas, areas with a high ratio between coastline length and surface area, and areas with a relatively large river outflow to the sea. In

Figure 5.3, the global distribution over land and sea areas of nitrobenzene is represented for emissions to air and agricultural soil in Afghanistan and New Zealand, respectively. Afghanistan and New Zealand are countries with comparable environmental temperatures. Afghanistan is fully enclosed by other countries, while New Zealand is fully surrounded by sea. Total amounts of nitrobenzene residing in the environment hardly differ between comparable emissions to both countries, but, although a remarkable part of air emission ends up in sea areas even for Afghanistan, the distribution ratio between land and sea areas turns out to be quite different.

a. emission to air

b. emission to agricultural soil

Figure 5.3 Distribution of nitrobenzene over land and sea areas for emissions in Afghanistan and New Zealand.

A decrease in environmental temperature is associated with lower volatility values – which can lead to 'cold condensation' (Wania and Mackay, 1993) – and with decreased environmental degradation rates. In Figure 5.4, the distribution of nitrobenzene over the different environmental compartments after emissions to air and agricultural soil, respectively, is shown for Mali and Mongolia: two landlocked countries with comparable rain rates but distinctly different average environmental temperatures.

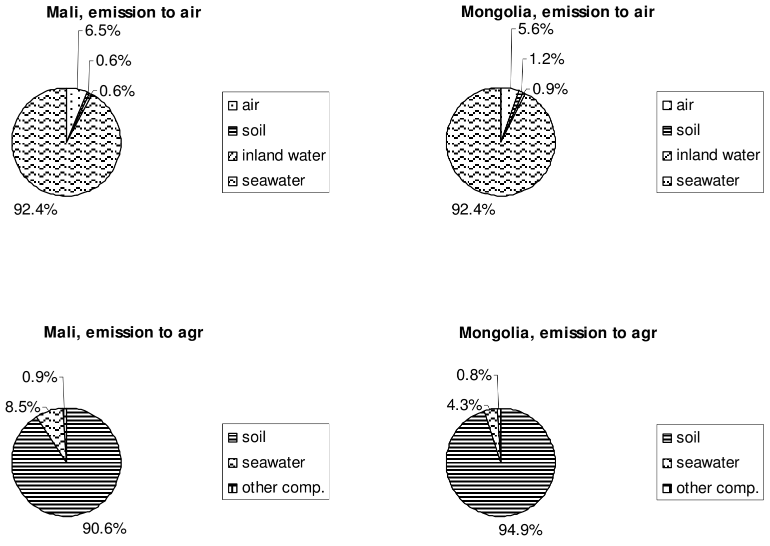

Figure 5.4 Distribution of nitrobenzene over different environmental compartments for emissions to air and agricultural soil in Mali and Mongolia.

If nitrobenzene is released to air, whether this happens in Mali or in Mongolia, more than 90% turns out to end up in seawater, despite the fact that both countries are landlocked. Total environmental amounts are almost equal: 9266 and 9258 t in the steady state situation for emissions of 1 kg/s nitrobenzene to air in Mali and Mongolia, respectively. The relative amounts, present in inland water and soil, are larger in Mongolia by factors 2 (1.2% versus 0.6%) and 1.5 (0.9% versus 0.6%), respectively. This may indicate either cold condensation or delayed degradation in these two compartments occurs in cold regions – or both. In case of emission to agricultural soil, the bulk part of the total environmental amount turns out to remain in the soil compartment, with a slightly larger part in Mongolia. The relative amount, ending up in seawater, is a factor 2 higher for Mali than for Mongolia. Remarkably, total environmental amounts differ by more than an order of magnitude: 3028 and 36692 t for emissions of 1 kg/s nitrobenzene to agricultural soil in Mali and Mongolia, respectively. This forms a strong indication for a substantial influence of the temperature-dependent increase of soil residence times on accumulation of chemicals in cold regions – at least for nitrobenzene.

According to the data in Table 5.6, variations with respect to drinking water purification (fraction of population with access to safe drinking water) have hardly any influence on characterisation factors for human toxicity. Such a lack of influence of a certain parameter can have several reasons:

- the parameter plays a subordinate role in the model, compared to other parameters
- parameter variations between regions are relatively small
- the parameter refers to an exposure route that is relatively unimportant for the chemical under study.

In Figure 5.5, the relative magnitudes of human exposure routes are represented for the case of an emission to Dutch air, leading to exposure in all inhabited countries.

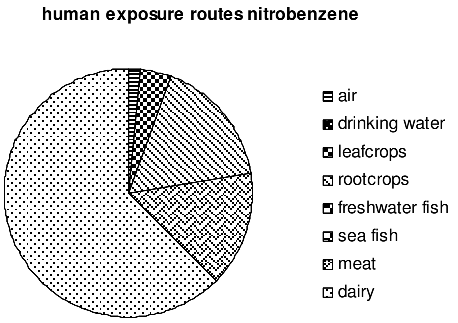

Figure 5.5 Relative magnitude of human exposure routes to nitrobenzene for Dutch air emissions.

Drinking water turns out to be only a minor exposure route for nitrobenzene. For other chemicals, this may be different, and the parameter that represents drinking water purification may be more important.

5.6.6 GDP weighting

From the analyses above, it is obvious that regional differentiation can have a large influence on the magnitude of characterisation factors. It is not yet clear, however, how important these differences are in the context of general LCA practice. The regions distinguished in the GLOBACK parameter set are very unequal, not only with respect to the magnitudes of areas and populations, but also regarding economic productivity, to which product life cycles are directly connected. In the context of LCA, it is important to know whether the regions for which characterisation factors deviate substantially from 'standard' characterisation factors represent a significant part of the global economic system, resulting in a relatively large share of regional processes in global product life cycles. The relative importance of different countries with respect to their CFs has therefore been approached by the application of weighting with their economic productivity in terms of their GDP (CIA, 2009), arguing that GDP is a good measure for a country's influence on the world market, and thus of its contribution to global economic productivity reflected by summed product life cycles.

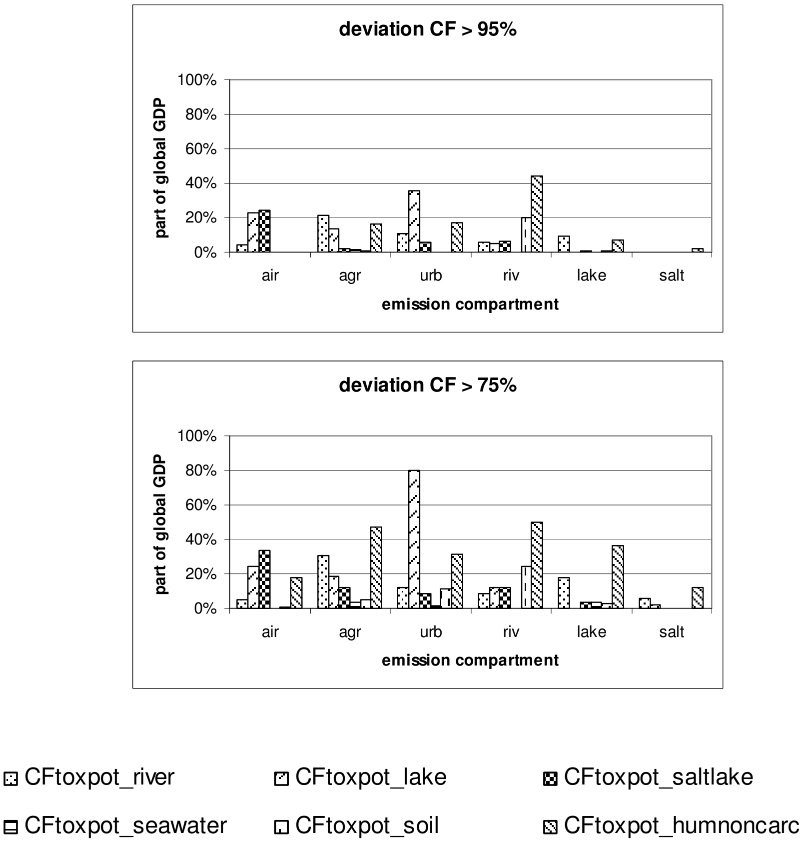

Figure 5.6 Part of the global GDP, produced in countries with a nitrobenzene CF that deviates more than 75 and 95 percent respectively from the European GDP-weighted mean nitrobenzene CF for different impact categories and emission compartments.

To test CFs for the relative importance of spatial deviation, GDP-weighted average values for the EU-27 were constructed for all characterisation factors, to act as European standard CFs. Subsequently, the countries for which individual CFs deviated more than 75% from the European standard CF were grouped, their GDPs were added, and the total GDP of these countries together was compared to the total world GDP. The same procedure was applied to countries with CFs that deviated more than 95% from the European standard CF. The results of this analysis are shown in Figure 5.6.

Figure 5.6 shows that regions with characterisation factors that deviate substantially from European standard CF values represent a substantial part of global GDP for several impact category/emission compartment combinations. This implies that the use of spatially differentiated characterisation factors may bring about an important refinement in the assessment, not just for processes that take place in small, 'exotic' countries, but for a substantial part of the global economic production.

5.7 Discussion

5.7.1 The influence of spatial differentiation

The main goal of the GLOBOX model is to increase the accuracy of LCA toxicity characterisation factors by accounting for spatial environmental differences. In a general sense, it has been clearly shown by the calculations on the test chemical nitrobenzene that the application of spatial differentiation can make a large difference between characterisation factors for different countries, especially for emissions to water and soil – with ranges of up to 5 orders of magnitude between different countries for nitrobenzene. Extremely low CF values are found for small, geographically isolated islands, such as Fiji. Extremely high CF values are found for countries for which emissions affect relatively large shares of certain ecosystems or large human populations, especially in combination with relatively high residence times in the country itself or in surrounding areas with equal environmental circumstances. A number of examples, referring to atmospheric emissions, are:

- The top-3 countries with respect to the CF for aquatic ecotoxicity for rivers are Colombia, Bolivia and Peru, all countries where the Amazon rises.
- The top-3 countries with respect to the CF for human toxicity are the Czech Republic, Slovakia and Poland, all centrally positioned in densely populated Europe.
- The top-3 countries with respect to the CF for aquatic ecotoxicity for salt lakes are Kyrgyzstan, Uzbekistan and Tajikistan, all countries of which river flows end up in the Aral Sea.

In general, the highest characterisation factors indicate which regions on earth are the most vulnerable to pollution with respect to a certain environmental impact. Important parameters with respect to spatial differentiation include geographic position, lake parameters (area, volume, and water residence time), environmental temperature, and rain rate. For human toxicity, population density and dietary intake play a major role as well.

The choice to differentiate at the level of countries and seas has advantages with respect to data availability, but a drawback of this choice is the fact that the regions distinguished are very different in size. Large countries like the United States, Canada, Russia and China, which are characterised by a wide variation in environmental parameters, need a refinement of this approach to decrease uncertainty in their CFs. Such refinement would be a desirable next step in the further development of the GLOBOX model. A further refinement could consist of making a distinction between urban and rural areas, which, according to other publications, could make a difference in human intake of a factor 3 (Huijbregts *et al.*, 2005) up to more than an order of magnitude (Humbert *et al.*, 2009).

The question can be posed whether the deviation of spatially differentiated characterisation factors (CF_i) from a reference value – *e.g.* a non-differentiated alternative characterisation factor (CF_{ref}) – should be expressed in terms of orders of magnitude deviation

$$\frac{CF_i}{CF_{ref}}$$

or in terms of percentage difference

$$\frac{CF_i - CF_{ref}}{CF_{ref}} \times 100\%$$

Since the difference in terms of percentage gives a better and more symmetrical reflection of the relative under- or overestimation of effects in absolute terms, this latter form has been chosen as the best option for this specific purpose, with deviations of 75 and 95 percent of the GDP-weighted average CF as a measure. For other purposes, such as the indication of ranges of CF values, orders of magnitude have been used.

The use of spatial differentiation makes sense if it results in a fairly large overlap of ranges of characterisation factors between different chemicals. An overlap in range between two chemicals indicates that the answer to the question which of the chemicals should be preferred in case of equal emissions is region-dependent. Since the environmental profiles of product alternatives are often dominated by a relatively small number of chemicals, an error with respect to the question which chemicals are to be preferred can potentially reverse the outcomes of comparative

LCA studies. In these cases, spatial differentiation is essential for the reliability of LCA results, in terms of the ranking of product alternatives. A small overlap indicates that a reverse ranking applies to extremes only, *e.g.* 'chemical A is preferred to chemical B, except for the situation that chemical A is released in Iceland and chemical B in Bolivia'. The larger the overlap, the more likely rank reversal will be. This can be illustrated by comparing the ranges of non-differentiated CFs for different chemicals to the ranges of spatially differentiated CFs for one chemical. The USES-LCA 2.0 spreadsheet program offers the possibility to calculate midpoint and endpoint characterisation factors for a number of different toxicity-related impact categories for 3396 chemicals (Van Zelm *et al.*, 2009). In Table 5.9, the ranges of a number of selected series of midpoint CFs, calculated with USES-LCA 2.0, are given.[*] In the third and fourth column, full CF ranges are compared to the ratio between the third and the first quartile of these CFs (Q_3/Q_1), spanning the central 50% of chemicals.

Table 5.9 Ranges of midpoint CFs in USES-LCA 2.0 (3396 chemicals) and GLOBOX (nitrobenzene).

		USES-LCA (3396 chem.)	USES-LCA (3396 chem.)	GLOBOX (nitrobenzene)
impact category	emission compartment	full range CFs	range CFs of central 50% (Q_3/Q_1)	range CFs of 50% with highest GDP[a]
terrestrial ecotoxicity	air	9.78×10^{14}	279	11
human toxicity	air	5.71×10^{10}	69	21
freshwater ecotoxicity	freshwater/lake	2.85×10^{12}	83	25
freshwater ecotoxicity	freshwater/river	2.85×10^{12}	83	86
soil ecotoxicity	agricultural soil	1.41×10^{14}	44	37
human toxicity	agricultural soil	8.01×10^{46}	72	3 815

[a] These countries are considered to cover the main part of world economic production, and thus, their CFs are considered to be of relative importance to LCA.

While the full range of the these series of characterisation factors spans between 10 and 46 orders of magnitude, the ratios between the third and the first quartiles (Q_3/Q_1) vary between 44 and 279, indicating that the characterisation factors for half the number of chemicals lie together within ranges of just one or two orders of magnitude, depending on impact category and emission compartment. In the fifth column, the ranges of spatially differentiated GLOBOX-CFs that represent

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[*] Scenario options chosen: fate and exposure: emission compartments: air, freshwater and agricultural soil (respectively); time horizon: steady state; bioaccumulation metals: yes; include ocean for essential metals: yes; human effect and damage: effect endpoint: DALY; carcinogenic substances: all; ecological effect: method freshwater ecological effect: linear; minimum nr of tested species: 1.

the 50% of the countries with the highest GDP values (together representing 99% of the global GDP) are given. These factors vary between 11 and 3815. This means that for the central group of chemicals with CF values between Q_1 and Q_3, spatial characteristics have an influence on the CF that is comparable to the influence of chemical properties or larger, at least for these selected combinations of impact categories and emission compartments.

It can be concluded from this example that spatial differentiation is of large importance. The differences between spatially differentiated CFs for nitrobenzene of up to 5 orders of magnitude, as found in this study, are in good accordance with the findings of other authors, who report differences of up to 1 or 2 orders of magnitude for differentiation at the level of continents (Huijbregts *et al.*, 2003 for fate and exposure factors; Rochat *et al.*, 2006 for intake fractions), differences of up to around 3, 5 or 8 orders of magnitude between smaller regions within continents (MacLeod *et al.*, 2004; Pennington *et al.*, 2005; Humbert *et al.*, 2009; all for intake fractions), and a noticeable increase of differences with increasing level of spatial model resolution (Manneh *et al.*, 2009 for intake fractions).

Besides spatial model resolution, the range of calculated model results is also influenced by internal model properties:

The parameters to which spatial differentiation has been applied
In the GLOBOX model, spatial differentiation has been applied not only to fate parameters, population and food production areas, but also to intake parameters concerning dietary pattern, body weight, fraction of drinking water that has been purified, and fraction of drinking water that is ground- and surface water, respectively. Especially dietary patterns turned out to have a marked influence on CFs.

The inclusion of spatially differing parameters in the model equations
Model equations were largely taken from the EUSES 2.0 model, which, in contrast to the earlier model version EUSES 1.0, included temperature-dependency of environmental degradation rates. The relatively large influence of temperature variations on CFs found in this study may be largely due to this model property, which stresses the importance of model equations to adequately reflect possible spatial dependencies.

The number of environmental compartments distinguished
The number of aquatic environmental compartments in the GLOBOX model is larger than in most multimedia models. Rivers, freshwater lakes, salt lakes and groundwater are distinguished as separate compartments. Regarding the differences in characterisation factors of more than an order of magnitude on average between freshwater lake CFs on the one hand and salt lake and river water CFs on the other (for emissions to the respective compartments concerned), it can be concluded that a separate distinction of these compartments does make sense.

Hollander (2009), concludes from a European study that substance properties are more influential than environmental properties with respect to environmental concentrations. This author bases her conclusion on full concentration ranges. As mentioned above, however, there exists a large discrepancy between the full range (10 to 46 orders of magnitude) and the range of the central 50% Q_3/Q_1 (one or two orders of magnitude) of USES-LCA characterisation factors for the given combinations of impact category and emission compartment. While the full concentration ranges, found by Hollander (2009) may be largely due to chemical properties, it is very well possible that at the same time, the variation of the central 50% of these concentrations display a much smaller range as well. In other words: even though chemical properties may be more influential than environmental properties on average, it is very well possible that for a substantial number of chemicals, spatial characteristics of environmental properties have a comparable or larger influence on environmental concentrations than chemical properties.

More chemicals should be tested with the GLOBOX model in order to obtain a detailed image of the general influence of spatial differentiation on the range of characterisation factors. Yet, it can be concluded from the calculations with nitrobenzene that spatial variation in environmental and human exposure parameters on toxicity-related LCA characterisation factors can be substantial. Summarising, the following findings on nitrobenzene can be reported:

- Characterisation factors for nitrobenzene vary up to 5 orders of magnitude – with corresponding interquartile ranges up to 2 orders of magnitude – due to spatial differentiation.
- Geographic and flow parameters alone cause characterisation factors to vary up to 3 orders of magnitude.
- Environmental parameters or parameter categories that cause the characterisation factor for one or more impact category/emission compartment combinations to deviate more than 25 percent from the median value of the interquartile range include area division natural/agricultural/urban soil, lake parameters, river volume, ice cover, temperature, wind speed and rain rate. Intake parameters that cause human toxicity characterisation factors to show a similar deviation include population and dietary intake. Most of these parameters can be demonstrated to have a sound correlation with at least one impact category/emission compartment combination, either with the Pearson correlation coefficient (*r*) or with the Spearman rank order correlation coefficient, or with both.
- The distribution of nitrobenzene between land and sea areas after emission seems to depend largely on the geographic location of the country of emission, with emissions in landlocked countries tending to reside for a comparatively large part in land areas, especially after emission to soil.

- The environmental temperature seems to have an important influence on the distribution of nitrobenzene between the different compartments, with lower temperatures being in favour of lower air concentrations and higher concentrations in water and soil. This may be largely explained by the seemingly decisive influence of environmental temperature on soil residence times.
- Lack of spatial differentiation causes characterisation factors for nitrobenzene to be more than 95 percent wrong for countries that together represent up to 40 percent of world GDP, and for more than 75 percent wrong for countries representing up to 80 percent of world GDP, compared to GDP-weighted average EU characterisation factors.
- The range of the spatially differentiated characterisation factors for nitrobenzene has the same order of magnitude as the range of the central 50% of USES-LCA midpoint characterisation factors for 3396 chemicals (Van Zelm *et al.*, 2009) for at least a number of impact category/emission compartment combinations.

From these findings, it can be concluded that at least for nitrobenzene, spatial differentiation has an important influence on toxicity-related LCA characterisation factors, that a fair number of environmental and human intake parameters are involved, and that lack of spatial differentiation may cause rank reversal and thus erroneous outcomes of LCA characterisation.

5.7.2 Practical application of GLOBOX in life cycle impact assessment

For LCA practice, spatial differentiation has two important consequences: in the first place, the use of spatially differentiated characterisation factors requires region-specific emission data. And in the second place, spatial differentiation on this scale results in a dramatic increase in the number of characterisation factors. This increase is proportional to the number of regions distinguished in the characterisation model – 289 in the case of GLOBOX. Distinguishing between actual and potential impacts will cause a further increase by a factor 2. The requirement of region-specific emission data refers to the process data in the LCA inventory. Existing LCA databases may have to be adapted by the spatial specification of emissions. The format of the inventory table will have to be supplemented with the emission location. The current EcoSpold format that is used for the ecoinvent data, for instance, allows for a geographical tag to processes and to products, but not to emissions, and would thus have to be adapted. A summation of emissions that take place in different regions will no longer be appropriate. As a consequence, the inventory table will largely increase in size. Despite the increases in the number of inventory data and characterisation factors, spatial differentiation has no influence on the eventual number of category indicator results, since for each impact category, all region-specific outcomes are summed to one overall impact score.

5.7.3 Broader application

Although the GLOBOX model has been primarily developed for the calculation of LCA toxicity characterisation factors, it is basically a multimedia model for fate, exposure and effect modelling, with a much broader range of application than just LCA. One of the possible applications is the analysis of distribution and exposure patterns, resulting from the emission profile of a certain chemical in a certain region. Different substances with specific chemical properties can thus be compared with respect to their distribution patterns. Distribution can be determined over different countries or over different environmental compartments. This type of analysis can for instance be used to calculate the distribution patterns of POPs on a global scale. With respect to cold areas, the findings about large differences in environmental amounts of nitrobenzene, following soil emissions to respectively Mali and Mongolia, are in good accordance with the global fractionation theory on accumulation of POPs in cold regions (Wania and Mackay, 1993), which is also confirmed by the findings of Toose *et al.* (2004). Another type of application is for supporting scenario studies, in which an entire emission profile for one or more regions is an intermediate result. For instance, the EXIOPOL project (Tukker *et al.*, 2009) provides a multi-region environmentally extended input-output table on the level of (more than forty) countries, easily connectible to the GLOBOX model when there is a need to move from the substance level to the impact level.

5.7.4 Future outlook

The current GLOBOX model is a steady state multimedia model. For the calculation of LCA characterisation factors, this is sufficient (Heijungs, 1995). A drawback of steady state models is, however, that they are more difficult to validate, since it requires well-documented steady state situations, caused by emissions of globally distributed chemicals. Developing a dynamic variant of the GLOBOX model would open up better possibilities for model validation, and is therefore considered as a desirable next step. This step would also broaden the applicability of the GLOBOX model for further environmental analyses of the global distribution patterns of chemicals. Yet, the main goal of the GLOBOX model remains the calculation of spatially differentiated LCA toxicity characterisation factors on a global scale. A logical next step would be the extension of the GLOBOX model with other impact categories such as global warming and acidification, including the specific environmental processes involved, and thus the creation of an integrated system for global spatial differentiation in life cycle impact assessment.

Acknowledgement

The authors thank Helias Udo de Haes for his useful comments, and also the three (anonymous) reviewers, who all took much effort, and whose comments added substantially to the quality of this chapter. Finally, they thank Unilever for financing the PhD-project of the first author, in the context of which this chapter has been written.

Appendix: Supplementary data

Supplementary data associated with this chapter can be found, in the online version, at doi:10.1016/j.scitotenv.2010.02.044.

References

Babkin VI (2003) *The World and its Physical Features.* In: Shiklomanov IA, Rodda JC (eds.) *World Water Resources at the Beginning of the Twenty-First Century.* International Hydrology Series, Cambridge University Press. Cambridge, UK, pp. 1-18

Bennett DH, McKone TE, Evans JS, Nazaroff WM, Margni MD, Jolliet O, Smith KR (2002) Defining Intake Fraction. *Environ Sci Technol* **36** (9): A206-211

CIA (2000) *The World Factbook 2000.* Central Intelligence Agency (CIA), Washington DC, 2000. Online version. Visited 2000 at:
http://www.odci.gov/cia/publications/factbook/index.html

CIA (2004) *The World Factbook 2004.* Central Intelligence Agency (CIA), Washington DC, 2004. Online version. Visited 2004 at:
http://www.odci.gov/cia/publications/factbook/index.html

EC (2004) *European Union System for the Evaluation of Substances 2.0 (EUSES 2.0).* Prepared for the European Chemicals Bureau by the National Institute of Public Health and the Environment. RIVM Report no. 601900005, RIVM, Bilthoven, The Netherlands. 18 + 206 + 222 pp. + appendices

FAO (2000) *FAOSTAT, FAO Statistical Databases. Nutrition. Food Balance Sheets 1998.* Food and Agriculture Organization of the United Nations (FAO), Rome, Italy. Visited September 2000 at:
http://faostat.fao.org/faostat/form?collection=FBS&Domain=FBS&servlet=1&hasbulk=&version=ext&language=EN

FAO (2004) *Computation of renewable water resources by country (in km3/year, average). FAO AQUASTAT 2003. FAO's Information System on Water and Agriculture.* Food and Agriculture Organization of the United Nations (FAO), Geneva, 2004. Series of datasheets by country, downloaded September 2004 from:
http://www.fao.org/ag/agl/aglw/aquastat/dbase

Gleick PH (ed.) (1993) *Water in Crisis. A Guide to the World's Fresh Water Resources. Section B. Rivers, lakes, and waterfalls. Tables B.1 II, B.1 IV, B.2.* Oxford University Press, New York, USA. 473 pp.

Guinée J, Heijungs R (1993) A Proposal for the Classification of Toxic Substances within the Framework of Life Cycle Assessment of Products. *Chemosphere* **26** (10): 1925-1944

Hauschild M, Potting J (2005) *Spatial differentiation in life cycle impact assessment. The EDIP2003 methodology.* Environmental News No. 80, 2005. Environmental Protection Agency, Danish Ministry of the Environment, Copenhagen, Denmark. 194 pp.

Heijungs R (1995) Harmonization of Methods for Impact Assessment. *Environ Sci Pollut Res* **2** (4): 217-224

Hertwich EG, Jolliet O, Pennington DW, Hauschild M, Schulze C, Krewitt W, Huijbregts M (2002) *Fate and Exposure Assessment in the Life-Cycle Impact Assessment of Toxic Chemicals.* In: Udo de Haes HA (ed.) *Life-Cycle Impact Assessment: Striving towards Best Practice.* Society of Environmental Toxicology and Chemistry (SETAC), Pensacola, Florida and Brussels, Belgium, pp. 101-122

Hertwich EG, Mateles SF, Pease WS, McKone TE (2001) Human toxicity potentials for life-cycle assessment and toxics release inventory risk screening. *Environ Toxicol Chem* **20** (4): 928-939

Hollander (2009) *A. Spatial Variation in Multimedia Mass Balance Models. The Influence of Environmental Characteristics on Chemical Concentrations.* PhD Thesis. Radboud University Nijmegen, The Netherlands. 243 pp.

Huijbregts MAJ, Lundi S, McKone TE, Van de Meent D (2003) Geographical Scenario Uncertainty in Generic Fate and Exposure Factors of Toxic Pollutants for Life-Cycle Impact Assessment. *Chemosphere* **51**: 501-508

Huijbregts MAJ , Struijs J, Goedkoop M, Heijungs R, Hendriks AJ, Van de Meent D (2005) Human Population Intake Fractions and Environmental Fate Factors of Toxic Pollutants in Life Cycle Impact Assessment. *Chemosphere* **61**: 1495-1504

Huijbregts MAJ, Thissen UMJ, Guinée JB, Jager T, Kalf D, Van de Meent D, Ragas AMJ, Wegener Sleeswijk A, Reijnders L (2000) Priority Assessment of Toxic Substances in Life Cycle Assessment. Part I: Calculation of Toxicity Potentials for 181 Substances with the Nested Multi-Media Fate, Exposure and Effects Model USES-LCA. *Chemosphere* **41**: 541-573

Humbert S, Manneh R, Shaked S, Wannaz C, Horvath A, Deschênes L, Jolliet O, Margni M (2009) Assessing regional intake fractions in North America. *Sci Total Environ* **407**: 4812-4820

IHO (1986) *IHO 23-4th: Limits of Oceans and Seas. Special Publication 23, 4th Draft, Edition 1986.* International Hydrographic Organization (IHO). International Hydrographic Bureau of the International Hydrographic Organization, Monaco

ILEC/UNEP (1994) *Data Book of World Lake Environments – a Survey of the State of World Lakes. Volume 1. Asia and Oceania.* International Lake Environment Committee, United Nations Environment Programme (ILEC/UNEP), Tokyo. Online version. Visited 2004 at: http://www.ilec.or.jp/database/database.html

Ibidem (1995) Volume 2. Africa and Europe.

Ibidem (1996)Volume 3. The Americas.

ISO (2006a) *Environmental Management – Life Cycle Assessment – Principles and Framework. Second edition, 2006-07-01.* ISO 14040: 2006, Geneva, Switzerland. 20 pp.

ISO (2006b) Environmental management – Life Cycle Assessment – Requirements and Guidelines. First edition, 2006-07-01. ISO 14044: 2006, Geneva, Switzerland. 46 pp.

Korzoun VI, Sokolov AA, Budyko MI, Voskresensky KP, Kalinin GP, Konoplyantsev ES, Lvovich MI, Editors (1977) *Atlas of World Water Balance.* The UNESCO Press, Paris, France. 34 pp. + 65 maps

Krewitt W, Trukenmüller A, Bachmann TM, Heck T (2001) Country specific damage factors for air pollutants—a step towards site dependent life cycle impact assessment. *Int J LCA* **6**: 199-210.

LakeNet (2004) *World Lakes Network. Lakes Global Lake Database. Online version 2004.* Annapolis, Maryland, 2004. Visited 2004 at:
http://www.worldlakes.org/lakes.asp

Mackay D (1991) *Multimedia Environmental Models. The Fugacity Approach.* Lewish Publishers, Chelsea, Michigan, USA. 257 pp.

MacLeod M, Bennett DH, Perem M, Maddalena RL, McKone TE, Mackay D (2004) Dependence of Intake Fraction on Release Location in a Multimedia Framework. A Case Study of Four Contaminants in North America. *J Ind Ecol* **8** (3): 89-102

MacLeod M, Riley WJ, McKone TE (2005) Assessing the Influence of Climate Variability on Atmospheric Concentrations of Polychlorinated Biphenyls using a Global-Scale Mass Balance Model (BETR-global). *Environ Sci Technol* **39** (17): 6749-6756

MacLeod M, Woodfine DG, Mackay D, McKone T, Bennett D, Maddalena R (2001) BETR North America: A Regionally Segmented Multimedia Contaminant Fate Model for North America. *Environ Sci Pollut Res* **8** (3): 156-163

Manneh R, Margni M, Deschênes L (2009) *Spatial Variability and Optimal Regional Scale for Intake Fractions linked to a Canadian Emission.* Abstract. p. 30. In: ACLCA. *Life Cycle Assessment IX. Toward the Global Life Cycle Economy.* Joint North American Life Cycle Conference. Boston September 29 to October 2nd 2009, Boston, USA. 237 pp.

McKone TE, Bodnar A, Hertwich EG (2000) *Development and Evaluation of State-Specific Landscape Data Sets for Life-Cycle Analysis.* Report LBNL-43722. Lawrence Berkeley National Laboratory, Berkeley, USA. 53 pp. + appendices

Nellestijn J, Dekker K (1998) *Wereld Klimaat Informatie (WKI). Versie 2.0.* KNMI, De Bilt, The Netherlands. (In Dutch.) Downloadable from: http://www.knmi.nl/kd/normalen1971-2000/wki.html

Nigge K-M (2000) *Life cycle assessment of natural gas vehicles: development and application of site-dependent impact indicators.* PhD Thesis. Springer, Berlin, Germany. 165 pp.

Pennington DW, Margni M, Ammann C, Jolliet O (2005) Multimedia Fate and Human Intake Modeling: Spatial versus Nonspatial Insights for Chemical Emissions in Western Europe. *Environ Sci Technol* **39** (4): 1119-1128

Pennington DW, Margni M, Payet J, Jolliet O (2006) Risk and Regulatory Hazard-Based Toxicological Effect Indicators in Life-Cycle Assessment (LCA). *Hum Ecol Risk Assess* **12** (3): 450-475

Potting J, Schöpp W, Blok K, Hauschild M (1998) Site-Dependent Life-Cycle Impact Assessment of Acidification. *J Ind Ecol* **2**: 63-87

Potting J (2000) *Spatial Differentiation in Life Cycle Impact Assessment. A Framework, and Site-dependent Factors to Assess Acidification and Human Exposure.* PhD thesis Utrecht University, Utrecht, The Netherlands. 177 pp.

Potting J, Hauschild M (2005) *Background for spatial differentiation in life cycle impact assessment. The EDIP2003 methodology.* Environmental News No. 996, 2005. Environmental Protection Agency, Danish Ministry of the Environment, Copenhagen, Denmark. 293 pp.

Prevedouros K, MacLeod M, Jones KC, Sweetman AJ (2004) Modelling the Fate of Persistent Organic Pollutants in Europe: Parameterisation of a Gridded Distribution Model. *Environ Pollut* **128**: 251-261

Rochat D, Margni M, Jolliet O (2006) Continent-specific Intake Fractions and Characterization Factors for Toxic Emissions: Does it make a Difference? *Int J LCA* **11** (Special Issue 1): 55-63

Rosenbaum R, Margni M, Jolliet O (2007) A Flexible Matrix Algebra Framework for the Multimedia Multipathway Modeling of Emission to Impacts. *Environment International* **33** (5): 624-634

Rosenbaum RK, Bachmann TM, Gold LS, Huijbregts M, Jolliet O, Juraske R, Koehler A, Larsen HF, MacLeod M, Margni M, McKone TE, Payet J, Schuhmacher M, Van de Meent D, Hauschild, MZ (2008) USEtox – The UNEP-SETAC toxicity model: recommended characterisation factors for human toxicity and freshwater ecotoxicity in Life Cycle Impact Assessment. *Int J LCA* **13** (7): 532-546

Schulze C (2001) Modelling and evaluating the aquatic fate of detergents. PhD Thesis. University of Osnabrück, Osnabrück, Germany. 191 pp.

Shiklomanov IA, Rodda JC (eds.) (2003) *World Water Resources at the Beginning of the Twenty-First Century.* Cambridge University Press, Cambridge, UK. 452 pp.

Statistics Finland (2004) *World in Figures. Tables. Geographical Data by Theme. Version 04.02.2004.* Statistics Finland, Helsinki, Finland. Visited 2004 at: http://www.stat.fi/tk/tp/maailmanumeroina/index_en.html

SWCSMH (2004) *Saline Lakes. The Largest, Highest & Lowest Lakes of the World!* Soil & Water Conservation Society of Metro Halifax (SWCSMH), Halifax, Nova Scotia, Canada. Visited 2004 at: http://lakes.chebucto.org/saline1.html

Toose L, Woodfine DG, MacLeod M, Mackay D, Gouin J (2004) BETR-World: a geographically explicit model of chemical fate: application to transport of α-HCH to the Arctic. *Environmental Pollution* **128** (1-2): 223-240

Troll C, Paffen KH (1966) Seasonal Climates of the Earth. Map No. 5. In: Rodenwaldt E, Jusatz HJ (eds.) *World Maps of Climatology. Third Edition.* Springer Verlag, Berlin [etc], Germany. 28 pp.

Tukker A, Poliakov E, Heijungs R, Hawkins T, Neuwahl F, Rueda-Cantuche JM, Giljum S, Moll S, Oosterhaven J, Bouwmeester M (2009) Towards a global multi-regional environmentally extended input-output database. *Ecological Economics* **68** (7): 1928-1937.

UNSD (2004) *Statistical Databases. Social Indicators. Indicators on Water Supply and Sanitation. Last updated 12 July 2004.* United Nations Statistics Division (UNSD). New York, USA. Visited 2004 at: http://unstats.un.org/unsd/demographic/products/socind/watsan.htm

UNSD (2007) *Social indicators. Indicators on human settlements.* United Nations Statistic Division (UNSD), New York, USA. Visited 2007 at: http://unstats.un.org/unsd/demographic/products/socind/hum-sets.htm

Van der Leeden F, Troise FL, Todd DK (1990) *The Water Encyclopedia. (Tables 3-54, 3-57, and 3-58).* Second Edition. Lewis Publishers, Chelsea, Michigan, USA. 808 pp.

Van Zelm R, Huijbregts MAJ, Van de Meent D (2009) USES-LCA 2.0 – a Global Nested Multi-Media Fate, Exposure, and Effects model. *In J LCA* **14**: 282–284

Wania F, Mackay D (1995) A Global Distribution Model for Persistent Organic Chemicals. *Sci Total Environ* **160/161**: 211-232

Wania F, Mackay D Tracking the Distribution of Persistent Organic Pollutants. Control strategies for these contaminants will require a better understanding of how they move around the globe. *Environ Sci & Technol* **30** (9): 390A-396A

Webster E, Mackay D, Di Guardo A, Kane D, Woodfine D (2004) Regional Differences in Chemical Fate Model Outcome. *Chemosphere* **55**: 1361-1376

Wegener Sleeswijk A General Prevention and Risk Minimization in LCA. A Combined Approach. *Environ Sci Pollut Res* **10** (1): 69-77

White P, De Smet B, Udo de Haes HA, Heijungs R (1995) LCA Back on Track. But Is It One Track or Two? *LCA News* **5** (3): 2-4

World Bank (2000) *World Development Indicators 2000*. World Bank, Washington DC, USA. 389 pp.

WRI (2000) *World Resources 2000-2001. People and Ecosystems: The Fraying Web of Life.* World Resources Institute (WRI), Washington DC, USA, 400 pp.

WRI (2004) *EarthTrends. The Environmental Information Portal. Data Tables. Freshwater Resources 2003*. World Resources Institute (WRI), Washington DC. Downloaded 2004 from: http://earthtrends.wri.org/pdf_library/data_tables/fre1_2003.PDF

6

Normalisation in product life cycle assessment: an LCA of the global and European economic systems in the year 2000*

Abstract

In the methodological context of the interpretation of environmental life cycle assessment (LCA) results, a normalisation study was performed. 15 impact categories were accounted for, including climate change, acidification, eutrophication, human toxicity, ecotoxicity, depletion of fossil energy resources, and land use. The year 2000 was chosen as a reference year, and information was gathered on two spatial levels: the global and the European level. From the 860 environmental interventions collected, 48 interventions turned out to account for at least 75% of the impact scores of all impact categories. All non-toxicity related, emission dependent impacts are fully dominated by the bulk emissions of only 10 substances or substance groups: CO_2, CH_4, SO_2, NO_x, NH_3, PM_{10}, NMVOC, and (H)CFCs emissions to air and emissions of N- and P-compounds to freshwater. For the toxicity-related emissions (pesticides, organics, metal compounds and some specific inorganics), the availability of information was still very limited, leading to large uncertainty in the corresponding normalisation factors. Apart from their usefulness as a reference for LCA studies, the results of this study stress the importance of efficient measures to combat bulk emissions and to promote the registration of potentially toxic emissions on a more comprehensive scale.

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* This chapter has been published as: Wegener Sleeswijk A, Van Oers LFCM, Guinée JB, Struijs J, Huijbregts MAJ (2008) Normalisation in Product Life Cycle Assessment: An LCA of the Global and European Economic Systems in the Year 2000. *Science of the Total Environment* **390**: 227-240.

Keywords

LCA, normalisation, economic system, impact categories, global assessment

6.1 Introduction

Life cycle assessment of products (LCA) has become a widely recognised method for quantifying the environmental performances of products (c.f. EC, 2001; Curran, 2006). Numerical scores make it possible to compare product alternatives on the aspects of climate change, ozone depletion, acidification, eutrophication, toxicity, fossil energy resource depletion, and more environmental impact categories. All environmental releases, fossil energy resource extractions and land use activities that belong to a product life cycle are translated and aggregated in the right proportions to deliver an environmental profile in terms of the overall contribution of the product to a limited number of impact categories (Guinée *et al.*, 2002). A comparison of environmental profiles reveals the relative environmental performance of product alternatives in the context of every single impact category. Despite their apparent simplicity, however, LCA profiles are not in every respect interpreted so easily. Impact scores are expressed in complex units, and reflect environmental impacts in a way that does not correspond directly to perceptible problems or prevailing threats. Their absolute value as an assessment measure remains difficult to interpret as long as it is not placed in an adequate environmental context. This is what LCA normalisation aims at.

LCA normalisation offers a reference situation of the pressure on the environment for each environmental impact category. Normalisation makes it possible to translate abstract impact scores for every impact category into relative contributions of the product to a reference situation. This reference situation consists of an environmental profile on a higher scale – that is, the environmental profile of an economic system that the product life cycle is considered to be part of. The fact that the normalisation results are expressed in the same unit for each impact score makes it easier to make comparisons between impact scores of different impact categories (Norris, 2001). Since product life cycles often have a global coverage – *e.g.* including resource extractions in diverse geographic regions – the global system is the most promising candidate to act as a reference situation (Guinée *et al.*, 2002).

A number of normalisation methods have appeared during the past 10 years. An overview is given in Table 6.1. Some methods are shown to be specific for a limited region or for a limited number of impact categories.

Table 6.1 Overview of LCA normalisation methods.

literature reference	reference areas	reference years	intervention types	number of impact categories
Wenzel *et al.* (1997)	Denmark	1990	emissions	11
Breedveld *et al.* (1999)	The Netherlands	1993/1994	general	13
	EU_{15+3}	1990/1994	general	12
Huijbregts *et al.* (2003)	The Netherlands	1997/1998	general	13
	EU_{15}	1995	general	13
	world	1990/1995	general	13
Strauss *et al.* (2006)	South Africa	2001	abiotic resource extraction	2
Stranddorf *et al.* (2005A & B)	Denmark	1994	emissions	11
	EU_{15}	1994	emissions	11
	world	1994	emissions	11
Bare *et al.* (2006)	United States	1999	general	10
Lundie *et al.* (2007)	Australia	2002/2003	toxic emissions	5
this chapter	EU_{25+3}	2000	general	15
	world	2000	general	15

This study can be considered as a follow-up of the study by Huijbregts *et al.* (2003), in which 1995 was used as the reference year, and which distinguished economic systems on three levels: the world, Western Europe, and The Netherlands. A follow-up was considered necessary for three reasons:

- Acquiring more up-to-date emission and extraction data (year 2000 instead of 1995) and more up-to-date boundaries for the European region (28 instead of 15 countries);
- Extending the number and improving the quality of emissions and extractions (although the availability and quality of the data for toxic emissions appeared to be still limited);
- Including more up-to-date impact assessment models in the normalisation factor calculations for many impact categories, including global warming, ozone depletion, toxicity and acidification.

The outcomes of this normalisation study can be interpreted as an LCA study of the economic systems as a whole on both the European and the global level. LCAs of economic systems can also be used in a broader context than normalisation, for instance by comparing the impacts of different economic systems with each other and by identifying the most important emissions or extractions within a specific impact impact category or economic system. Both aspects will be discussed and quantified.

6.2 General methodological choices

6.2.1 Reference system

Although the global economic system may be considered as the most justifiable reference system for normalisation from a scientific point of view, policy makers are often interested in reference systems on a lower geographic level, since this provides a more direct link to political goals. In this study, we accounted for the group of 28 European countries, formed by the 25 countries of the European Union in 2006, supplemented with Iceland, Norway and Switzerland, as an alternative reference system besides the world economic system. This European system will be further referred to as EU_{25+3}.

With respect to demarcation in time, different alternatives exist. In the most usual approach, emissions that have occurred during the reference year are used as the reference emissions. In an alternative, approach, the reference system is not the year of emission as such, but the year during which the emission has been caused initially. This last approach accounts for the delay between production and use on the one hand and waste treatment and emission on the other, that occurs for certain emissions. While the first approach has the practical advantages of relative simplicity, transparency and feasibility, the second approach is the most correct one in a theoretical sense, since this approach creates a reference system that corresponds to the product-oriented LCA approach. Differences will be negligible for processes with a small time delay or a constant character, but may become distinct if production processes with long-lived emissions show abrupt changes (*e.g.* CFC production) or for future processes handling current products as waste and differing substantially from current waste treatment processes.

In this study, we have headed for a combination of theoretical correctness and practical feasibility. This implies that the second approach is used in those cases where the difference between both approaches is clear and information of future emissions, caused by products of the year 2000, can be obtained with reasonable reliability. For this reason, emissions of ozone-depleting substances are set equal to their production rates in the year 2000, and emissions of the anti-fouling agent tributyltin (TBT) are set equal to releases, estimated to result from TBT that has been applied in the year 2000. For both types of chemicals, these emissions are much lower than the actual emission level in 2000, which is largely caused by leakage from formerly produced products. For processes of which future emissions are unknown, emission levels in the year 2000 are used as a 'best estimate'. This is the case for emissions from waste incineration and landfill seepage.

6.2.2 Units

The assessment unit in LCA – a *functional unit* of product –is usually expressed in terms of a certain *amount* of product. This implies that emissions and extractions in LCA are also most commonly expressed in these terms: they are emission and extraction amounts (in kg), rather than the continuous emission flows (in kg/year) that form the direct link between economic activity and environmental impacts or risks.

If normalisation is considered as an LCA study – as we propose – it seems almost self-evident that outcomes of the normalisation step should be expressed in terms of fractions. This is not, however, common practice. Heijungs (2005) explicitly defends the use of time units such as years – implying that the reference interventions in normalisation should be expressed in units per year. The apparent advantage of this last approach is the fact that the normalisation outcomes will be independent of the (arbitrarily chosen) time period to which the reference interventions in normalisation apply. We have chosen to follow the approach as proposed by Heijungs (2005), which theoretically implies that in this study, both the functional unit (the economic system) and the corresponding interventions should be considered as rates, rather than the more commonly used absolute magnitudes.

Following this line of reasoning, multiplying emission and extraction magnitudes by the corresponding LCA characterisation factors for each LCA impact category gives:

$$A_{e,s} = \sum_i \sum_x Q_{e,x,i} \times M_{x,i,s} \tag{6.1}$$

where $A_{e,s}$ (*e.g.* in kg-eq./yr) is the normalisation factor for impact category e in reference system s, $Q_{e,x,i}$ (*e.g.* in kg-eq./kg) is the characterisation factor related to impact category e for substance x released to or extracted from environmental compartment i, and $M_{x,i,s}$ (*e.g.* in kg/yr) is the release or extraction of substance x to compartment i in reference system s.

6.2.3 Impact category classes

In LCA characterisation, a distinction is made between two classes of impact categories: the so-called *midpoint* and *endpoint* categories, respectively (Jolliet *et al.*, 2004). Midpoint categories represent homogeneous classes of impacts with respect to effect type or mechanism. These categories largely correspond to the focus points of environmental policy. *Climate change*, *acidification* and *aquatic ecotoxicity* are examples of impact categories at the midpoint level. Endpoint categories are formulated on a more functional basis: they represent the ultimate environmental values, eventually damaged by anthropogenic interventions. In this study, we focus on the calculation of normalisation scores for impact categories on the midpoint level. Table 6.2 gives an overview of the impact categories considered, and of the characterisation methods used for the different categories. Most of these characterisation factors are updates of the characterisation factors, published in the *Handbook on Life Cycle Assessment* by Guinée *et al.* (2002). The new factors are to be included in the new impact assessment method ReCiPe (Heijungs *et al.*, 2003).

Table 6.2 Overview of the impact categories covered by this study.

impact category	characterisation factor	unit of CF	ref.
climate change	global warming potential	kg CO_2-eq./kg	[1]
ozone depletion	ozone depletion potential	kg CFC-11-eq./kg	[2]
acidification	acidification potential	kg SO_2-eq./kg	[3,4]
freshwater eutrophication	freshwater eutrophication potential	kg P-eq./kg (to freshwater)	[5]
marine eutrophication	marine eutrophication potential	kg N-eq/kg (to freshwater)	[5]
human toxicity	human toxicity potential	kg 1,4-DCB eq./kg (to urban air)	[6-10]
photochemical oxidant formation	photochemical oxidant formation potential	kg NMVOC-eq./kg	[11,12]
particulate matter formation	particulate matter formation potential	kg PM_{10}-eq./kg	[11,12]
terrestrial ecotoxicity	terrestrial ecotoxicity potential	kg 1,4-DCB eq./kg (to industrial soil)	[6-10]
freshwater ecotoxicity	freshwater ecotoxicity potential	kg 1,4-DCB eq./kg (to freshwater)	[6-10]
marine ecotoxicity	marine ecotoxicity potential	kg 1,4-DCB eq./kg (to seawater)	[6-10]
ionising radiation	ionising radiation potential	kBq U-235 eq./kg (to air)	[13]
agricultural land occupation	land occupation potentials	–	[14]
urban land occupation	land occupation potentials	–	[14]
fossil energy resource depletion	fossil energy resource depletion potential	kg oil eq./kg (nat. gas: MJ/kg oil eq./m^3)	[15]

[1] IPCC (2001); [2] WMO (1999); [3] Van Zelm *et al.* (2007b); [4] Van Zelm *et al.* (2007c); [5] Struijs *et al.* (2007); [6] Huijbregts *et al.* (2005b); [7] Huijbregts *et al.* (2005a); [8] Van de Meent & Huijbregts (2005); [9] Van Zelm *et al.* (2007a); [10] Huijbregts *et al.* (2007); [11] Van Zelm *et al.* (*in press*); [12] Van Zelm *et al.* (2007d); [13] Frischknecht *et al.* (2001); [14] De Schrijver and Goedkoop (*in press*); [15] Frischknecht *et al.* (2004).

6.2.4 Boundary between inventory and characterisation

Normalisation largely consists of a two-step procedure: *inventory analysis* of environmental interventions (Rebitzer *et al.*, 2004) and numerical *characterisation* of these interventions by multiplying them with the characterisation factors in the context of the applicable impact categories (Pennington *et al.*, 2004). Although environmental fate analysis is considered as a part of the LCA characterisation, it is not always clear where the inventory analysis ends and the characterisation starts – that is, in which terms the interventions should be expressed. Ammonia emissions from manure and fertiliser to air, reported extensively in literature, are in this study considered as emissions of nitrogen compounds to soil, with subsequent volatilisation in the field situation. Emissions of nitrous oxide – again reported extensively in emission databases – result from environmental fate processes in the soil after the application of manure or fertiliser. In this study, these emissions are accounted for as direct emissions, since the process of denitrification is not yet included in the characterisation factors used. In general, we accounted for fate in the inventory analysis only if the fate process concerned was not included in the characterisation factors (see Table 6.3).

Table 6.3 Level of emissions at the boundary between *inventory* and *characterisation*.

substance	emission source	original release compartment	inventory level emission compartment	possible subsequent (characterisation level) residence compartments
ammonia/ ammonium	manure, fertiliser	air or agricultural soil	agricultural soil	air
nitrous oxide	manure, fertiliser	agricultural soil (as N)	air	–
minerals	manure, fertiliser	agricultural soil	agricultural soil	freshwater, crops
heavy metals	manure, fertiliser	agricultural soil	agricultural soil	freshwater, crops
pesticides	direct application	agricultural soil	agricultural soil	air, freshwater

6.2.5 Boundary between economic system and environment

When soils are used for economic activities, the boundary between the economic and the environmental system is not always clear cut. For normalisation, we need to define the environmental soil system in order to be able to distinguish between soil emissions and transfer processes within the economic system. For industrial soil, we considered landfills as part of the economic system, but the underlying soil as part of the environmental system. Agricultural soil was assumed to be part of the environmental system, but crops were considered as part of the economic system. This corresponds with the calculation routine for fate and exposure factors of toxic pollutants, as elaborated in Huijbregts *et al.* (2005b).

6.2.6 Emissions, caused by physical interventions

Besides resource extraction, production, use, and waste treatment, physical interventions too are part of many product life cycles. Physical interventions include forest clearing, mine exploitation and other landscape-transforming processes that are performed for the sake of economic production. Besides direct landscape transformation, these interventions can also cause emissions. While the emission of carbon dioxide by forest burning is easily recognised, more hidden, long-lasting emissions may occur as well, especially as a result of transformed soil physics and chemistry. These emissions include increased levels of soil carbon dioxide release (Marland and Schlamadinger, 1995; Schulze *et al.*, 2000) and increased phosphorous compound loss as a result of a boosted soil erosion level (Smil, 2002). The magnitude of this type of emissions is expected to be considerable, but estimates are still uncertain. The question in which way such interventions should be allocated to an LCA functional unit has been discussed by Reijnders and Huijbregts (2003). For reasons of present uncertainty on the emission magnitudes, emissions that are caused by physical interventions have not been included in this study.

6.3 Guidelines for data source prioritisation and data estimation

6.3.1 Procedures

It occasionally happens that different literature resources are available on the same releases and extractions. In these cases, it is necessary to make a choice between different data sources. Additionally, data on environmental releases and extractions are most often not available in the form or at the geographical scale that exactly corresponds to the specific needs for an LCA normalisation study. Therefore, the use of data estimates is inevitable in LCA normalisation.

For reasons of consistency, it is important to use explicit criteria for the prioritisation of data sources and the estimation of data. The criteria developed for use in this project can be considered as a proposal for the establishment of a general set of guidelines for data source prioritisation and data estimation in LCA normalisation. A detailed overview of impact categories, intervention data collected, data types used, data estimation procedures applied, and literature resources consulted, can be found in the *Supporting information* (part 1).

6.3.2 Data source prioritisation

The following criteria for data source prioritisation have been used in this study, and are proposed as general guidelines:

1. Authorativeness of literature sources

Authorative literature sources were preferred to less authorative sources. Independent scientific journals were considered as the most authorative data sources, followed by databases provided by independent, large international organisations, particularly if the databases concerned were updated regularly and were generally recognised as a basis for international environmental policy.

2. Number of emission sources covered

Data covering a large proportion of emission source categories were preferred to data which covered only a limited number of source categories.

3. Measured values versus scenario estimates

Measured values were preferred to scenario estimates.

4. Measured values versus expert estimates

Expert estimates on the basis of measured values were preferred to measured values as such.

5. Independency of data sources

Independently collected data was preferred to data, reported by stakeholders.

6. Number of countries covered
Data sources, covering a large number of countries, were preferred to sources with a smaller spatial coverage.

7. Normalisation as a 100% reference
Data, linked to emissions *caused by* production in the reference year, chosen for the normalisation at stake, were preferred to emission data as such for the same year.

6.3.3 Emission factors

Emission factors can be used if the relationship between the magnitude of a source and the release from this source is known or can be derived. For some source-substance combinations, emission factors are readily available. In this study, we used ammonia emission factors for different types of fertiliser, as defined by FAO (2006a), Bouwman *et al.* (1997, 2002), and IFA (2006), and an emission factor for the release of the anti-fouling agent tributyltin (TBT) from ship surfaces (Van de Plassche and Van der Aa, 2004). If emission factors are not readily available, they can be constructed from information on the magnitude and composition of releases. In this study, we constructed emission factors for the release of ammonia from animal manure and for the release of phosphorous compounds and heavy metals from both animal manure and fertilisers on the basis of livestock statistics (FAO, 2006b), manure excretion data (Bouwman *et al.*, 1997, Van Bruggen, 2004), the use of fertiliser and manure (FAO, 2006a,b,c) and the assumed heavy metal content of manure and fertilisers (Delahaye *et al.*, 2003).

6.3.4 Production and consumption data

If emissions and emission factors are unknown, production or consumption data can be used instead. This is only possible for chemicals of which the largest part of production of consumption will eventually be released to the environment. In this study, we used consumption data of CFCs, HCFCs, halons, 1,1,1-dichloroethane, and tetrachloromethane (UNEP, 2002) as an approach for the corresponding (future) emissions. For aldrin, dieldrin, DDT and cyclohexatin, we used production data from a UNEP/FAO study (1995) as estimates for global emissions to agricultural soil. For bromomethane, consumption data (UNEP, 2002) was used as an estimate for the emission to agricultural soil.

6.3.5 Estimation factors

If emissions and emission factors are unknown and production or consumption data are not applicable, so-called estimation factors can be used instead. In contrast to emission factors, estimation factors are not applied to individual emission source types, but directly to emission totals. Estimation factors should preferably bear a clear functional relationship to the emission or extraction to be estimated. Depending on the type of emission or extraction to be assessed, many different types of estimation factors are possible. In this project, we used the following estimation factors:

- *GDP* (gross domestic product), assumed to be related to industrial production and release
- *crop production area*, assumed to be related to crop-dependent ammonia emissions and pesticide use
- *population magnitude*, assumed to be related to human waste production of N and P
- *nuclear power capacity*, assumed to be related to the release of radio-active substances
- *estimated length of polluted coastline*, assumed to be related to metal releases in the marine environment

The estimation factors were applied to extrapolate or interpolate in space or time.

6.3.6 Estimation types

Space

Extrapolation in space can be used if information is available on just a part of the assessment region. As an example, information on emissions or extractions in a number of European countries can be extrapolated to the level the European region as a whole, and information on emissions and extractions in a number of individual countries can be extrapolated to the global level. In this study, extrapolation in space was mainly applied to industrial emissions of toxic chemicals, in particular on the global scale. The national PRTRs (Pollutant Release and Transfer Registers) of the United States, Canada, Japan and Australia (US-EPA, 2006; EC, 2006; NITE, 2006; AG-DEH, 2006) and the European emission databases EMEP (2006) and EPER (2006) were the most important data sources used for this purpose.

Interpolation in space can be used if information is available on a higher spatial level than the assessment region. As an example, information on emissions or extractions on the global level can be interpolated to the level of the European region. In this study, data on the emissions of HFCs on the European scale was interpolated from global scale data (AFEAS, 2006), while data on the emissions of phosphorous compounds to freshwater on the European scale was interpolated from the global scale information, provided by Smil (2002).

Time

Extrapolation in time can be used if information is available on an earlier year than the assessment year. In this project, we extrapolated air emissions of ammonia in the year 1990 to the reference year 2000.

Interpolation in time can be used if information is available on a later year than the assessment year, *e.g.* on emissions and extractions in the year 2005 instead of 2000. In this project, we did not use interpolation in time.

Parallel equivalency assumptions
Parallel equivalency assumptions can be used if information is available on another region than the assessment region, *e.g.* on emissions and extractions in the United States instead of Europe. In this project, we used parallel equivalency assumptions to estimate European pesticide emissions from estimated pesticide emissions in The Netherlands (CBS, 2006), the United Kingdom (CSL, 2006), and the United States (Gianessi and Marcelli, 2000; Kiely *et al.*, 2004).

6.3.7 Statistical analysis

The reliability of estimation factors depends on the strength of the correlation between the emission or extraction on the one side and the specific estimation factor on the other. If information is available on a number of emissions/extractions, it can be valuable to calculate correlation factors for two or more alternative estimation factors. In this project, we applied statistical analysis to the emission data of PM_{10} and to pesticide consumption data.

For the emission of PM10, we had emission data to our disposal for most European countries and a small number of Asian countries, provided by EMEP (2006). The correlation between GDP values and PM_{10} emissions for these countries turned out to be rather weak (r^2 = 0.291). An analysis of alternative extrapolation bases showed that it was possible to find a better correlation alternative by dividing countries in three different income groups, based on a classification by the World Bank (2000): *high*, *upper-middle* and *lower-middle* plus *low* (r^2 = 0.544 by the application of ANOVA).

Outliers were eliminated by use of Chauvenet's criterion (Bevington and Robinson, 1992). Within each income group, the ratio between PM_{10} emission and GDP turned out to be reasonably constant, with large differences between income groups. The ratio between PM_{10}/GDP ratios was 3:20:600 for high, upper-middle and lower-middle plus low income groups, respectively, suggesting that the investments in cleaner technologies are larger in the more prosperous countries. Average PM_{10}/GDP ratios for the 3 income groups were applied to calculate estimates for PM_{10} emissions for all world countries on the basis of the combination of their respective GDP values and income groups.

Specific attention was paid to the estimation of pesticide emissions. FAO (2006d) provides data on the consumption of different pesticide groups for a reasonably large number of European countries. Although these group data could not be used as emission estimates for individual pesticides, they were useful for checking the validity of alternative estimation factors. The correlation between the data for overall pesticide use and GDP values turned out to be rather weak (r^2 = 0.318), suggesting that another variable might be more determinative. Crop production showed a better correlation with total pesticide use ($r^2 = 0.507$). Still better became the image when we used a more specific approach by dividing pesticides into different classes, and calculated correlations separately for each class. For the use of different classes of pesticides, we analysed correlation coefficients between pesticide use on the one hand and GDP values and crop production areas on the other, respectively. It turned out that for insecticide consumption, the correlation coefficient with the crop production area ($r^2 = 0.62$) was much higher than the correlation coefficient with the GDP value ($r^2 = 0.075$), while for herbicide, fungicide and bactericide, and other pesticide consumption, it was the other way around: higher correlation coefficients with GDP values ($r^2 = 0.701$, $r^2 = 0.336$ and $r^2 = 0.562$, respectively) than with crop production areas ($r^2 = 0.67$, $r^2 = 0.163$ and $r^2 = 0.101$, respectively). Outliers were eliminated by use of Chauvenet's criterion (Bevington and Robinson, 1992) for all correlation calculations. Estimation factors were chosen in correspondence with the results of the correlation analyses for the individual pesticides in each of the pesticide classes. The use of individual pesticides on both the global and the European scale was derived from pesticide consumption data in The Netherlands (CBS, 2006), the United Kingdom (CSL, 2006), and the United States (Gianessi and Marcelli, 2000; Kiely *et al.*, 2004).

6.4 Results

A total number of 860 environmental interventions were collected for both the European and the global system: 854 emission totals, 4 fossil energy resource extraction totals and 2 land occupation totals. An emission total consists of the summed emissions of a substance to a specific compartment in one of the geographic systems. Fossil energy resource extraction totals refer to summed extractions of a certain fossil energy resource. Land occupation totals comprise the summed area occupied for a certain type of use. The results of LCA normalisation are acquired by multiplication of each reference intervention for each environmental system with the applicable characterisation factors for all impact categories. The resulting normalisation factors are listed in Table 6.4. This table also gives an overview of the relative environmental load of the European economic system, compared to the world economic system, for each separate impact category.

Table 6.4 Normalisation factors.

impact category	unit	EU_{25+3}	world	EU_{25+3} (% of world)
climate change				
TH = 20 yr	kg CO_2 eq.	6.57E+12	5.76E+13	11
TH = 100 yr	kg CO_2 eq.	5.21E+12	4.18E+13	12
TH = 500 yr	kg CO_2 eq.	4.49E+12	3.36E+13	13
ozone depletion	kg CFC-11 eq.	6.79E+06	2.10E+08	3
acidification				
TH = 20 yr	kg SO_2 eq.	2.23E+10	3.01E+11	7
TH = 100 yr	kg SO_2 eq.	2.36E+10	3.18E+11	7
TH = 100 yr	kg SO_2 eq.	2.49E+10	3.36E+11	7
TH = 500 yr	kg SO_2 eq.	2.84E+10	3.78E+11	8
freshwater eutrophication	kg P eq. (to freshwater)	3.47E+08	3.77E+09	9
marine eutrophication	kg N eq. (to freshwater)	5.89E+09	5.71E+10	10
respiratory effects				
photochemical oxidant formation	kg NMVOC eq.	2.80E+10	3.51E+11	8
particulate matter formation	kg PM_{10} eq.	8.12E+09	9.92E+10	8
human toxicity				
TH = 100 yr	kg 1,4-DCB eq. (to urban air)	1.24E+11	1.20E+12	10
TH = infinite	kg 1,4-DCB eq. (to urban air)	2.27E+12	8.86E+12	26
freshwater ecotoxicity				
TH = 100 yr	kg 1,4-DCB eq. (to freshwater)	5.83E+09	2.94E+10	20
TH = infinite	kg 1,4-DCB eq. (to freshwater)	6.03E+09	3.07E+10	20
marine ecotoxicity				
TH = 100 yr	kg 1,4-DCB eq. (to seawater)	8.98E+09	2.85E+10	32
TH = infinite	kg 1,4-DCB eq. (to seawater)	1.78E+12	6.24E+12	29
terrestrial ecotoxicity				
TH = 100 yr	kg 1,4-DCB eq. (to industrial soil)	4.07E+09	3.72E+10	11
TH = infinite	kg 1,4-DCB eq. (to industrial soil)	6.37E+09	5.09E+10	13
ionising radiation	kBq U-235 eq. (to air)	2.90E+12	7.97E+12	36
agricultural land occupation	m^2×year	2.10E+12	3.30E+13	6
urban land occupation	m^2×year	1.89E+11	4.71E+12	4
fossil energy resource depletion	kg Sb eq.	7.23E+11	7.78E+12	9

An overview of the most important environmental interventions with respect to each impact category is shown in Table 6.5 and Table 6.6, which list all interventions that contribute to a joint share of at least 75% of the total result. Total contributions of important substance groups are listed as well. For impact categories with different sets of factors for different time horizons, a default time horizon was chosen for this table: 100 years for climate change, 500 years for acidification, and 'infinite' for al toxicity-related impact categories. A complete representation of all data for all impact categories and time horizons can be found in the *Supporting information* (part 2). It turns out that a relatively small number of interventions are responsible for the dominant results: 52 emission totals, 4 fossil energy resource extraction totals, and 2 land occupation totals.

Table 6.5 Contributions of individual impacts to normalisation factors for the EU25+3/world: emission related impact categories (TH = time horizon).

substance	emission compartment	climate change (TH 100 years)	ozone depletion (infinite TH)	acidification (TH 500 years)	freshwater eutrophication	marine eutrophication	photochemical oxidant formation	particulate matter formation	human toxicity (infinite TH)	freshwater ecotoxicity (infinite TH)	marine ecotoxicity (infinite TH)	terrestrial ecotoxicity (infinite TH)	ionising radiation
CO_2	air	77/68											
CH_4	air	10/18											
HCFC-22	air		41/7										
CFC-12	air		26/48										
CFC-11	air		11/19										
Halon-1211			2/14										
HCFCs (total)	*air*		*57/10*										
CFCs (total)	*air*		*39/70*										
halons			*3/20*										
SO_2	air			31/35				22/26					
NO_x (as NO_2)	air			30/22		27/27	42/33	32/26					
N from pig manure	agricultural soil			8/3									
N from dairy cattle manure	agricultural soil			7/3									
NH_3 (direct)	air			3/12									
manure-N (total)	*agricultural soil*			27/20		*13/15*		*11/9*					
fertiliser-N (total)				9/11		*14/11*							
NH_3 (total)	*air/agricultural soil*			40/44		*28/29*		*14/17*					
P-total	freshwater				66/80								
P-total	agricultural soil				34/20								
N-total (direct)	freshwater					47/43							
N from non-specified fertiliser	agricultural soil					6/1							
urea	agricultural soil					3/6							
NMVOC	air						42/48						
PM_{10}	air							31/29					
selenium	air								31/21		17/13		
lead	air								17/9				
arsenic	air								15/12				
mercury	air								5/3				
zinc	agricultural soil								4/13			5/7	
barium	industrial soil								3/3				

substance	emission compartment	climate change (TH 100 years)	ozone depletion (infinite TH)	acidification (TH 500 years)	freshwater eutrophication	marine eutrophication	photochemical oxidant formation	particulate matter formation	human toxicity (infinite TH)	freshwater ecotoxicity (infinite TH)	marine ecotoxicity (infinite TH)	terrestrial ecotoxicity (infinite TH)	ionising radiation
bromomethane	air								2/8				
cadmium	agricultural soil								3/7				
chlorine	freshwater									68/60			
atrazine	agricultural soil									15/10		17/8	
nickel	air										22/11		
copper	air										16/23	6/4	
vanadium	air										16/17		
zinc	air										6/3	5/1	
cypermethrin	agricultural soil									3/7		16/26	
copper	marine water										3/3		
nickel	agricultural soil										3/3		
copper	agricultural soil										3/3	9/2	
copper	industrial soil											5/2	
aldicarb	agricultural soil											5/7	
chloropicrin	agricultural soil											4/6	
terbufos	agricultural soil											4/6	
pesticides (total)	*agricultural soil*								*1/8*	*24/30*		*59/68*	
carbon^{14}	air												73/73
cesium^{137}	freshwater												25/25

Data in *italics* refer to intervention groups.

Table 6.6 Contributions of individual impacts to normalisation factors for the EU_{25+3}/world: non-emission related impact categories.

land use intervention or substance extracted	intervention type	agricultural land occupation	urban land occupation	fossil energy resource depletion
agricultural land occupation	agricultural land use	100/100		
urban land occupation	urban land use		100/100	
natural gas	fossil energy resource depletion			37/31
crude oil	fossil energy resource depletion			38/44
hard coal	fossil energy resource depletion			14/23
lignite	fossil energy resource depletion			11/2

For *climate change*, CO_2 and CH_4 together account for around 85% of the effect on both scales. CO_2 alone is responsible for almost 70% of the impact on the global scale and for more than 75% of the impact on the European scale.

For *ozone depletion*, CFC emissions are responsible for 66% of ozone depletion on the global scale in the year 2000. Halons are the second cause, with a contribution of 19%. On the European scale, however, HCFCs take the leading role with a contribution of 65%, and the contribution of halons is less than 5%.

Characterisation factors for *acidification* on both the global and the European scale are defined for SO_2, NO_x, and NH_3. Each of these substances contributes significantly. Emissions of NH_3 have been split up between different sources: Emissions of all different types of manure and fertiliser are considered separately, and distinguished from direct ammonia emissions from other sources. Manure and fertilisers together form the largest sources of NH_3 on both scales. Total NH_3 emissions form the dominant cause of acidification on both scales.

Eutrophication is split up into *freshwater* and *marine eutrophication*. While *freshwater eutrophication* is caused by emissions of phosphorous compounds, either directly to the freshwater compartment or to agricultural soil, *marine eutrophication* is caused by a number of different nitrogen compounds to different compartments. Human waste emissions of phosphorous compounds and point emissions of nitrogen compounds to the freshwater compartments are identified as the dominant causes for freshwater and marine eutrophication, respectively.

Photochemical oxidant formation is caused for more than 80% by the combination of non-methane volatile organic chemicals (NMVOCs) and NO_x in both geographic systems. *Particulate matter* formation is dominated not only by the direct emission of PM_{10} (particles with a diameter of 10 μm or less), but also to a considerable extent by the emissions of SO_2, NO_x and NH_3 in both systems.

Human toxicity impacts are fully dominated by heavy metals in both geographic systems. Air emissions of heavy metals are specifically large contributors to human toxicity, with selenium air emissions as the largest contributor for both the global (21%) and the European (31%) system. Apart from heavy metals, only pesticide emissions to agricultural soil contribute for more the 5% to one of the environmental profiles: 8% for the global system. This last contribution is almost fully determined by bromomethane.

For *freshwater ecotoxicity*, chlorine emissions to the freshwater compartment play a dominant role with a contribution of more than 50% for both systems. Pesticide emissions to agricultural soil are the other important factor. *Marine ecotoxicity* is fully dominated by emissions of heavy metals, largely to air. *Terrestrial ecotoxicity* is dominated by pesticide emissions to agricultural soil.

For *ionising radiation*, emissions of carbon-14 are fully dominant, with a contribution of 73% to the total impact on both geographical scales.

For LCA characterisation and normalisation purposes, the impact categories of agricultural and urban land occupation have been split up here. On the global scale, direct data for both categories was available from the World Resources Institute (WRI, 2000). On the European scale, these categories have been composed from classes in the CORINE system (EEA, 2006).

Finally, for *fossil energy resource depletion*, the extractions of natural gas and crude oil form the determinative impacts.

6.5 Discussion

6.5.1 Interpretation of results

The results of this study show that only a relatively small proportion of the total number of interventions is responsible for a large proportion of potential environmental impacts. From the 858 environmental interventions collected, 46 interventions account for at least 75% of the impact scores of all impact categories. All non-toxicity related, emission dependent impacts are fully dominated by the bulk emissions of 10 substances or substance groups: CO_2, CH_4, SO_2, NO_x, NH_3, CO, PM_{10}, NMVOC, and(H)CFCs emissions to air and emissions of N- and P-compounds to freshwater.

Comparing our results with the study of Huijbregts *et al.* (2003), it was found that for climate change, acidification and resource extraction, the overall results for year 2000 have remained largely the same as for 1995. For ozone depletion, the toxicity-related impact categories and ionising radiation, the results have substantially changed. The total impact score for ozone depletion has been largely reduced between 1995 and 2000. CFC emissions still dominate the global normalisation score. On the European level, however, HCFCs have taken over the leading role of CFCs as the dominant cause of ozone depletion. It should be remarked, however, that the normalisation results for 1995 and 2000 are not fully comparable. Especially for these ozone-depleting emissions, the methodological choice to shift from emissions, taking place in the reference year to emissions, caused by production in this year, results in a considerable reduction.

For eutrophication and photochemical oxidant formation, the results between the two studies are difficult to compare, because the characterisation method has been adapted for these impact categories. Particulate matter formation is a new impact category that was not accounted for in the 1995 study.

The present human toxicity image, with a dominant role for heavy metal emissions, is different from the 1995 image, in which non-halogenated hydrocarbons were fully dominant. For aquatic ecotoxicity, chlorine emissions to freshwater, that dominate the results in the present study, were not accounted for in 1995, and pesticide emissions to agricultural soil then dominated the impact score. For marine ecotoxicity, heavy metal emissions were dominant as well in 1995, but differences exist in the relative importance of individual metals, and direct emissions to seawater played a more important role. For terrestrial ecotoxicity, heavy metal and pesticide emissions to agricultural soil changed places between 1995 and 2000: a dominant role for the pesticides and a secondary role for heavy metals in the present study, and the inverse image in the 1995 study. Here too, the relative importance of individual metals differs between the 1995 and the 2000 studies. The large differences between 1995 and 2000 results indicate that the uncertainties for the toxicity-related impact categories are probably very high. For these impact categories, the dominance of an emission should be considered only as an indication that further investigation could be interesting. Whether the dominant emissions (*e.g.* chlorine emissions to freshwater and bromomethane emissions to agricultural soil) actually play a dominant role in potential environmental toxicity is a question for more specific research.

For ionising radiation, the results for year 2000 are similar to the results for the year 1995: a dominant role for the emission of carbon-14 to air.

With respect to the LCA results of both economic systems as a whole, it turns out that the European economic system is responsible for relatively large contributions to most of the toxicity-related impact categories, and to ionising radiation. For ionising radiation, this is due to the relatively high nuclear capacity of the European region, which has been used as an estimation parameter for emissions. For the toxicity-related impact categories, the ratios found are most probably a reflection of the percentage of 27% of world GDP for which the European region is responsible, since GDP has been used as an extrapolation factor for many toxic emissions. This finding emphasizes the relatively high uncertainty of the normalisation factors for toxicity in both Europe and the world. Considering the relatively high European GDP, the European contribution to other impact categories – mostly around 10% or less – is rather low. For the emission-related impact categories, this may be due to the use of cleaner technologies in this region.

6.5.2 Uncertainty

Uncertainty in normalisation results is caused by a combination of uncertainty in emission data and uncertainty in characterisation factors. Establishing quantitative estimates of uncertainty in normalisation factors is considered out of the scope of this study, as uncertainty margins for most emissions, extractions and characterisation factors were not readily available. Instead, we focus on a qualitative assessment of the most important uncertainties in the normalisation factors.

The highest level of uncertainty applies to emission data that is extrapolated from emissions in a limited number of countries. This is the case for virtually all data that refer to *toxicity*-related impact categories, to the impact category *ionising radiation*, to emissions of the substances 1,1,1,-trichloroethane (methyl chloroform) and tetrachloromethane (carbon tetrachloride) – that contribute to *ozone depletion* – and to emissions of PM_{10} – that is important in the context of the impact category *particulate matter formation*. An intermediate level of uncertainty is expected to apply to all other types of estimates that are based on a combination of reported data and estimation factors: emission estimates for CFCs, HCFCs and halons, European emission estimates for HFCs, estimated point emissions of nitrogen compounds, and emission estimates for phosphorous compounds. The lowest level of uncertainty is assumed to apply to the emission and extraction data, taken directly from official data reports: European data on *climate change*, European SO_2 and NO_x emission data, land occupation data, and resource depletion data. Emission estimates or scenarios, derived from reported emission data in earlier years or calculated from manure and fertiliser application, are also considered to have a relatively low level of uncertainty: global, non-European data on *climate change* and on SO_2 and NO_x emissions, as well as all NH_3, CO and NMVOC emission data.

Apart from emission data, characterisation factors can also be a source of uncertainty for normalisation. The largest uncertainties with respect to characterisation factors probably apply to fate modelling of heavy metals, resulting in uncertainty in the corresponding toxicity-related characterisation factors (Heijungs *et al.*, 2004). Since the emission data for heavy metals have a high factor of uncertainty as well, the relative importance of the role of heavy metals with respect to different toxicity-related impact categories is still very difficult to assess.

The most important overall cause of uncertainty in emission data is most probably the absence of toxic release inventories in most countries. The absence of characterisation factors for some substances further adds to uncertainty of the results of normalisation.

Expansion of emission registration by international policy can be considered as one of the most effective measures to diminish uncertainty. The foundation of an Intergovernmental Panel on Chemical Pollution, as recently suggested by Scheringer (2007), would be a way to implement this in a formalised and unambiguous way. An independent reviewing procedure for all types of release data could improve data quality and thus further reduce uncertainty.

6.5.3 Bias

Systematic over- or underestimation are considered as bias, rather than uncertainty. Heijungs *et al.* (2007) pointed out that data gaps in the inventory or in the list of characterisation factors may cause not only uncertainty, but also bias in normalisation. The authors give a systematic overview of all possibilities of over- or underestimation, according to the type of data that is lacking.

In this study, we had to deal with two types of data gaps: missing characterisation factors for expectedly toxic substances on which emission data was available, and missing emission data for potentially toxic substances that were included in the list of characterisation factors. Despite a large increase in the number of available characterisation factors for toxic impacts, data gaps are still considerable. 30% of the total load of emissions to air and freshwater, reported by the national PRTRs (Protocols on Pollutant Release and Transfer Register) of Canada, Japan and the United States (EC, 2006; NITE, 2006; US-EPA, 2006) could not be covered by characterisation factors for at least one toxic impact category. Almost all reported emissions are expected to refer to potentially toxic substances. As a result of this gap in toxicity characterisation factors, both characterisation and normalisation will often apply to a limited part of total emission – depending on the exact emission profile of the product under study. This should be kept in mind if conclusions are drawn from the results. Especially if a substance causes a high impact score in characterisation, while this substance has not been accounted for in the normalisation factor, the normalisation score may become disproportionally high. This bias can be prevented either by leaving the characterisation score of the substance out of the impact score in the normalisation step, or by the (*ad hoc*) construction of a new normalisation factor that includes the total environmental emission of the substance at stake.

A possible cause of bias that has not been mentioned by Heijungs *et al.* (2007) is connected to the demarcation of non-global reference systems. Geographical boundaries do not automatically correspond to the system boundaries in LCA. The life cycle of a European product, for instance, will often exceed the geographic European boundaries. In other words: the environmental impacts, connected to the European *ecological footprint* (Wackernagel and Rees, 1996) will probably be different from the environmental impacts occurring within the European geographic boundaries. If normalisation should be consistent with the LCAs of the composing product systems, it should reflect the impacts, connected to this ecological footprint, rather than to the European geographic region. This issue has been addressed by Breedveld *et al.* (1999), who defined normalisation factors for the Netherlands on two different bases: geographic boundaries versus final consumption – representing 'all environmental interventions in one year (1993/1994) related to the consumption of Dutch end consumers, including the total chains of production and waste processes that result from this consumption'. In the present study, we used the geographic boundaries as system boundaries. A possible future implementation of the 'ecological footprint' principle could be reached by the use of input–output models (*e.g.* Hubacek and Giljum, 2003; Suh, 2004).

The methodological choice to prefer emissions, caused by production in the year 2000, above emission during the year 2000 as such, can be an extra cause of bias. Future emissions of CFCs, HCFCs, and halons, are presumed to equal consumption in the year 2000, while in reality, combustion or destruction are other possibilities to handle these substances. Recycling of 'old' CFCs and HCFCs in the year 2000 and the question how this should be analysed and allocated further adds to methodological complexity and further risk of bias. Future emissions, caused by usage and waste treatment of products, were presumed to equal the equivalent emissions in the year 2000, with only a few exceptions for mainly (H)CFCs. This assumption may be biased, especially for those substances that are largely emitted by usage and waste treatment related processes. For the majority of substances, however, differences between both emission types are expected to be relatively small.

6.5.4 Perceived and actual versus potential and prolonged

The results of an LCA study do not always reflect the ratios of perceived environmental problems. This becomes specifically clear if not just one product, but the economic system as a whole is subjected to the analysis. High impact scores may be connected to substances that are perceived as being not that problematic, while substances that are known to be connected to real environmental problems may receive amazingly low scores in the LCA environmental profile. This phenomenon is caused by two specific properties of LCA characterisation: first, the convention to assess potential environmental impacts, and second, the integration of environmental concentrations over time.

The concept of potential problems – or the 'less is better approach' – refers to the fact that emissions in LCA are assessed on the basis of a combination of potential harmfulness, environmental residence time and – if applicable – overall human intake. Environmental concentrations or average daily intake rates cannot be coupled to the summed emission totals that LCA characterisation is about. LCA therefore leaves risks and average human intake rates out of consideration. Environmental emissions are directly combined with environmental residence times to deliver time-integrated exposure totals. This makes LCA results independent of dilution, not only in the spatial sense, but also in terms of time. Environmental threshold values – that are so determinative for risk assessment – are not accounted for in LCA. Low but long-remaining concentrations of potentially toxic substances will deliver the same outcome as concentration peaks, as long as the time-integrated concentrations are the same. In general, this may result in an unexpectedly high LCA impact scores for poorly degradable chemicals, despite their relatively low environmental concentrations. For the normalisation step in an individual case study, it means that normalisation scores for these chemicals, and for chemicals that are released in near-to-threshold concentrations, will be relatively high, compared to their relative risk that they cause. Therefore, the prioritisation of desired environmental measures should not be based on LCA normalisation alone. Normalisation scores form an indication, but should be checked with measurements before conclusions on corresponding risk levels can be drawn.

6.6 Conclusions

This study has been performed in the context of LCA methodology, but the relevance of the results ranges much further. For LCA, this normalisation study is not only an update in the sense that it refers to a time step of 5 years in comparison to our former study (Huijbregts *et al.*, 2003). Much more important is the fact that a large reduction in uncertainty could be reached by the increased data availability, resulting from a growing international awareness of the urgency of emission data reporting. Another important feature of these updated normalisation data is in their correspondence to up-to-date LCA midpoint characterisation factors.

Although intended as a methodological step in LCA, this normalisation study can also be considered as an LCA case study in itself – with the economic system as the functional unit. The results of this study clearly indicate that the environmental profile of the global and European economic systems appears to be dominated to a large extent by only a small number of substances, released in bulk quantities.

Large uncertainties remain to exist with respect to toxic substances. Current toxic release inventories are available for developed countries only. Releases in developing countries are very difficult to estimate, even by approximation. Moreover, characterisation factors are still lacking for many toxic chemicals, most probably because no or insufficient toxicity data is available. This combination makes it impossible to assess the magnitude of overall toxicity of chemicals, released to the environment, and thus to construct reliable normalisation factors for toxicity-related impact categories in LCA. An update of this normalisation study is recommended as soon as either supplemental emission information or new characterisation factors have become available.

With a fast growing world economy, new, strictly controlled procedures for the abatement of bulk releases and the inventory of toxic releases, coupled to the identification of key toxic substances, are recognised to be of prior importance for global environmental management in the context of sustainability.

References

AFEAS (2006) *AFEAS Data Download.* Alternative Fluorocarbons Environmental Acceptability Study (AFEAS), Arlington, VA, USA. Downloadable from: http://afeas.org/prodsales_download.html

AG-DEH (2006) *National Pollutant Inventory (NPI) Australia.* Australian Government - Department of Environment and Heritage (AG-DEH), Canberra, Australia. At: http://www.npi.gov.au/

Bare J, Gloria Th, Norris G (2006) Development of the Method and U.S. Normalization Database for Life Cycle Impact Assessment and Sustainability Metrics. *Environ Sci Technol* **40** (16): 5108 -5115

Bevington PhR, Robinson DK (1992) *Data Reduction and Error Analysis for the Physical Sciences. Second edition.* McGraw-Hill, Inc., New York [etc.], USA. 328 pp.

Bouwman AF, Boumans LJM, Batjes NH (2002) Estimation of Global NH_3 Volatilization Loss from Synthetic Fertilizers and Animal Manure Applied to Arable Lands and Grasslands. *Global Biogeoch Cycles* **16** (2): 8-1 - 8-15

Bouwman AF, Lee DS, Asman WAH, Dentener FJ, Van der Hoek KW, Olivier JGJ (1997) A Global High Resolution Emission Inventory for Ammonia. *Global Biogeochemical Cycles* **11**: 561-587

Breedveld L, Lafleur M, Blonk H (1999) A Framework for Actualising Normalisation Data in LCA: Experiences in the Netherlands. *Int J LCA* **4** (4): 213-220

CBS (2006) *Statline.* Centraal Bureau voor de Statistiek (CBS), Voorburg/Heerlen, The Netherlands. At:
http://statline.cbs.nl/StatWeb/start.asp?lp=Selection2FApplet2FSelectPage

CSL (2006) *Pesticide Usage Statistics.* Central Science Laboratory (CSL), York, UK. At: http://pusstats.csl.gov.uk/myindex.cfm

Curran, MA (2006) *Life Cycle Assessment: Principles and Practice. EPA/600/R-06/060.* U.S. Environmental protection agency (EPA), Cincinnati, OH, USA. 80 pp. Downloadable from: http://www.epa.gov/nrmrl/lcaccess/pdfs/600r06060.pdf

Delahaye R, Fong PKN, Van Eerdt MM, Van der Hoek KW, Olsthoorn CSM (2003) *Emissie van zeven zware metalen naar landbouwgrond. Emission of seven heavy metals to the agricultural soil.* (In Dutch.). Centraal Bureau voor de Statistiek (CBS), Voorburg/Heerlen, The Netherlands. 33 pp. Downloadable from:
http://www.cbs.nl/NR/rdonlyres/837282FD-9AC2-4529-AB2C-340444892528/0/zwaremetaleneindrapport.pdf

De Schrijver A, Goedkoop M (*in press*) *Land use.* In: Goedkoop M, Heijungs R, Huijbregts M, De Schrijver A, Struijs J, Van Zelm R. *Towards a life cycle impact assessment method which comprises category indicators at the midpoint and the endpoint level. Report of the second project phase: Implementation of the new method.* RIVM, Bilthoven, The Netherlands

EA (2006) *Pollution Inventory Data Trends Spreadsheet.* Environment Agency (EA), London, UK. At:
http://www.environment-agency.gov.uk/commondata/103601/pi_summ_proc_05v3prot_862571.xls

EC (2001) *Green Paper on Integrated Product Policy.* Commission of the European Communities (EC), Brussels, Belgium. 32 pp. Downloadable from:
http://www.iwoe.unisg.ch/org/iwo/web.nsf/SysWebRessources/EU_IPP.pdf/$FILE/EU_IPP.pdf

EC (2006) *National Pollutant Release Inventory (NPRI).* Environment Canada (EC), Ottawa, Ontario, Canada. At: http://www.ec.gc.ca/pdb/npri/npri_home_e.cfm

EEA (2006) *EPER. The European Pollutant Emission Register*. European Environment Agency (EEA), Copenhagen, Denmark. At: http://www.eper.cec.eu.int/eper/default.asp

EMEP (2006) *UNECE/EMEP activity data and emission database. WebDab 2005*. EMEP, Oslo, Norway. At: http://webdab.emep.int/

FAO (2006A) *FAOSTAT Statistical Data. Fertilizer*. Food and Agriculture Organization of the United Nations (FAO), Rome, Italy. At: http://faostat.fao.org/site/422/default.aspx

FAO (2006b) *FAOSTAT Statistical Data. Production. Live animals*. Food and Agriculture Organization of the United Nations (FAO), Rome, Italy. At: http://faostat.fao.org/site/409/default.aspx

FAO (2006c) *FAOSTAT. Agricultural data. Agricultural & Food Trade. Milk Fresh*. Food and Agriculture Organization of the United Nations (FAO), Rome, Italy. At: http://faostat.fao.org/faostat/form?collection=Trade.CropsLivestockProducts&Domain=Trade&servlet=1&hasbulk=0&version=ext&language=EN

FAO (2006d) *FAOSTAT. Statistical data. Pesticide consumption*. Food and Agriculture Organization of the United Nations (FAO), Rome, Italy. At: http://faostat.fao.org/site/424/DesktopDefault.aspx?PageID=424

Frischknecht R, Braunschweig A, Hofstetter P, Suter P (2001) Human Health Damages due to Ionising Radiation in Life Cycle Impact Assessment. *Environ Impact Assessment Rev* **20**: 159-189

Frischknecht R, Jungbluth N, Althaus H-J, Doka G, Dones R, Hirschier R, Hellweg S, Humbert S, Margni M, Nemecek T, Spielmann M (2004) *Implementation of Life Cycle Impact Assessment Methods. ecoinvent report No. 3*. Swiss Centre for Life Cycle Inventories, Dübendorf, Switzerland

Gianessi LP, Marcelli MB (2000) *Pesticide use in U.S. crop production: 1997. National Summary Report*. National Center for Food and Agricultural Policy (NCFAP), Washington DC, USA. 101 pp. Downloadable from: http://www.ncfap.org/ncfap/nationalsummary1997.pdf

Guinée JB, Gorrée M, Heijungs R, Huppes G, Kleijn R, De Koning A, Van Oers L, Wegener Sleeswijk A, Suh S, Udo de Haes, De Bruijn H, Van Duin, Huijbregts MAJ (2002) *Handbook on Life Cycle Assessment. Operational Guide to the ISO Standards*. Kluwer Academic Publishers, Dordrecht [etc.], The Netherlands. 704 pp.

Heijungs R (2005) On the Use of Units in LCA. *Int J LCA* **10** (3): 173-176.

Heijungs R, Goedkoop M, Struijs J, Effting S, Sevenster M, Huppes G (2003) *Towards a life cycle impact assessment method which comprises category indicators at the midpoint and the endpoint level. Report of the first project phase: Design of the new method*. VROM

Report. Netherlands Ministry of Housing, Spatial Planning and the Environment (VROM), The Hague, The Netherlands. 74 pp. Downloadable from: http://www.leidenuniv.nl/cml/ssp/publications/recipe_phase1.pdf

Heijungs R, Guinée JB, Kleijn R Rovers V (2007) Bias in Normalization: Causes, Consequences, Detection and Remedies. *Int J LCA* **12** (4): 211-216

Heijungs R, De Koning A, Ligthart T, Korenromp R (2004) *Improvement of LCA characterization factors and LCA practice for metals.* TNO-report R 2004/347. TNO, Apeldoorn, The Netherlands. 67 pp. Downloadable from: http://www.leidenuniv.nl/interfac/cml/ssp/projects/finalreportmetals.pdf

Hubacek K, Giljum S (2003) Applying physical input-output analysis to estimate land appropriation (ecological footprints) of international trade activities. *Ecological Economics* **44**: 137-151

Huijbregts MAJ, Breedveld L, Huppes G, De Koning A, Van Oers L, Suh S (2003) Normalisation Figures for Environmental Life-Cycle Assessment: The Netherlands (1997/1998), Western Europe (1995) and the World (1990 and 1995). *Journal of Cleaner Production* **11** (7): 737-748

Huijbregts MAJ, Rombouts LJA, Ragas AMJ, Van de Meent D (2005a) Human-toxicological effect and damage factors of carcinogenic and non-carcinogenic chemicals for life cycle impact assessment. *Integrated Environmental Assessment and Management* **1** (3): 181-244

Huijbregts MAJ, Struijs J, Goedkoop M, Heijungs R, Hendriks JA, Van de Meent D (2005b) Human Population Intake Fractions and Environmental Fate Factors for Toxic Pollutants in Life Cycle Impact Assessment. *Chemosphere* **61** (10): 1495-1504

Huijbregts MAJ, Van Zelm R, Van de Meent D (2007) *Human and ecological impacts of toxic chemicals in life-cycle impact assessment.* LCA Expertise Centre, RIVM, Bilthoven, The Netherlands

IFA (2006) Statistics > Nitrogen fertilizer nutrient consumption - Million tonnes N. International Fertilizer Industry Association (IFA), Paris, France. At: http://www.fertilizer.org/ifa/statistics/indicators/tablen.asp

IPCC (2001) *Climate Change 2000. The science of climate change. Contribution of working group I to the third assessment report of the Intergovernmental Panel on Climate Change.* Cambridge University Press, Cambridge, UK. 881 pp.

Jolliet O, Müller-Wenk R, Bare J, Brent A, Goedkoop M, Heijungs R, Itsubo, Peña C, Pennington D, Potting J, Rebitzer G, Stewart M, Udo de Haes H, Weidema B (2004) The LCIA Midpoint-Damage Framework of the UNEP/SETAC Life Cycle Initiative *Int J LCA* **9** (6): 394-404

Kiely T, Donaldson D, Grube A (2004) *Pesticides Industry Sales and Usage: 2000 and 2001 Market Estimates.* U.S. Environmental Protection Agency (US-EPA), Office of Pesticide Programs, Office of Prevention, Pesticides, and Toxic Substances (OPPTS), Biologocal and Economic Analysis Division. Washington DC, USA. 33 pp. Downloadable from:
http://www.epa.gov/oppbead1/pestsales/01pestsales/market_estimates2001.pdf

Lundie S, Huijbregts MAJ, Rowley HV, Mohr NJ, Feitz AJ (2007) Australian Characterisation Factors and Normalisation Figures for Human Toxicity and Ecotoxicity. *Journal of Cleaner Production* **15**: 819-832

Marland G, Schlamadinger B (1995) Biomass fuels and forest-management strategies: how do we calculate the greenhouse-gas emissions benefits? *Energy* **20**: 1131-1140

NITE (2006) PRTR data 2001. National Institute of Technology and Evaluation (NITE), Japan. At: http://www.safe.nite.go.jp/english/index.html

Norris GA (2001) The Requirement for Congruence in Normalisation. *Int J LCA* **6** (2): 85-88

Pennington DW, Potting J, Finnveden G, Lindeijer E, Jolliet O, Rydberg T, Rebitzer G (2004) Life cycle assessment. Part 2: Current impact assessment practice. *Environment International* **30**: 721-739

Rebitzer G, Ekvall T, Frischknecht R, Hunkeler D, Norris G, Rydberg T, Schmidt W-P, Suh S, Weidema BP, Pennington DW (2004) Life cycle assessment. Part 1: Framework, goal and scope definition, inventory analysis, and applications. *Environment International* **30**: 701-720

Reijnders L, Huijbregts MAJ (2003) Choices in calculating life cycle emissions of carbon containing gases associated with forest derived biofuels. *Journal of Cleaner Production* **11**: 527-532

Scheringer M (2007) Towards in International Panel on Chemical Pollution (IPCP). *Chemosphere* **67**: 1682-1683

Schulze ED, Wirth C, Hellman M (2000) Managing forests after Kyoto. *Science* **28**: 2058–2059

Smil, V (2002) *Phosphorus: Global Transfers.* In: Munn T (ed.) *Encyclopedia of Global Environmental Change.* Douglas I (Ed.) *Volume 3: Causes and consequences of global environmental change.* John Wiley & Sons, Ltd, Chichester, UK, pp. 536-542. Downloadable from: http://home.cc.umanitoba.ca/~vsmil/pdf_pubs/EGEC-1.pdf

Stranddorf HK, Hoffmann L, Schmidt A (2005a) *Impact categories, normalisation and weighting in LCA. Updated on selected EDIP97-data.* Environmental news No. 78. Danish Ministry of the Environment. Environmental Protection Agency. Copenhagen, Denmark. 90 pp. Downloadable from:

http://www2.mst.dk/udgiv/publications/2005/87-7614-574-3/pdf/87-7614-575-1.pdf

Stranddorf HK, Hoffmann L, Schmidt A (2005b) *Update on Impact Categories, Normalisation and Weighting in LCA. Selected EDIP97-data.* Environmental Project Nr. 995 2005. Miljøprojekt. Danish Ministry of the Environment. Environmental Protection Agency. Copenhagen, Denmark. 290 pp. Downloadable from:
http://www2.mst.dk/udgiv/Publications/2005/87-7614-570-0/pdf/87-7614-571-9.PDF

Strauss K, Brent A, Hietkamp S (2006) Characterisation and Normalisation Factors for Life Cycle Impact Assessment Mined Abiotic Resources Categories in South Africa: The manufacturing of catalytic converter exhaust systems as a case study. *Int J LCA* **11** (3): 162-171

Struijs J, Beusen A, Huijbregts MAJ (2007) *Environmental impacts of nutrients in life-cycle impact assessment.* LCA Expertise Centre, RIVM, Bilthoven, The Netherlands

Suh S (2004) A note on the calculus for physical input-output analysis and its application to land appropriation of international trade activities. *Ecological Economics* **48**: 9-17

UNEP (2002) *Production and Consumption of Ozone Depleting Substances under the Montreal Protocol 1986-2000.* United Nations Environment Programme (UNEP). Ozone Secretariat, Nairobi, Kenya. 75 pp. Downloadable from:
http://hq.unep.org/ozone/Publications/Production_and_consumption2005.pdf

UNEP/FAO (1995) *Study on International Trade of Widely Prohibited Chemicals. Summary. UNEP/FAO/PIC/INC.1/9.* United Nations Environment Programme (UNEP)/Food and Agriculture Organization of the United Nations (FAO), Brussels, Belgium. 7 pp. Downloadable from:
http://www.pic.int/INCs/Inc1/i9)/English/1-9.pdf

US-EPA (2006) *Toxics Release Inventory (TRI) Program. TRI Explorer.* United States Environmental Protection Agency (US-EPA), Washington DC, USA. At:
http://www.epa.gov/triexplorer/

Van Bruggen C (2004) *Dierlijke mest en mineralen 2002.* Centraal Bureau voor de Statistiek (CBS), Voorburg/Heerlen, The Netherlands. (In Dutch.). 18 pp. Downloadable from:
http://www.cbs.nl/NR/rdonlyres/EF9A77E2-C0DB-43F3-B412-FC0216668E49/0/2005dierlijkemestenmineralenart.pdf

Van de Meent D, Huijbregts, MAJ (2005) Evaluating ecotoxicological effect factors based on the Potentially Affected Fraction of species. *Environ Toxicol Chem* **24** (6): 1573-1578

Van de Plassche E, Van der Aa E (2004) *Harmonisation of Environmental Emission Scenarios: An Emission Scenario Document for Antifouling Products in OECD Countries.* European Commission, Directorate-General Environment, Final Report 9M2892.01. Royal Haskoning, Nijmegen, The Netherlands. 137 pp. + appendices.

Van Zelm R, Huijbregts MAJ, Den Hollander HA, Van Jaarsveld HA, Sauter FJ, Struijs J, Van Wijnen HJ, Van de Meent D (*in press*) European characterization factors for respiratory health damage due to PM_{10} and ozone in life cycle impact assessment. *Atmospheric Environment* (accepted)

Van Zelm R, Huijbregts MAJ, Harbers JV, Wintersen A, Struijs J, Posthuma L, Van de Meent D (2007a) Uncertainty in msPAF-based ecotoxicological freshwater effect factors for chemicals with a non-specific mode of action in life cycle impact assessment. *Integrated Environmental Assessment and Management* **3**: 203-210.

Van Zelm R, Huijbregts MAJ, Van Jaarsveld HA, Reinds GJ, De Zwart D, Struijs J, Van de Meent D (2007b) Time horizon dependent characterization factors for acidification in life-cycle assessment based on forest plant species occurrence in Europe. *Environ Sci Technol* **41**: 922-927

Van Zelm R, Reinds GJ, Van Jaarsveld H, Huijbregts MAJ (2007c) *Environmental impacts of acidifying substances in life-cycle impact assessment.* LCA Expertise Centre, RIVM, Bilthoven, The Netherlands

Van Zelm R, Sauter F, Van Jaarsveld H, Huijbregts MAJ (2007d) *Human impacts of priority air pollutants in life-cycle impact assessment.* LCA Expertise Centre, RIVM, Bilthoven, The Netherlands

Wackernagel M, Rees W (1996) *Our Ecological Footprint: Reducing Human Impact on the Earth.* New Society Publishers, Gabriola Islands, BC, Canada. 176 pp.

Wenzel H, Hauschild M, Alting L (1997) *Environmental Assessment of Products. Vol. 1: Methodology, Tools and Case Studies in Product Development.* Chapman & Hall, London, UK. 517 pp.

WMO (1999) *Scientific Assessment of Ozone Depletion: 1998. Global Ozone Research and Monitoring Project - Report No. 44.* World Meteorological Organization (WMO), Geneva, Switzerland. 700 pp.

World Bank (2000) *World Development Indicators 2000.* World Bank, Washington DC, USA. 389 pp.

WRI (2000) *World Resources 2000-2001.* United Nations Development Programme, United Nations Environment Programme, World Bank, World Resources Institute (WRI), Washington, DC, USA. Downloadable from:
http://www.wri.org/biodiv/pubs_description.cfm?pid=3027

7

General discussion and conclusions

7.1 Introduction

This final chapter provides an integration of the previous chapters, which were written as independent journal articles, into one coherent PhD thesis. The topics discussed so far – actual versus potential impacts, life cycle assessment versus risk assessment, metals in the marine environment, regionalisation of fate, exposure and effect models, and normalisation – may seem to be quite different in character. In this chapter, it will be shown that all these topics are in fact intimately related, and that they can be integrated both conceptually and in a practical sense.

First, I will revisit the main arguments of the various preceding chapters, but in a different order, and with cross-references added. Then, I will list the main conclusions and new findings and insights. The chapter also includes some personal views and historical lines.

7.2 Actual versus potential impacts in connection to LCA and RA

The issue of actual versus potential impacts, which takes a central position in chapter 2, has served as a leading theme throughout a large part of this thesis. Potential impacts are based on a chemical's relative toxicity, environmental distribution and human exposure characteristics as such, without accounting for environmental thresholds or environmental sensitivity. In 1995, White *et al.* stated that the assessment of chemicals, based on threshold exceeding, was not applicable to LCA. Although shortly thereafter, this statement became outdated in practice by the work of Hogan *et al.* (1996) and Potting *et al.* (1998), the tradition of assessing potential impacts with LCA has still remained in most LCIA-methods (*cf.* popular impact assessment methods, such as CML 2002 (Guinée *et al.*, 2002), IMPACT 2002 (Pennington *et al.*, 2005), TRACI (Bare, 2002), and Eco-indicator 99 (Goedkoop & Spriensma, 2003)). This is in part due to the fact that environmental impacts in LCA cannot be described in terms of risks (*cf.* Owens, 1997), at least not the type of risks that have traditionally been assessed with conventional risk assessment methods (Udo de Haes & Owens, 1998). Another ground is that environmental thresholds and sensitivity are location-dependent issues while most LCA characterisation methods are location-independent.

The fact that LCA cannot be used for the assessment of risks has two main reasons. The first reason is that most industrial processes – and the connected risks – are only partially included in the life cycle of a given product. A power plant, for instance, may cause a number of environmental risks, that may be analysed and quantified in the context of chemical risk assessment. For the production of a product – for example, a can of paint – only a certain amount of electricity is needed, not that of the whole plant. Although both the risks of the power plant and the amount of electricity needed for the production of a can of paint may be well described, neither risk assessment nor LCA provides the context for describing the risk of one can of paint. In more general terms: risks are connected to (continuous) economic processes in their full extent, while LCA accounts for the impacts of partial processes in a product life cycle, for example, 'paint production' in a certain paint factory. This applies not only to upstream processes in the product life cycle, but also to the direct production process itself. This incongruousness can only be solved if we express the contribution by the given can of paint to the risk that is caused by the plant as a whole in terms of time (Heijungs & Guinée, 1994), for instance, during its production time of 2 seconds, the can of paint was responsible for the full risk of the plant. Or, alternatively, during a year, the can of paint was responsible 1/1,500,000 part of the total risk of the plant (with a production capacity of 1,500,000 cans of paint a year). This is a modification that is not part of the conventional risk assessment procedure. The second reason why LCA cannot be used for risk assessment is the fact that upstream processes in the product life cycle are often dedicated to several downstream processes, for example, steel production is dedicated not only to the production of paint cans, but also to the production of cars, dust bins, cutlery and all other kinds of steel objects. The contribution of a paint can to the environmental risks, caused by a steel production plant, could again be expressed in terms of time – *e.g.*, the time that the full process is needed for the production of the amount of steel, used for the production of one paint can – but it should be noted that the full risk is connected not only to paint cans, but to many other products as well.

The location-independent character of traditional LCA – not allowing for the inclusion of any location dependent threshold exceeding – has raised the question whether LCA could make any sense at all in the context of toxicity assessment (*cf.* Owens, 1997). This issue has been discussed in terms of 'less is better' versus 'only above threshold' (White *et al.*, 1995) and 'general prevention' versus 'risk minimisation' (Barnthouse *et al.*, 1997). Potential impacts in LCA are based on the 'general prevention' principle that the release of toxic chemicals into the environment is undesirable and should be prevented per se, whether or not concentrations exceed environmental threshold values. Although I agree with this statement, I feel that concentrations that do exceed thresholds should be handled with priority; they should therefore be recognisable in LCIA, and get more emphasis in the assessment. This is the reason for which I worked out a method to distinguish between potential and actual impact in LCA toxicity assessment.

My ideas on risk assessment versus LCA and actual versus potential impacts are reflected in several chapters of this thesis. In chapter 2, a conceptual framework is described for the inclusion of contributions to risks in LCA. These contributions are together considered as the summed 'actual impacts', as opposed to the conventional 'potential impacts'. A detailed discussion on the similarities and differences between LCA and human and environmental risk assessment (HERA) can be found in chapter 3. The conclusion from this chapter is that the functional unit, as the only fundamental difference between LCA and HERA, forms the background of the fact that summed 'actual impacts' or 'risk contributions' in LCA remain different from the 'full risks' assessed with HERA, but that both could be combined in a common software tool that produces both HERA and LCA results in a consistent fashion. Chapter 5 contains a description of how the method for the assessment of 'actual impacts', proposed in chapter 2, has been implemented in the GLOBOX model. To this end, two new factors have been introduced: a *sensitivity factor* (SF) and a *threshold factor* (TF), respectively. The sensitivity factor reflects the fraction of a certain region that contains ecosystems that are sensitive to the chemical to be assessed, while the threshold factor reflects the fraction of the total region where the background concentration of this chemical exceeds the toxicological no-effect level. The user of the GLOBOX-model can choose whether actual or potential impacts, or both, should be calculated by the model. 'Actual' impacts are then expressed as the impact scores for the sensitive, above-threshold part of the region. A problem that remains, however, is the limited availability of information, required for determining the sensitivity and threshold factors. This will be illustrated by an example below.

Around the year 2000, I was involved in a project, commissioned by the Netherlands Oil and Gas Exploration and Production Association (NOGEPA), that was meant to assess the emissions of oil platforms in the North Sea with LCA. To this end, we developed location-specific LCA characterisation factors for North Sea water, and alternative characterisation factors for ocean water (Wegener Sleeswijk *et al.*, 2003). The guidelines for the NOGEPA study included that we should assign zero values to the characterisation factors for metals in ocean water, since metal concentrations in oceans were well known to be far below environmental threshold values, and it was regarded useless to include non-existing impacts in the assessment of the companies' activities. What was asked, in fact, was to deviate from our convention to assess potential impacts, and to switch to the assessment of actual impacts. With the newly developed GLOBOX model, this seems to be easy: just set the threshold factor to a zero value for metal emissions to oceans. It should be kept in mind, however, that the user should be keen to make a consistent choice. If the choice is made to account for actual impacts, this should be done for all chemicals involved in the study, and for all emission and distribution compartments in all regions. This requires a substantial amount of information, which is not always easily available. For LCA, this is much more complex than for risk assessment, because a product life cycle is not limited to one single process, neither to one single substance, to one single region or to one single year.

The GLOBOX model contains specific settings to account for actual environmental impacts in LCA toxicity characterisation. The development of a data set concerning regional environmental sensitivities and background concentrations would be a desirable next step.

7.3 LCA characterisation factors for metals

In the 1992 CML Guide on LCA (Heijungs *et al.*, 1992), characterisation factors for toxicity assessment were based on toxicity as such, combined with human intake for human toxicity assessment. In the years that followed, the possibilities of for the inclusion of multimedia transport and environmental degradation in LCA toxicity assessment were investigated (*cf.* Guinée & Heijungs, 1993). This had consequences for the ratios between characterisation factors, putting relatively more weight on persistent chemicals. In 1996, Guinée *et al.* published a study that included a list of LCA toxicity characterisation factors for about 100 chemicals, based on the Dutch RIVM multimedia fate model USES 1.0. On the basis of this same model, Huijbregts *et al.* (2000) developed a specific LCA multimedia fate model called USES-LCA. With this model, LCA toxicity characterisation factors for 181 substances were calculated, which were later on included in the LCA Handbook of CML (Guinée *et al.*, 2002). Although the USES 1.0 model has originally been designed for organic chemicals, characterisation factors for metals were calculated with the same USES and USES-LCA models, respectively, by the way of specific parameter settings. As a result of the non-degradability and very low rates of disappearance of metals from the environmental system, the calculations showed a strong accumulation of metals, especially in the seawater compartments, which acted as a sink. This resulted in extremely high characterisation factors for metals, and as a consequence, in environmental profiles which in most LCA cases studies were fully dominated by metal emissions.

These results drew the attention of specialists on the environmental chemistry of metals, who remarked that metal-specific environmental chemistry was not included in the model. At an expert meeting with experts from the fields of both LCA and environmental metal chemistry in Apeldoorn (The Netherlands) in May 2004, it was agreed upon that characterisation factors for metals had to be adapted, as was briefly laid down in the so-called 'Apeldoorn Declaration' (Aboussouan *et al.*, 2004). In the mean time, a workshop had been organised in Montréal (Canada) where experts from both fields could exchange ideas. It is for this workshop that chapter 4 of this thesis has been prepared, as a proposal for the improvement of LCA characterisation factors for the ecotoxicity assessment of metals in seawater.

It was clear from the international discussion that the process of a better, science based inclusion of metals in LCIA would be a laborious and time-consuming task. The goal of the study in chapter 4 was to start this process by making a simple, transparent method with which the most urgent problems would be solved. Two metal-related issues were addressed:

- metal speciation in freshwater and seawater;
- vertical transport of metals to deeper water layers in seawater.

Free metal ion fractions of different metals in water were collected from literature and introduced in a preliminary version of the GLOBOX model. For metals, emitted in inorganic forms, bio-availability was assumed to be limited to these free ion fractions, according to the so-called *free ion activity model* (FIAM) (Morel, 1983). Regarding the vertical transport of metals, the seawater compartment was split into two parts: an upper mixed layer of 100 m and a lower layer, which was considered not to be part of the environmental system. As a consequence, the sedimentation process resulted in a reasonably fast elimination of metals from the environmental system. These two relatively simple modifications brought about that the values of metal characterisation factors dropped dramatically, thus no longer unduly causing metals to dominate environmental profiles because of their environmental persistence.

The original calculations reported in chapter 4 were executed with a preliminary version of the GLOBOX model. The fully differentiated version discussed in chapter 5 contains the same adaptations: temperature-dependent speciation, the inclusion of activity coefficients and the distinction between an upper mixed layer and a lower layer in the seawater compartment.

Further improvement of metal characterisation factors could be achieved by accounting for metal-specific environmental processes in other environmental compartments too. Especially for soil compartments, it will be necessary to adapt model parameters to local circumstances. How this should be fitted into a global LCA model would be a subject for further study. Within the water compartments, modelling could be improved by replacement of the FIAM by the biotic ligand model (BLM) (Di Toro, 2001), which accounts for bioavailability in a more refined way. An advanced model that has been specifically designed to account for the behaviour of metals in both aquatic and terrestrial environments is the Canadian TRANSPEC model (Bhavsar *et al.*, 2004 and 2008). In a project, commissioned by the International Council on Mining & Metals (ICMM) and executed by a number of collaborating institutes in The Netherlands and Canada, these issues are now being elaborated in the context of LCA (*cf.* Gandhi *et al.*, 2008).

7.4 Regional differentiation

Characterisation factors connected to substances released to the environment aim to reflect the relative environmental harmfulness of emissions of these substances in comparison to each other, assuming they are released in equal amounts. Environmental characteristics of the specific regions where the emissions take place are generally not accounted for in LCA characterisation factors. It has been demonstrated in this thesis that for the test substance nitrobenzene, when region dependent characteristics are included, the toxicity characterisation factor may show differences of up to 5 orders of magnitude for different countries. These findings are in good accordance with those of other authors, who report differences of up to 1 or 2 orders of magnitude for differentiation at the level of continents (Huijbregts *et al.*, 2003b, for fate and exposure factors; Rochat *et al.*, 2006, for intake fractions), and differences of up to around 3, 5 or 8 orders of magnitude for differentiation at the level of smaller regions within continents (MacLeod *et al.*, 2004; Pennington *et al.* 2005; Humbert *et al.*, 2009; all for intake fractions). Manneh *et al.* (2009) report a noticeable increase of differences with increasing level of spatial model resolution, which may explain why the differences, found at the level of small regions, are considerably higher than the differences, found at the level of continents.

Leaving out spatial information from LCA characterisation may cause the introduction of major inaccuracies in environmental profiles of product alternatives – and thus in the environmental ranking of product alternatives – since the emissions of the product life cycles to be compared may take place at different locations, not only for the different product alternatives, but also for the different processes within one product life cycle. Product life cycles usually consist of hundreds of processes, that may together span the world with respect to their regional origin. The lack of spatial differentiation may well reverse the outcome of an LCA study with respect to the question which product alternative should be preferred.

Spatial differentiation of toxicity assessment refers to three different issues: environmental fate, human intake, and effect. The environmental fate of chemicals depends on a large number of parameters: geographic parameters (for example, the relative surface area covered by water), geophysical parameters (*e.g.,* the organic carbon content of soils), climatological parameters (*e.g.,* temperature, rain rate and wind speed) and flow parameters (*e.g.,* river in- and outflows). Human intake depends on population density, food and drinking water consumption patterns, drinking water origin, drinking water purification characteristics, and body weight. Ecotoxicological effects depend on regional species sensitivities, and both human and ecotoxicological effects depend on background concentrations in relation to toxicological threshold values. The degree to which a certain environmental parameter influences LCA outcomes will be chemical-dependent; for instance, there will be a relatively high influence of drinking water related parameters on LCA on characterisation factors of chemicals that tend to reside in the water compartments.

In order to test whether spatial differentiation matters or not, three conditions should be met:

1. All possibly influential parameters should be spatially differentiated with respect to environmental fate, human intake and human and ecotoxicological effects.
2. Fate, exposure and effect models should contain equations that reflect all possibly relevant spatial dependencies.
3. The environmental system tested should be sufficiently broad and varied to represent the given spatial variation of model parameters.

The GLOBOX model for LCA toxicity assessment has been designed according to these conditions. A central characteristic of the model is the combination of its large number of spatially differentiated parameters with a global range and a relatively high level of spatial differentiation. The exemplifying calculations with nitrobenzene as a test chemical show that many of the spatially differentiated parameters do matter, and that the influence of spatial differentiation is comparable to the influence of chemical characteristics.

A question that can be posed is whether the traditional, non-differentiated toxicity-related characterisation factors make any sense at all if spatial differentiation is indeed so important. I think the answer is that they do make sense if they are handled with care, that is: if they are used only for the assessment of product life cycles of which the main processes are located in the area to which the model parameters apply, *e.g.,* to Western Europe for the USES-LCA factors (Van Zelm *et al*, 2009) or to North America for the CALtox factors (McKone *et al.*, 2001). This implies that for other countries, the use of spatial differentiation *or* the replacement of region-dependent parameters by the applicable values is necessary for acquiring reliable characterisation factors.

It should be kept in mind that a regionalised model can address both actual impacts and potential impacts, as discussed above. Potential impacts can thus be calculated either with a non-regionalised model or with a regionalised model. A regionalised model is expected to improve the results for potential impacts, without pretending to make them more actual. For actual impacts, a regionalised model is indispensible.

I believe that the development models like USEtox (Rosenbaum *et al.*, 2008), resulting from the harmonisation of a number of existing models, are very useful for the enhancement of model reliability with respect to their selective power considering model structure, equations and parameter construction. A parsimonious approach, defended by the designers of the USEtox model, can be useful in this context. In my view, however, parsimony should be considered as an intermediate stage, that serves the goal of disposing the model of bugs and flaws. After this, the improved model should be tooled up again with spatial characteristics and other information that makes the model reflect reality as well as possible. The ideal model should reflect the world as it is, in its full complexity. The challenge for the modeller is to develop sufficient knowledge on relevant details to allow for building a construction that produces perhaps unpredictable but yet plausible results in relevant model situations.

7.5 Normalisation

The primary goal of LCA normalisation is to translate the abstract impact scores of the environmental profile into more imaginable indicators, that relate each score to a concrete reference situation. A typical choice for the reference is the collection of global emissions of potentially harmful substances in a certain year. A normalised environmental profile gives an image of the relative contributions of a functional unit of product to the different environmental problems as they are occurring.

The goal of the normalisation study described in chapter 6 of this thesis was to update the formerly published normalisation factors for the reference year 1995 (Huijbregts *et al.*, 2003a), to the new reference year 2000. Normalisation factors were determined at two levels: the EU (plus Switzerland, Norway and Iceland) in the year 2000, and the world. This has been done for all impact categories which had been elaborated in the LCIA ReCiPe-project (Goedkoop *et al.*, 2009) by that time, in the context or which this normalisation study was performed.

It should be noted that the ReCiPe-characterisation factors for the toxicity-related impact categories differ from the characterisation factors that could be derived with the GLOBOX-model. Differences largely apply to environmental modelling parameters – especially in relation to spatial differentiation – and to the way in which the characterisation factors for metals have been derived. This last issue also influences the relative weight of the normalisation factors for metals.

When I started collecting data on emissions in this new reference year, I encountered the discrepancy between production data and emission data for CFCs, caused by the recent ban on CFC. On the one hand there were the low emission rates, related to the adaption of production processes to the new legislation, and on the other hand the still high rates of actually emitted CFCs, due to the use and waste treatment of formerly produced refrigerators, air conditioners, etc. The question was whether for ozone depletion, the actual CFC emissions in the year 2000 would form the right reference if the goal of normalisation were to assess the contribution of the environmental impacts of a certain product to the impacts of all products together. CFC emissions in the year 2000 formed an inheritance of past economic systems, rather than resulting from the life cycles of products produced in the chosen reference year. Inversely, it was the question whether it was correct that new chemicals, produced in the year 2000 but released in later years, would not be taken into account for products produced in the year 2000 by traditional normalisation factors. In the traditional approach, normalisation scores (or 'contributions') of single products could in theory even become more than 100% of the total. Thus, the question presented itself whether LCA normalisation should take environmental interventions *taking place* in the reference year, or, alternatively, the interventions *caused by economic activities* in this same year, should be quantified as reference interventions. Personally, I felt we had not been right by choosing the first of these two options in our former normalisation activities. If we wanted to use normalisation as a reference for assessing the relative contribution of the environmental impacts of a product to 'total' environmental impacts, this 'total' should reflect the impacts of all product life cycles together, in their proper magnitudes. And this corresponds in my view to the second option: that of the interventions, caused by economic activities in the reference year. This is what we aimed at in our updated normalisation study.

Different sources of uncertainty and bias were identified in our normalisation study. Data gaps in LCA inventory were identified as the most important cause of both uncertainty and bias. If normalisation factors are uncertain, this enhances the risk of biased results in case studies (Heijungs *et al.*, 2007). With respect to missing emission data, the foundation of an independent organisation that aims to register emissions in a systematic way, as suggested by Scheringer (2007), could offer the possibility to make a step forward in this respect.

Another type of bias can be caused if a discrepancy exists between the reference region for normalisation (used for the construction of a normalisation factor) and the 'ecological footprint' (Wackernagel & Rees, 1996) of this same region (in which product life cycles may extend). This issue has been addressed by Breedveld *et al.* (1999), who defined normalisation factors for the Netherlands on two different bases: geographic boundaries versus final consumption – representing 'all environmental interventions in one year (1993/1994) related to the consumption of Dutch end consumers, including the total chains of production and waste processes that result from this consumption'. In fact, a footprint approach seems to offer the most complete figure. Most normalisation studies – including the present study – use geographic boundaries as system boundaries, thus being prone to this type of bias. A possible future implementation of the 'ecological footprint' principle could be reached by the use of economic input-output models (*e.g.*, Hubacek, & Giljum, 2003; Suh, 2004) to estimate the emissions due to a region's consumption.

7.6 Main achievements and conclusions

This thesis reports an attempt to improve the reliability of LCA toxicity assessment and normalisation. In the introduction, five goals were presented:

1. Contributing to an optimal reliability of LCA toxicity assessment by creating a flexible, reasonably detailed system for spatial differentiation of LCA toxicity assessment on a global scale.
2. Enhancing the accuracy of LCA modelling with respect to the behaviour of metals in the environment.
3. The introduction of a method for the assessment of contributions of the product life cycle to toxic risks or *actual impacts*, along with the conventional assessment of *potential impacts*.
4. Analysing the influence of spatial differentiation on LCA characterisation factors for human toxicity and ecotoxity by calculations on a test substance.
5. Creating an updated, global LCA normalisation sytem.

The five goals have been achieved as follows:

With respect to toxicity assessment, the software tool GLOBOX has been developed, in which three concepts have been implemented:

- spatial differentiation on a global scale (1);
- a specific approach for the calculation of the fate of metals in the oceans (2);
- a distinction between potential and actual impacts (3).

The GLOBOX model has been tested by calculations on the test substance nitrobenzene, with an analysis of the relevance of spatial differentiation (4).

Normalisation has been updated at two scales: the Western European scale and the global scale (5).

From the calculations with the test substance nitrobenzene, it has been shown that spatial differentiation can indeed make a large difference, and that lack of spatial differentiation may lead to rank reversal of chemicals with respect to the harmfulness of their emissions.

Metal characterisation factors have been shown to fall dramatically if speciation is accounted for, and if only the upper mixed layer of the seas is regarded as part of environmental system.

Actual impacts have not yet been calculated, but after a discussion of many years about whether this is possible in LCA at all, a first step has now been set by rendering the assessment of actual impacts possible, in the GLOBOX model, both conceptually and implemented in the model software.

Normalisation has been founded on a new principle: the idea that normalisation factors should be based on the production processes in the given year, rather than on the actual emissions taking place in that year, in order to remain in line with the characterisation of a product, which is also about the processes for which this product (by itself being produced in a certain year) is responsible. All products together, produced in a certain year, are thus forming the basis for the normalisation factors.

Apart from the practical achievements, this thesis can also be viewed from a more abstract perspective. It can be considered as a plea for not avoiding complexity in environmental science. Quoting Einstein: *Everything should be made as simple as possible, but not simpler*. Spatial differentiation causes multimedia models to become more complex, and thus less easy to understand, but this enables them to much better reflect reality and lead to relevant results.

In my view, three levels can be distinguished in the relation between environmental science and policy. The highest level is the level of implementation of environmental measures, such as an emission tax or the banning of chemicals. At this level, a balance should be found between scientific environmental information, feasibility in terms of funding and time, and social and economic interests. This is primarily a political issue in which scientific knowledge only plays a role as source of essential information.

One level below is the level of environmental tools like LCA and HERA. At this level, a scientific foundation is an absolute requirement. In the mean time, it is important that the instrument remains manageable for the user. Tools that can be handled by experts only, that require input that is not easily available, or that are very time-consuming in use, will not become popular. Again, a balance will have to be found, this time between scientific accuracy on the one hand and practicability on the other. Since practicability is more easily recognizable than scientific accuracy, safeguarding the latter is a special point of attention. Attractively designed tools of which the results are not sufficiently detailed or even scientifically incorrect are of little use and may even be harmful. Smart software may help to include the necessary scientific details in environmental tools while preserving user friendliness, practicability and elegance.

The basic level on which both environmental measures and environmental tools rest is the level of scientific modelling. At this level, scientific accuracy is the main purpose. Scientific models should reflect reality as well as possible. On this basis, choices can be made about the details that can be omitted from practical tools if desirable – without giving in too much on scientific quality – and about details that are indispensible and should be included anyhow. It is at this level that the GLOBOX model has been designed, built on the conviction that environmental practice should always be based on sound scientific grounds.

One final remark. Despite the importance of the environmental improvement of products, it is my personal belief that the most urgent step forward towards a sustainable economy is in a decrease of industrial production. It may be questioned what the eventual goal of production should be, and how this relates to the fulfilling of human needs, both in a material and in a financial-economic sense. In environmental discussions, the emphasis is often placed on a decrease in consumption, but if consumption levels are largely driven by production and marketing, these should also be the subject of environmental management.

References

Aboussouan L, Saft RJ, Schönnenbeck M, Hauschild M, Delbeke K, Struijs J, Russell A, Udo de Haes H, Atherton J, Van Tilborg W, Karman C, Korenromp R, Sap G, Baukloh A, Dubreuil A, Adams W, Heijungs R, Jolliet O, De Koning A, Chapman P, Ligthart T, Van de Meent D, Kuyper J, Van der Loos R, Eikelboom R, Verdonck F (2004) Declaration of Apeldoorn on LCIA of non-ferro metals. *SETAC Globe* **5** (4): 46-47

Bare JC, Norris GA, Pennington DW, McKone T (2003) TRACI. The Tool for the Reduction and Assessment of Chemical and Other Environmental Impacts. *J Ind Ecol* **6** (3-4): 49-78

Barnthouse L, Fava J, Humphreys K, Hunt R, Laibson L, Noesen S, Owens J, Todd J, Vigon B, Weitz K, Young J (eds.) (1997) *Life-Cycle Impact Assessment: The State-of-the-Art.* SETAC, Pensacola, FL, USA

Bhavsar SP, Diamond ML, Gandhi N, Nilsen J (2004) Dynamic Coupled Metal Transport–Speciation Model: Application to Assess a Zinc-Contaminated Lake *Environmental Toxicology and Chemistry* **23** (10): 2410–2420

Bhavsar SP, Gandhi N, Diamond ML (2008) Extension of Coupled Multispecies Metal Transport and Speciation (TRANSPEC) Model to Soil. *Chemosphere* **70** (5): 914-924

Breedveld L, Lafleur M, Blonk H (1999) A Framework for Actualising Normalisation Data in LCA: Experiences in the Netherlands. *Int J LCA* **4** (4): 213-220

De Koning, A, Guinée JB, Pennington DW, Wegener Sleeswijk A, Hauschild MZ, Molander S, Nyström B, Pant R, Schowanek D (2002) *Methods and typology report Part A: Inventory and classification of LCA characterisation methods for assessing toxic releases. Contribution to Work-package 7 of the OMNIITOX Project as part A of appropriate deliverable D11.* Centre of Environmental Science (CML), Leiden University, Leiden, The Netherlands

Di Toro, DM, Allen HE, Bergman HL, Meyer JS, Paquin PR, Santore RC (2001) Biotic ligand model of the acute toxicity of metals. 1. Technical basis. *Environ Toxicol Chem* **20**: 2383-2396

EC (2002) *The World Summit on Sustainable Development: People, Planet, Prosperity.* European Commission (EC). Office for Official Publications of the European Communities, Luxembourg

Gandhi N, Diamond ML, Van de Meent D, Huijbregts M, Peijnenburg W, Guinée J, Koelmans B (2008) *New method for calculating metal characterization factors in life cycle impact assessment.* In: Abstract book SETAC North America 29th Annual Meeting, 16-20 November 2008, Tampa, FL, USA

Goedkoop M, Heijungs R, Huijbregts M, De Schryver A, Struijs J, Van Zelm R (2009) *ReCiPe 2008. A life cycle impact assessment method which comprises harmonised category indicators at the midpoint and the endpoint level. First edition. Report I: Characterisation.* Ministerie van Volkshuisvesting, Ruimtelijke Ordening en Milieubeheer. The Hague, The Netherlands

Goedkoop M, Spriensma R (2001) *The Eco-indicator 99. A Damage-Oriented Method for Life Cycle Impact Assessment. Methodology Report.* Third edition. Ministerie van Volkshuisvesting, Ruimtelijke Ordening en Milieubeheer. The Hague, The Netherlands

Guinée JB, Gorrée M, Heijungs R, Huppes G, Kleijn R, De Koning A, Van Oers L, Wegener Sleeswijk A, Suh S, Udo de Haes HA, De Bruijn H, Van Duin R, Huijbregts MAJ (2002) *Handbook on Life Cycle Assessment. Operational Guide to the ISO Standards.* Kluwer Academic Publishers, Dordrecht, The Netherlands

Guinée J, Heijungs R, Van Oers L, Wegener Sleeswijk A, Van de Meent D, Vermeire Th, Rikken M (1996) USES – Uniform System for the Evaluation of Substances. Inclusion of Fate in LCA Characterisation of Toxic Releases Applying USES 1.0. *Int J LCA* **1**: 133-138

Guinée J, Heijungs R (1993) A proposal for the classification of toxic substances within the framework of life cycle assessment of products. *Chemosphere* **26** (10): 1925-1944

Heijungs R, Guinée JB (1994): The Flux-Pulse Problem in LCA. *LCA News* **4**: 6-7

Heijungs R, Guinée JB, Huppes G, Lankreijer RM, Udo de Haes HA, Wegener Sleeswijk A, Ansems AMM, Eggels PG, Van Duin R, De Goede HP (1992) *Environmental Life Cycle Assessment of Products. Guide & Backgrounds – October 1992.* NOH report 9267. Centre of Environmental Science Leiden University (CML), Leiden, The Netherlands

Heijungs R, Guinée JB, Kleijn R, Rovers V (2007) Bias in Normalization: Causes, Consequences, Detection and Remedies. *Int J LCA* **12** (4): 211-216

Hogan LM, Beal RT, Hunt RJ (1996) Threshold inventory interpretation methodology - A case study of three juice container systems. *In J LCA* **1** (3): 159-167

Hubacek K, Giljum S (2003) Applying physical input-output analysis to estimate land appropriation (ecological footprints) of international trade activities. *Ecological Economics* **44**: 137-151

Huijbregts MAJ, Breedveld L, Huppes G, De Koning A, Van Oers L, Suh S (2003a) Normalisation Figures for Environmental Life-Cycle Assessment: The Netherlands (1997/1998), Western Europe (1995) and the World (1990 and 1995). *Journal of Cleaner Production* **11** (7): 737-748

Huijbregts, MAJ, Lundi S, McKone TE, Van de Meent D (2003b) Geographical Scenario Uncertainty in Generic Fate and Exposure Factors of Toxic Pollutants for Life-Cycle Impact Assessment. *Chemosphere* **51**: 501-508

Huijbregts MAJ, Thissen UMJ, Guinée JB, Jager T, Kalf D, Van de Meent D, Ragas AMJ, Wegener Sleeswijk A, Reijnders L (2000): Priority Assessment of Toxic Substances in Life Cycle Assessment. Part I: Calculation of Toxicity Potentials for 181 Substances with the Nested Multi-Media Fate, Exposure and Effects Model USES-LCA. *Chemosphere* **41**: 541-573

Humbert S, Manneh R, Shaked S, Wannaz C, Horvath A, Deschênes L, Jolliet O, Margni M (2009) Assessing regional intake fractions in North America. *Sci Total Environ* **407**: 4812-4820

MacLeod M, Bennett DH, Perem M, Maddalena TL, McKone TE, Mackay D (2004) Dependence of Intake Fraction on Release Location in a Multimedia Framework. A Case Study of Four Contaminants in North America. *J Ind Ecol* **8** (3): 89-102

Manneh, R, Margni M, Deschênes L (2009) *Spatial Variability and Optimal Regional Scale for Intake Fractions linked to a Canadian Emission. Abstract. p. 30.* In: ACLCA *Life Cycle Assessment IX. Toward the Global Life Cycle Economy.* Joint North American Life Cycle Conference. Boston September 29 to October 2nd 2009, Boston, USA. 237 pp.

McKone T, Bennett D, Maddalena R (2001) *CalTOX 4.0 Technical Support Document, Vol. 1.* LBNL - 47254, Lawrence Berkeley National Laboratory, Berkeley, CA, USA

Meeusen-Van Onna MJG, Leneman H, Wegener Sleeswijk A, Kleijn R, Van Zeijts H, Reus JAWA (1996) *Toepassing van LCA voor agrarische produkten. 4b. Ervaringen met de methodiek in de case melkveehouderij.* Landbouw-Economisch Instituut (LEI-DLO), Den Haag; Centrum voor Milieukunde (CML), Leiden University, Leiden; Centrum voor Landbouw en Milieu (CLM), Utrecht, The Netherlands. (In Dutch.)

Morel FMM (1983) *Principles of Aquatic Chemistry.* Wiley-Interscience, New York, USA

Owens JW (1997) Life-Cycle Assessment. Constraints on Moving from Inventory to Impact Assessment. *J Ind Ecol* **1** (1): 37-49

Pennington DW, Margni M, Ammann C, Jolliet O (2005) Multimedia Fate and Human Intake Modeling: Spatial versus Nonspatial Insights for Chemical Emissions in Western Europe. *Environ Sci Technol* **39** (4): 1119-1128

Potting J, Schöpp W, Blok K, Hauschild M (1998) Site-Dependent Life-Cycle Impact Assessment of Acidification. *J Ind Ecol* **2**: 63-87

Rochat D, Margni M, Jolliet O (2006) Continent-specific Intake Fractions and Characterization Factors for Toxic Emissions: Does it make a Difference? *Int J LCA* **11** (Special Issue 1): 55-63

Rosenbaum RK, Bachmann TM, Gold LS, Huijbregts M, Jolliet O, Juraske R, Koehler A, Larsen HF, MacLeod M, Margni M, McKone TE, Payet J, Schuhmacher M, Van de Meent D, Hauschild MZ (2008) USEtox – The UNEP-SETAC toxicity model: recommended characterisation factors for human toxicity and freshwater ecotoxicity in Life Cycle Impact Assessment. *Int J LCA* **13** (7): 532-546

Scheringer M (2007) Towards an International Panel on Chemical Pollution (IPCP). *Chemosphere* **67**: 1682-1683

Sengers HHWJM, Meeusen-Van Onna MJG, Wegener Sleeswijk A, Kleijn R, Van Zeijts H, Reus JAWA (1996) *Toepassing van LCA voor agrarische produkten. 4c. Ervaringen met de methodiek in de case bio-energie.* Landbouw-Economisch Instituut (LEI-DLO), Den Haag; Centrum voor Milieukunde (CML), Leiden University, Leiden; Centrum voor Landbouw en Milieu (CLM), Utrecht, The Netherlands. (In Dutch.)

Suh S (2004) A Note on the Calculus for Physical Input-Output Analysis and its Application to Land Appropriation of International Trade Activities. *Ecological Economics* **48**: 9-17

Udo de Haes HA, Owens JW (1998) *Evolution and Development of the Conceptual Framework and Methodology of Life-Cycle Impact Assessment.* Society of Environmental Toxicology and Chemistry, Pensacola, FL, USA

Van Zeijts H, Lenenman H, Wegener Sleeswijk A (1999) Fitting Fertilisation in LCA: Allocation to Crops in a Cropping Plan. *J Cleaner Prod* **7**: 69-74

Van Zeijts H, Reus JAWA, Wegener Sleeswijk A, Kleijn R, Meeusen-Van Onna MJG, Leneman H, Sengers HHWJM(1996) *Toepassing van LCA voor agrarische produkten. 4a. Ervaringen met de methodiek in de case akkerbouw.* Landbouw-Economisch Instituut (LEI-DLO), Den Haag; Centrum voor Milieukunde (CML), Leiden University, Leiden; Centrum voor Landbouw en Milieu (CLM), Utrecht, The Netherlands. (In Dutch.)

Van Zelm R, Huijbregts MAJ, Van de Meent D (2009) USES-LCA 2.0—a Global Nested Multi-Media Fate, Exposure, and Effects model. *In J LCA* **14**: 282–284

Wackernagel M, Rees W (1996) *Our Ecological Footprint: Reducing Human Impact on the Earth.* New Society Publishers, Gabriola Islands, BC, Canada. 176 pp.

Wegener Sleeswijk A, Lankreijer RM, Van der Voet E (1992) *Tarwe en milieu: hoe boert de Zeeuwse Vlegel? Een levenscyclusanalyse van de milieueffecten van tarweteelt bij verschillende wijzen van bemesting en gewasbescherming.* Wetenschapswinkel, Rijksuniversiteit Leiden, The Netherlands. (In Dutch.)

Wegener Sleeswijk A (1993) *Life cycle Assessment of Wheat Fertilization: Methodological Aspects and Results.* In: Pedersen Weidema B (ed.) *Life Cycle Assessment of Food Products. Proceedings of the 1st European Invitational Expert Seminar on Life Cycle Assessment of Food Products. 22d-23d of November 1993.* The Ecological Food Project, Interdisciplinary Centre, Technical University of Denmark, Lyngby, Denmark

Wegener Sleeswijk A (1996) *LCA of agricultural products.* In: Ceuterick D (ed.) (1996) *International Conference on Application of Life Cycle Assessment in Agriculture, Food and Non-Food Agro-Industry and Forestry: Achievements and Prospects.* Preprints. 4-5 April 1996, Brussels, Belgium. VITO, Mol, Belgium

Wegener Sleeswijk A, Huppes G (1995) *Leerpuntenverslag van het project 'LCA fosfogips'.* Ministerie van V&W, Dienst Weg- en Waterbouwkunde, intern verslag MAO-R-94035, Delft. (In Dutch.)

Wegener Sleeswijk A, Kleijn R, Karman C, Bernhard R, Van der Vlies L (2003) *REIMSEA: an LCA Toxicity Characterization Model for the North Sea. Supplement to 'REIM: LCA-based Ranking of Environmental Models' Including Toxicity Characterization Factors for 12 Organics and 7 Metals.* CML Report 159. Centre of Environmental Science, Leiden University, Leiden, The Netherlands

Wegener Sleeswijk A, Kleijn R, Meeusen-Van Onna MJG, Leneman H, Sengers HHWJM, Van Zeijts H, Reus JAWA (1996) *Application of LCA to agricultural products. 1. Core methodological issues. 2. Supplement to the LCA Guide. 3. Methodological background.* CML report 130. Centre of Environmental Science (CML), Leiden University, Leiden, The Netherlands

White P, De Smet B, Udo de Haes HA, Heijungs R (1995) LCA Back on Track. But Is It One Track or Two? *LCA News* **5** (3): 2-4

Samenvatting

Levencyclusanalyse van producten (LCA) is een methode waarmee de milieueffecten van producten kunnen worden beoordeeld. Drie begrippen staan daarbij centraal: de *levenscyclus* van het product, *karakterisatiefactoren* en de zogenaamde *functionele eenheid*. De *levenscyclus* of levensketen van het product omvat naast de productie en het gebruik van het product ook alle processen die daar direct of indirect mee samenhangen, zoals de winning van grondstoffen, de verwerking van het afgedankte product en de productie van energie en hulpstoffen die nodig zijn om het product te maken en/of te gebruiken. *Karakterisatiefactoren* zijn getallen die aangeven hoeveel een standaardhoeveelheid van een stof in het milieu bijdraagt aan een bepaald type milieueffect. De verschillende typen milieueffecten zijn ondergebracht in *effectcategorieën* zoals de uitputting van grondstoffen, landgebruik, het broeikaseffect, verzuring, vermesting, humane toxiciteit en ecotoxiciteit. Een product dat met LCA wordt beoordeeld ontvangt per effectcategorie een *effectscore*. De *functionele eenheid*, tenslotte, is een maat voor de hoeveelheid product waarop de beoordeling betrekking heeft. Het functionele aspect is vooral van belang bij het vergelijken van verschillende producten met dezelfde functie: daarbij dient niet de fysieke hoeveelheid product als vergelijkingsbasis, maar de mate waarin een hoeveelheid product de benodigde functie kan vervullen. Zo is bij een milieuanalyse van melkverpakkingen ‘de verpakking van 1000 liter melk’ een mogelijke functionele eenheid, en zullen 1000 melkpakken daarbij vergeleken worden met 25 statiegeldflessen – gesteld dat zo’n fles 40 keer meegaat. De verpakkingen worden beoordeeld op de mate waarin ze bijdragen aan de verschillende effectcategorieën, gedurende de levenscyclus die loopt van de winning van grondstoffen via productie, vervoer en (voor flessen) retourtransport en schoonmaak tot en met afvalverbranding en/of verwerking tot herbruikbare grondstoffen.

De analyse gebeurt in drie stappen: *inventarisatie*, *effectbeoordeling* en *interpretatie*. In de inventarisatie worden de kwantitatieve gegevens verzameld: de directe en indirecte bijdragen van de functionele eenheid aan de onttrekking van grondstoffen, aan landgebruik en aan de uitstoot – of *emissie* – van schadelijke stoffen naar lucht, water en bodem. Emissies en onttrekkingen samen worden aangeduid als *(milieu)-ingrepen*. In de effectbeoordeling (ook wel aangeduid al *LCIA – life cycle impact assessment*) worden de effectscores voor iedere effectcategorie berekend en gecombineerd tot een zogenaamd *milieuprofiel*. Omdat de effectscores als zodanig moeilijk te interpreteren zijn worden deze vaak genormaliseerd, dat wil zeggen dat ze worden uitgedrukt als fractie van het totale milieueffect op wereldschaal, op continentale schaal of in een bepaald land. Zo kan worden bepaald aan welke effectcategorieën het product een relatief grote bijdrage levert.

LCA gaat over kwantificeerbare milieueffecten, met name effecten die het gevolg zijn van emissies van milieuschadelijke stoffen, onttrekkingen van grondstoffen en landgebruik. In dit proefschrift staan de emissies van toxische stoffen centraal: stoffen die giftig zijn voor de mens of voor planten, dieren of micro-organismen. Een belangrijk kenmerk van deze stofgroep is dat het om een zeer groot aantal stoffen gaat. Dit in tegenstelling tot de stofgroepen die verantwoordelijk zijn voor het broeikaseffect, verzuring en vermesting: daarbij speelt voornamelijk een klein aantal 'bulk'emissies een rol: koolstofdioxide, methaan, zwaveldioxide, stikstofoxiden, ammoniak, nitraat en fosfaat.

Het aantal toxische stoffen dat in het milieu wordt geloosd bedraagt vele duizenden. Om het effect van deze stoffen te kunnen bepalen is het niet alleen nodig om te weten hoe toxisch ze zijn: ook de verspreiding en afbraak in het milieu en de mate waarin de mens deze stoffen via voedsel en drinkwater binnenkrijgt zal moeten worden gemeten of gemodelleerd. Het voordeel van meting is dat het meestal de nauwkeurigste manier is om concentraties in het milieu en in voedsel en drinkwater te bepalen. Modelleren heeft andere voordelen: het heeft een voorspellende waarde, het behoeft slechts eenmalig te gebeuren – waarna het model iedere keer opnieuw met emissiegegevens kan worden ingevuld – en het kan duidelijkheid bieden over de herkomst van de verontreiniging. De omvang van de bijdrage van een product met alle daaraan verbonden processen aan milieuverontreiniging kan niet worden gemeten. Voor LCA is modellering daarom de enige optie. In dit proefschrift staat de modellering van de verspreiding en afbraak van toxische stoffen en de blootstelling van mensen en ecosystemen aan die stoffen centraal.

Binnen de LCA vormt de toxiciteitsbeoordeling slechts een onderdeel van het geheel – naast de beoordeling op het gebied van milieuthema's zoals het broeikaseffect, de aantasting van de ozonlaag, verzuring, vermesting, landgebruik en de uitputting van grondstoffen. Een vakgebied waarin juist toxische stoffen in het milieu centraal staan is de risico-analyse van stoffen, ook wel *human and environmental risk assessment* (*HRA and ERA* of *HERA*) of *risk assessment of chemicals* (RA) genoemd.

De methoden die in de LC(I)A worden gebruikt voor de beoordeling van toxische effecten zijn meestal geënt op methoden uit de HERA. Omdat LCA andere eisen stelt dan HERA moeten deze methoden echter op bepaalde punten worden aangepast. Beide instrumenten leveren dan ook verschillende resultaten op. Omdat LCA en HERA beide worden gebruikt voor het maken van milieuverantwoorde keuzen kan het verwarrend zijn wanneer de resultaten van beide methoden tegenstrijdig zijn. Een nadere analyses van de verschillen tussen beide instrumenten en van de mogelijkheden tot stroomlijning en integratie is daarom noodzakelijk.

Voor het modelleren van de verspreiding en afbraak van stoffen in het milieu zijn verschillende typen modellen in omloop. Binnen de LCA wordt vaak gebruik gemaakt van de zogenaamde *multimediamodellen*. In deze modellen – die oorspronkelijk zijn ontwikkeld door Don Mackay van de Canadese *Trent University* – zijn de fysisch-chemische transportprocessen tussen lucht, water en bodem, en afbraakprocessen binnen elk van deze milieucompartimenten, gemodelleerd als functie van enerzijds de chemische eigenschappen van de betrokken stoffen zoals vluchtigheid en oplosbaarheid en anderzijds de fysisch-chemische milieueigenschappen zoals de omgevingstemperatuur en het organische-stofgehalte van de bodem. Binnen lucht, water en bodem worden de concentraties in principe verondersteld homogeen te zijn. Wel kunnen diverse 'eenheidswerelden', met elk hun eigen lucht-, water- en bodemcompartiment, aaneengeschakeld worden. Dit leidt ertoe dat er binnen hetzelfde medium verschillende compartimenten worden gedefinieerd. Uiteraard dient in dit geval ook het transport tussen dergelijke gelijksoortige compartimenten te worden gemodelleerd – bijvoorbeeld het stromingstransport tussen twee luchtcompartimenten als functie van de windsnelheid. Binnen ieder compartiment kan afbraak plaatsvinden. Daarnaast kunnen stoffen ook worden getransporteerd naar compartimenten die verondersteld worden geen deel uit te maken van het ecologisch systeem – bijvoorbeeld diepere bodem- of sedimentlagen. Omdat de stoffen daarmee uit het gemodelleerde milieusysteem verdwijnen heeft dit modelmatig hetzelfde effect als afbraak.

De multimediamodellen zijn ontworpen voor organische stoffen. Het bijzondere van deze modellen is dat ze voor iedere organische stof kunnen worden toegepast: het invoeren van een klein aantal chemische eigenschappen en afbraaksnelheden bij een standaardtemperatuur volstaat voor het uitvoeren van de berekeningen. Anorganische stoffen passen echter niet zonder meer in deze modellen. Met name metalen zijn lastig in te voeren, enerzijds omdat de metaalspecifieke speciatieprocessen – waarbij metalen zich in het milieu uitsplitsen in verschillende chemische vormen – niet in de bestaande multimediamodellen zijn opgenomen, en anderzijds omdat metalen niet afbreekbaar zijn, en daarom in principe altijd in het milieu aanwezig blijven.

De basale modellen voor multimediatransport, menselijke blootstelling en de toxische potentie van stoffen vormen een waardevolle basis voor het modelleren van toxische effecten in LCA. Toch moeten daarnaast nog een aantal LCA-specifieke problemen worden opgelost. Eén van de meest bekritiseerde aspecten van de toxiciteitsbeoordeling in LCA is het gebruik van de zogenaamde *potentiële effecten* in LCA milieuprofielen, als tegenhanger van de *actuele effecten* of risico's die met HERA worden geschat. De tegenstelling in karakter tussen de uitkomsten van respectievelijk LCA en HERA worden ook wel aangeduid met de termen *algemene* *preventie* versus *risicominimalisatie*, oftewel *minder is beter* versus *alleen boven de drempel.* In dit proefschrift worden de mogelijkheden en beperkingen verkend die betrekking hebben op de integratie van LCA en HERA. Aangetoond wordt dat de functionele eenheid – waarvan wordt beredeneerd dat deze het enige fundamentele verschil vormt tussen LCA en HERA – het onmogelijk maakt de beide instrumenten volledig met elkaar te integreren, dat wil zeggen: om LCA aan te vullen met een geïntegreerde risicobeoordeling. Wel wordt een methode voorgesteld voor het beoordelen van *risicobijdragen* van de productlevenscyclus in de context van LCA. Omdat de risico's afhankelijk zijn van de regionale verschillen voor wat betreft zowel de verspreiding en afbraak van als de menselijke blootstelling aan toxische stoffen, is zo'n beoordeling van risicobijdragen niet mogelijk zonder ruimtelijke differentiatie. Tegelijk is echter ook een wereldwijde dekking van alle milieumodelleringsaspecten een voorwaarde voor LCA, enerzijds omdat de productlevenscyclus zich willekeurig over de gehele wereld kan uitstrekken – ook voor producten die bijvoorbeeld in Nederland worden geproduceerd en gebruikt – en anderzijds omdat er steeds meer vraag komt naar methoden die geschikt zijn voor het beoordelen van producten die afkomstig zijn uit ieder willekeurig land. In het GLOBOX-model worden de beide genoemde principes verenigd: het is een wereldwijd model dat regionaal gedifferentieerd is op het niveau van individuele landen, territoria*, zeeën en oceanen. Deze basis voor differentiatie is gekozen omdat zowel emissiegegevens als gegevens die betrekking hebben op de parameters voor de modellering van multimediatransport en blootstelling vaak per land of regio beschikbaar zijn.

De kern van dit proefschrift wordt dus gevormd door het model GLOBOX: een speciaal voor LCA ontworpen combinatie van een multimediamodel, een blootstellingsmodel en een effectmodel, waarmee LCA-karakterisatiefactoren voor zowel de humaan-toxische als de eco-toxische effecten van stoffen kunnen worden berekend. GLOBOX onderscheidt zich van de reeds bestaande modellen doordat het ruimtelijk gedifferentieerd is en tegelijk de wereld als geheel bestrijkt.

Dit proefschrift heeft vijf doelen:

1. Het maken van een flexibel, redelijk fijnmazig model voor ruimtelijke differentiatie van de LCA toxiciteitsbeoordeling op wereldschaal, om daarmee bij te dragen aan een optimale betrouwbaarheid van de LCA toxiciteitsbeoordeling.
2. Het vergroten van de betrouwbaarheid van de LCA-modellering van het gedrag van metalen in het milieu.

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* Deze omvatten overzeese gebiedsdelen (zoals Réunion) en onbewoonde gebieden (zoals Antarctica).

3. De introductie van een methode voor het beoordelen van bijdragen van de productlevenscyclus aan toxische risico's of actuele effecten, naast de gebruikelijke beoordeling van potentiële effecten.
4. Het toetsen van de invloed van ruimtelijke differentiatie op LCA karakterisatiefactoren voor humane toxiciteit en ecotoxiciteit door middel van modelberekeningen aan een voorbeeldstof.
5. Het opstellen van een geactualiseerd, wereldwijd normalisatiesysteem.

In tegenstelling tot de bestaande LCA multimedia- en blootstellingsmodellen, die hun parameters vaak impliciet ontlenen aan de milieu- en blootstellingsgegevens in Europa, de Verenigde Staten en Japan, biedt het GLOBOX-model de mogelijkheid expliciet te kiezen voor emissies die plaatsvinden in gebieden buiten deze regio's. Daarmee wordt het mogelijk gemaakt om bij de beoordeling van producten die afkomstig zijn uit andere regio's – maar ook bij de beoordeling van niet-regionale processen binnen levenscycli van Europese, Amerikaanse en Japanse producten – recht te doen aan de ruimtelijke verschillen in milieu- en blootstellingsomstandigheden.

Naast het opstellen en aanpassen van modelvergelijkingen heeft ook het verzamelen en construeren van modelparameters een belangrijke rol gespeeld binnen het onderzoek dat aan dit proefschrift ten grondslag ligt. Het GLOBOX-model en de onderliggende parametersets (de GLOBACK achtergrondgegevens) zijn te vinden op http://cml.leiden.edu/software/software-globox.html en op http://www.globright.nl. Behalve een *executable* versie van model zelf zijn daar de volgende parametersets gepubliceerd:

- GLOBACK 2.0, deel 1 en 2
- aanvulling op deel 1 van GLOBACK 2.0, voor deelgebieden van de Verenigde Staten en Canada
- normalisatiegegevens

Deel 1 van GLOBACK 2.0 bevat alle ruimtelijk gedifferentieerde milieu- en blootstellingsparameters voor het GLOBOX-model, inclusief de parameters die de ruimtelijk gedifferentieerde hydrologische cyclus bepalen, en schattingen van het voedselconsumptiepatroon in de individuele landen. Deel 2 bevat parameters voor de grootte van de lucht- en waterstromingen tussen de verschillende gebieden. Voor een verdere opsplitsing van twee grote landen – de Verenigde Staten en Canada – is een groot deel van de parameters uit deel 1 van GLOBACK ook reeds verzameld. Na aanvulling met de nog ontbrekende parameters en de parameters uit deel 2 kunnen deze gebieden zonder meer in het GLOBOX-model worden opgenomen. De normalisatiegegevens vormen een verzameling schattingen van de emissies naar en onttrekkingen uit het milieu voor zo veel mogelijk stoffen op wereldschaal en op Europees niveau, veroorzaakt door de economische activiteiten in het jaar 2000. Daarnaast is ook een schatting van de diverse vormen van landgebruik gemaakt. Tezamen vormen deze parametersets een basis die niet alleen voor het GLOBOX-model en LCA-normalisatie, maar ook voor andere modellen en modelberekeningen kan worden ingezet.

Dit proefschrift bestaat uit zeven hoofdstukken. De hoofdstukken 1 en 7 zijn respectievelijk een inleiding en een discussie over het document als geheel. De overige vijf hoofdstukken zijn als gereviewde artikelen verschenen in internationale tijdschriften of – in het geval van hoofdstuk 4 – verschenen als gereviewd hoofdstuk van een boek. De hoofdstukken 2 en 3 vormen een theoretische inleiding. De hoofdstukken 4, 5 en 6 vormen tezamen een praktische handleiding voor de LCA-effectbeoordeling van toxische stoffen en de normalisatie van LCA-effectscores voor alle LCA-effectcategorieën. Hoofdstuk 5 is geïmplementeerd als softwaremodel (GLOBOX), dat als zodanig ook buiten de context van LCA bruikbaar is.

Hoofdstuk 2: Introductie van informatie over gevoeligheid en drempelwaarden in LCA
In hoofdstuk 2 wordt LCA beschouwd vanuit twee perspectieven: dat van de *algemene preventie* en dat van de *risicominimalisatie*. Het algemene-preventieprincipe berust op de overtuiging dat milieuverontreiniging altijd ongewenst is en dat het nastreven van een minimum aan milieuverontreiniging daarom als zodanig belangrijk is; dit wordt ook wel aangeduid met de term *minder is beter* ('less is better'). Het uitgangspunt van het risicominimalisatieprincipe is de overtuiging dat het minimaliseren van aantoonbare risico's bij het terugdringen van de milieuverontreiniging centraal zou moeten staan. Omdat vaak wordt aangenomen dat er voor veel toxische stoffen beneden bepaalde drempelwaarden niet of nauwelijks meer aantoonbare milieueffecten optreden wordt dit principe wel aangeduid met de term *alleen boven de drempel* ('only above threshold'). De algemene trend is dat de beoordelingsmethode in LCA geacht wordt te berusten op het algemene-preventieprincipe en die van de HERA op het risiciominimalisatieprincipe.

Het feit dat de uitkomsten van LCA hiermee niet direct betrekking hebben op risico's is door critici wel gebruikt om de betrouwbaarheid van LCA als zodanig in twijfel te trekken. In dit hoofdstuk wordt aangetoond dat de beide principes niet tegenover elkaar behoeven te staan, maar dat ze goed te verenigen zijn. Ook binnen LCA is het mogelijk beide principes tot uitdrukking te laten komen. Bepleit wordt voor dit doel twee nieuwe variabelen te introduceren in de LCA-toxiciteitsmodellering: een *gevoeligheidsfactor* en een *drempelfactor*. Omdat het hier gaat om regiospecifieke variabelen is ruimtelijke differentiatie voor deze benadering wel een noodzakelijke voorwaarde. Met de gevoeligheidsfactor wordt aangeduid in hoeverre de ecosystemen in een gebied gevoelig zijn voor een bepaalde stof, terwijl de drempelfactor een maat vormt voor de fractie van het gebied waar de norm of het *no effect level* reeds wordt overschreden. Alhoewel met LCA geen risico's kunnen worden berekend zou op deze manier wel een kwantitatieve maat ontstaan voor de bijdrage van een product aan toxische risico's in het algemeen. Per effectcategorie kan op deze manier een dubbele effectscore worden berekend: één volgens de traditionele methode in het kader van de algemene preventie en één volgens de nieuwe methode in het kader van de risicominimalisatie. Hiermee is het mogelijk LCA en HERA nader tot elkaar te brengen zonder dat dit ten koste gaat van de karakteristieke kenmerken van LCA.

Hoofdstuk 3: LCA verus HERA
In hoofdstuk 3 worden LCA en HERA naast elkaar gezet. In de bestaande literatuur beschouwen sommige auteurs deze twee modelbenaderingen als min of meer gelijk, terwijl anderen ze juist zien als twee totaal verschillende benaderingen. Om hierin meer helderheid te brengen worden LCA en HERA in dit hoofdstuk op drie niveaus met elkaar vergeleken.

Niveau 1 vertegenwoordigt de basisvergelijkingen die het gedrag van stoffen in het milieu en de dosis-responsrelaties beschrijft. Op dit gebied bestaat er nauwelijks verschil: in principe hebben beide instrumenten betrekking op dezelfde milieuprocessen, hanteren ze dezelfde wiskundige vergelijkingen om het verband tussen emissies enerzijds en concentraties in het milieu, menselijke inname, en milieueffecten anderzijds weer te geven en maken ze gebruik van dezelfde stof- en milieueigenschappen.

Niveau 2 vertegenwoordigt de globale modelstructuur van de beide instrumenten. Gesteld wordt dat LCA ten opzichte van HERA een tiental eigen karakteristieken bevat: het levenscyclusperspectief, het feit dat het onderwerp van de analyse wordt gevormd door producten in plaats van stoffen, het grote aantal betrokken economische processen, het grote aantal betrokken stoffen en effectcategorieën, de grote reikwijdte voor wat betreft de milieueffecten die in de beoordeling worden betrokken, het gebruik van karakterisatiefactoren, het sommeren van effecten van verschillende stoffen tot één gezamenlijke score, de onafhankelijkheid van plaats en tijd, de beoordeling van afzonderlijke emissiepulsen in plaats van continue fluxen, en het gebruik van een functionele eenheid als basis voor de beoordeling en het relatieve karakter van de beoordeling. Alhoewel LCA en HERA elk hun eigen modelstructuur hebben, zijn de meeste verschillen niet fundamenteel. De functionele eenheid vormt daarop echter een uitzondering. Dit blijkt cruciaal te zijn: de functionele eenheid maakt dat bij LCA de emissies van processen niet in hun volle omvang worden beoordeeld, maar uitsluitend met betrekking tot hun aandeel in de levenscyclus van een bepaalde hoeveelheid van een bepaalde 'functionele eenheid' product of dienst. Voor wat betreft de risico-analyse staat juist een beoordeling van processen in hun volle omvang centraal: alleen daarmee kunnen de veranderingen in milieuconcentraties in een bepaald gebied worden berekend, hetgeen nodig is voor toetsing aan een norm.

Niveau 3 is het toepassingsniveau, dat direct is verbonden met doelen en modelresultaten. Het centrale doel van LCA is het geven van een kwantitatieve beoordeling van de risico's die worden veroorzaakt door de emissie naar het milieu van een bepaalde stof of stofgroep, in het kader van productbeoordeling of als basis voor de keuze van het minst milieubelastende productalternatief. Het toepassingsgebied van HERA is anders: HERA wordt meestal toegepast om de toxische risico's in een bepaalde regio onder controle te houden door toetsing van concentraties van verontreinigingen aan de geldende normen. LCA en HERA zijn hier dus complementair.

Ondanks de verschillen wordt bepleit LCA en HERA onder te brengen in een gemeenschappelijk computermodel dat beide typen uitkomsten kan genereren. Een dergelijk model zou een optimale harmonisatie van LCA en HERA garanderen, met name voor wat betreft de gemeenschappelijke onderlinge modelstructuren en -parameters. Bovendien zou hiermee een breed instrument worden geschapen waarmee bedrijven hun milieuprestaties op diverse gebieden kunnen toetsen, als basis voor weloverwogen keuzes op het gebied van hun milieubeleid.

Hoofdstuk 4: metalen in multimediamodellen

Hoofdstuk 4 is gewijd aan de inpassing van metalen in de multimediamodellering. Oorspronkelijk zijn de multimediamodellen ontwikkeld ten behoeve van de modellering van het gedrag van organische stoffen. Voor metalen kunnen deze modellen niet zonder meer worden toegepast, omdat een aantal modelvergelijkingen niet van toepassing zijn op metalen en omdat sommige stofeigenschappen die door de gebruiker van het model moeten worden ingevoerd voor metalen niet gedefinieerd zijn. Hiervoor zijn echter oplossingen bedacht waardoor bepaalde vergelijkingen omzeild kunnen worden en waarbij sommige parameters een kunstmatige waarde krijgen toegekend. Met behulp van deze oplossingen zijn binnen de LCA in het verleden ook voor metalen karakterisatiefactoren ontwikkeld. In de praktijk bleken deze karakterisatiefactoren ordes van grootte hoger uit te pakken dan de karakterisatiefactoren voor vrijwel alle organische stoffen, met name ten gevolge van het feit dat metalen niet afbreekbaar zijn. Hierdoor werden er grote vraagtekens werden gezet bij de betrouwbaarheid van deze factoren. In dit hoofdstuk wordt de hypothese gelanceerd dat de bestaande karakterisatiefactoren voor metalen inderdaad te hoog zijn, en wel vanwege het feit dat een aantal voor metalen belangrijke processen, die mogelijk een sleutelrol spelen, niet in de multimediamodellen voorkomen of tekortkomingen vertonen op het gebied van processen die juist voor metalen belangrijk zijn. Het gaat daarbij met name om speciatie en sedimentatie in het mariene milieu. De term speciatie heeft betrekking op het feit dat metalen in een waterig milieu in verschillende chemische vormen kunnen voorkomen, en dat die vormen met elkaar in een dynamisch evenwicht verkeren. Wanneer metalen in een bepaalde vorm naar het milieu worden uitgestoten betekent dit dus nog niet dat ze in die vorm zullen blijven bestaan. Dit is belangrijk in de context van de effectbeoordeling, omdat niet alle vormen biologisch beschikbaar (en dus schadelijk). In dit model is aangenomen dat voor metalen die in anorganische vorm worden geëmitteerd, alleen de fractie die in vrije ionvorm in het milieu verschijnt biologisch beschikbaar is. Alleen voor metallisch kwik en methylkwik is een uitzondering gemaakt. Dit zijn beide zeer schadelijke vormen van kwik, de eerste met name in gasvorm en de tweede als een stof die regelmatig in het milieu ontstaat als omzettingsproduct van anorganische vormen van kwik.

Per metaal dient te worden ingevoerd welke fractie binnen het mariene milieu in deze vorm aanwezig is. Voor kwik is een geheel aparte benadering ontworpen, omdat niet alleen de vrije ionvorm, maar ook de organische en de metallische vorm van dit metaal zeer schadelijk zijn voor de gezondheid van zowel mensen als ecosystemen. Naast de speciatie is ook de sedimentatie aan een nadere analyse onderworpen. Voor een aantal bekende metalen is de berekening van de sedimentatiesnelheid in de bovenlaag van de oceanen vervangen door gemeten waarden in een vroege versie van het GLOBOX-model. Alhoewel deze waarden soms sterk afwijken van de gemodelleerde waarden is de belangrijkste toevoeging waarschijnlijk de modellering van twee lagen in de oceaan: een menglaag, die als deel van het milieusysteem wordt beschouwd, en een diepere laag, die verondersteld wordt geen deel uit te maken van het te beoordelen milieusysteem. Met deze diepere laag is een sink gecreëerd die de gemodelleerde verblijftijd van metalen in het milieusysteem sterk bekort. Door de ingevoerde verbeteringen is de kloof tussen de karakterisatiefactoren voor organische stoffen enerzijds en metalen anderzijds verdwenen, en kunnen de toxische effecten van metalen binnen de LCA op een meer geloofwaardige manier worden beoordeeld.

Hoofdstuk 5: Het GLOBOX model voor fate*, blootstelling en beoordeling van toxische effecten*
Hoofdstuk 5 vormt de kern van dit proefschrift. In dit hoofdstuk wordt het model GLOBOX besproken. GLOBOX is een model voor het berekenen van ruimtelijk gedifferentieerde LCA karakterisatiefactoren voor toxiciteit. GLOBOX onderscheidt zich van andere modellen op dit vlak door het feit dat het model sterk ruimtelijk gedifferentieerd is, doordat het een wereldwijde dekking heeft en doordat met dit model de bijdragen van een product aan actuele effecten of risico's beoordeeld kunnen worden, naast de gebruikelijk potentiële effecten. Het model als geheel bestaat uit drie submodellen of modules: een multimedia-*fate*module, een module voor menselijke blootstelling en een effectmodule. De multimedia-*fate*-module en de module voor menselijke blootstelling zijn gebaseerd op het EUSES-model (versie 2.0), dat ontwikkeld is voor de risicobeoordeling van emissies van organische stoffen naar het Europese milieu. De aanpassingen aan de multimedia-module en de module voor menselijke blootstelling van EUSES 2.0 betreffen met name de reikwijdte en de ruimtelijke differentiatie. Omdat de productlevenscyclus zich willekeurig over de wereld kan uitstrekken heeft het GLOBOX-model een wereldwijde dekking. Het model is ruimtelijk gedifferentieerd op het niveau van landen/territoria en zeeën/oceanen. Voor dit niveau van ruimtelijke differentiatie is om twee redenen gekozen: ten eerste omdat de milieu- en blootstellingsparameters waarop het model is gebaseerd sterk locatie-afhankelijk zijn, en ten tweede omdat processen in de levenscyclus het gemakkelijkst per land geloka-

liseerd kunnen worden Er worden 289 regio's onderscheiden: 239 landen/territoria en 50 zeeën/oceanen. Iedere regio is onderverdeeld in een aantal milieucompartmenten, waaronder lucht, rivieren, zoet- en zoutwatermeren, grondwater en een aantal bodem- en sedimentcompartimenten voor de landen en territoria en lucht, zeewater en zeesediment voor de zeeën en oceanen. Behalve transport tussen lucht-, water- en bodemcompartimenten vindt er ook transport plaats tussen gelijksoortige compartimenten van verschillende regio's, met name ten gevolge van de wind en van rivier- en zeestromingen. Ook is er transport tussen rivieren en zoetwatermeren, en van rivieren naar de zeeën en oceanen. De hydrologische cyclus – een bestaande, wereldwijde waterbalans – is ten behoeve van het GLOBOX-model regionaal gedifferentieerd, en is in het model geïntegreerd. Daarbij zijn ook de stromingen tussen de verschillende zeeën en oceanen in ogenschouw genomen. Behalve op het gebied van de parameters die aan waterstromingen zijn gerelateerd is de multimediamodule ruimtelijk gedifferentieerd op het gebied van geografische parameters (bijvoorbeeld het relatieve oppervlak van zoet- en zoutwatermeren, diverse bodemtypen en landijs per regio), geofysische parameters (bijvoorbeeld de gemiddelde diepte van meren), klimatologische parameters (bijvoorbeeld omgevingstemperatuur, windsnelheid, regenval en vorstperioden) en 'intermedia transfer' parameters (voor gebiedsafhankelijk multimediatransport).

Veel parameters zijn verzameld uit de literatuur of berekend aan de hand van literatuurgegevens. Waar parameters voor bepaalde gebieden ontbraken zijn deze geschat uit equivalente parameters voor andere gebieden. De parameters die betrekking hebben op de hydrologische cyclus zijn zodanig aangepast dat een gesloten waterkringloop ontstond die zo goed mogelijk in overeenstemming is met de gegevens van de hydrologische cyclus als geheel. Aan de oorspronkelijke EUSES-multimediatransportmodule zijn diverse parameters en vergelijkingen toegevoegd, met name om naast organische stoffen ook metalen in de berekeningen te kunnen betrekken, om een onderscheid tussen zoet- en zoutwatermeren en rivieren te kunnen maken, alsmede om rekening te kunnen houden met tijdelijke of permanente bevriezing van bodem-, grond- en oppervlaktewater in koude gebieden.

Ook de module voor menselijke blootstelling is ruimtelijk gedifferentieerd. Voor ieder land of territorium is een schatting gemaakt van het voedselconsumptiepatroon en van de herkomst en de kwaliteit van het drinkwater. Tevens zijn het gemiddelde lichaamsgewicht en het aandeel kinderen in de populatie geschat en in de analyse betrokken. In de effectmodule zijn de gevoeligheidsfactor en de drempelfactor in de vergelijkingen geïntroduceerd.

Alle ruimtelijk gedifferentieerde parameters zijn verzameld in een tweetal spreadsheets. Deel 1 van GLOBACK 2.0 bevat alle multimedia- en blootstellingsparameters, behalve de lucht- en waterstromingen tussen de verschillende regio's, die in deel 2 van deze parameterset worden weergegeven. De modelberekeningen van de multimediamodule resulteren uiteindelijk in een stelsel van circa 3000 vergelijkingen met evenzoveel onbekenden, die het wereldwijde multimedia-transport en de afbraak in elk van de 3000 compartimenten vertegenwoordigen. Deze vergelijkingen worden in het GLOBOX-model simultaan opgelost door middel van matrixinversie. De uitkomsten bestaan uit de over tijd en ruimte geïntegreerde concentraties in elk van de compartimenten ten gevolge van een standaardhoeveelheid van een stof die in één van de 3000 compartimenten is geloosd.

Voor het berekenen van karakterisatiefactoren voor ecotoxiciteit worden de geïntegreerde concentraties, die berekend zijn met de multimediamodule, vermenigvuldigd met de bijbehorende effectfactoren, die de output vormen van de effectmodule. Daarmee ontstaan per compartiment twee karakterisatiefactoren: één volgens het algemene preventieprincipe en één volgens het risicominimalisatie-principe. De effectfactoren die betrekking hebben op het algemene-preventie-principe bestaan uitsluitend uit een toxiciteitsmaat (bijvoorbeeld de EC_{50}) en zullen in het algemeen locatie-onafhankelijk zijn. Voor het verkrijgen van de effect-factoren volgens het risicominimalisatieprincipe wordt deze zelfde toxiciteitsmaat vermenigvuldigd met twee extra factoren: de gevoeligheidsfactor en de drempel-factor.

Voor de berekening van karakterisatiefactoren voor humane toxiciteit ligt het iets ingewikkelder: daarvoor moet de geïntegreerde concentratie ook nog worden vermenigvuldigd met een innamefactor, die per compartiment de relatie aangeeft tussen enerzijds de concentratie binnen dat compartiment en anderzijds de inname van de mens vanuit dat compartiment via voedsel, lucht of drinkwater.

Bij het uitvoeren van een LCA-productstudie wordt iedere emissie vermenigvuldigd met de bijbehorende karakterisatiefactoren. Daarbij ontstaan per effect-categorie voor elke emissie 3000 deeleffectscores per effectcategorie: één voor ieder compartiment. Deze deeleffectscores kunnen vervolgens voor alle stoffen samen per effectcategorie worden opgeteld tot één (totaal)effectscore, die de bijdrage van de levenscyclus aan betreffende type toxiciteit op wereldschaal vertegenwoordigt. Alhoewel het aantal karakterisatiefactoren ten gevolge van de ruimtelijke differentiatie dus sterk toeneemt, blijft het aantal effectscores uiteindelijk gelijk. De gebruiker van het GLOBOX-model behoeft voor iedere stof en voor iedere regio alleen maar de omvang van de emissies naar de diverse compartimenten op te geven, plus een beperkt aantal stofeigenschappen, om voor iedere toxiciteit-gerelateerde effectcategorie tot een ruimtelijk gedifferentieerde beoordeling van de betreffende toxische effecten op wereldschaal te komen.

Ruimtelijk gedifferentieerd karakterisatiefactoren blijken een grote mate van variatie tussen landen te vertonen, met name voor emissies naar binnenlandse wateren en bodemcompartimenten. De geografische positie, de verdeling van meren en rivieren en variaties in omgevingstemperatuur en regenval zijn parameters die bepalend blijken te zijn voor een aantal verschillende karakterisatiefactoren. Daarnaast spelen bevolkingsdichtheid en voedselinname een cruciale rol in de variatie van karakterisatiefactoren voor humane toxiciteit. De landen die opmerkelijke afwijkingen vertonen van de gemiddelde waarden van de karakterisatiefactoren vertegenwoordigen tezamen een belangrijk deel van het wereldwijde BNP. Geconcludeerd wordt dat ruimtelijke differentiatie tussen landen een belangrijke stap voorwaarts betekent bij de verbetering van de toxiciteitgerelateerde LCA.

Hoofdstuk 6: LCA-normalisatie
Hoofdstuk 6 beschrijft de laatste, facultatieve stap binnen de LCA-effectbeoordeling: de normalisatie. Door normalisatie krijgen de effectscores betekenis, omdat ze daarmee van abstracte getallen veranderen in relatieve bijdragen aan de verschillende typen effecten in hun totaliteit. In de normalisatie wordt iedere effectscore gedeeld door de effectscore van het economisch systeem als geheel in een bepaald referentiegebied en een bepaald jaar. Dit kan op verschillende schalen gebeuren, op wereldschaal of bijvoorbeeld op de schaal van een bepaald continent of een bepaald land. Omdat de levenscyclus van een product meestal een vrij grote geografische reikwijdte heeft is het verstandig de schaal niet al te klein te kiezen. In principe ligt een normalisatie op wereldschaal het meest voor de hand, maar wanneer de effectscores in het kader van bepaalde beleidsdoelen moeten worden geëvolueerd wordt vaak gekozen voor een schaal die overeenkomt met die van het geformuleerde beleid. In dit document is gekozen voor het uitwerken van de emissies op wereldschaal en op de schaal van de Europese Unie in 2006, uitgebreid met de landen Zwitserland, Noorwegen en IJsland – de 'EU25+3'. Als referentiejaar is het jaar 2000 gekozen.

Deze normalisatiestudie onderscheidt zich van eerdere normalisatiestudies doordat niet de emissies die *plaatsvonden* in het referentiejaar, maar de emissies die ten gevolge van de economische activiteiten in dat jaar zijn *veroorzaakt*, als uitgangspunt dienen. Dit betekent dat in deze benadering rekening wordt gehouden met de vertraging tussen productie en emissie, bijvoorbeeld in het geval van CFK's in koelkasten. Daarmee is de benadering in de normalisatie gelijk getrokken aan de benadering zoals die in het algemeen in LCA productstudies wordt toegepast, hetgeen van een echte referentie mag worden verwacht.

In tegenstelling tot de voorgaande hoofdstukken heeft hoofdstuk 6 niet alleen betrekking op de beoordeling van toxische effecten, maar op het gehele spectrum van effectcategorieën. De belangrijkste doelstelling van deze normalisatiestudie was het verzamelen van alle milieu-ingrepen – dat wil zeggen: de emissiegegevens van alle stoffen die door de mens in het milieu worden gebracht, de gegevens van de belangrijkste grondstofwinningen en de gegevens met betrekking tot landgebruik – zowel op wereldschaal als op de schaal van de EU25+3. Wanneer de emissie- of onttrekkingsgegevens voor een belangrijke stof niet op het juiste niveau bekend waren is gebruik gemaakt van extrapolatie- en interpolatiemethoden. In totaal konden gegevens worden verzameld over 860 typen milieu-ingrepen (d.w.z. typen emissies, onttrekkingen en landgebruik tezamen). Slechts 48 typen ingrepen bleken gezamenlijk verantwoordelijk te zijn voor 75 procent van alle effectscores voor de vijftien beschouwde effectcategorieën. Alle niet-toxiciteitsgebonden, emissiegerelateerde effecten bleken volledig te worden gedomineerd door de bulkemissies van slechts tien stoffen of stofgroepen: emissies van koolstofdioxide, methaan, zwaveldioxide, stikstofoxiden, ammoniak, fijn stof, vluchtige organische koolwaterstoffen exclusief methaan (NMVOC's) en (H)CFK's naar lucht en emissies van stikstof- en fosforverbindingen naar zoet water. Voor wat betreft de toxische stoffen was de beschikbaarheid van emissiegegevens zeer beperkt. De onzekerheid van de uitkomsten was daardoor voor de toxiciteitgerelateerde effectcategorieën erg groot. Een betere registratie van toxische emissies lijkt dus van groot belang, in de eerste plaats vanwege het onder controle houden van de milieueffecten van de betreffende stoffen, maar ook voor LCA.

Alhoewel dit document met name is bedoeld als referentiekader voor de effectbeoordeling in LCA kan het tegelijk ook zelf als een LCA-studie worden beschouwd: een analyse waarmee de milieueffecten van het economisch systeem als geheel worden geïdentificeerd. Als zodanig benadrukt deze studie dat het bestrijden van een beperkt aantal bulkemissies een belangrijke stap voorwaarts zou vormen voor het Europese en mondiale milieubeleid.

Conclusies

Alhoewel LCA en HERA complementaire instrumenten zijn kan de nauwkeurigheid van LCA sterk worden vergroot door het implementeren van een aantal elementen uit de humane risico-analyse en de milieu-risico-analyse: regionale differentiatie en daaraan gekoppeld een onderscheid tussen boven- en onderdrempeleffecten. Omdat de productlevenscyclus zich willekeurig over de wereld uitstrekt is daarvoor een wereldwijd model nodig. Het GLOBOX-model voldoet aan deze voorwaarden. Bovendien voorziet het model in een grote parameterset, GLOBACK, die in de vorm van een losse module ook als basis voor andere modellen gebruikt kan worden. Deze parameterset is reeds uitgebreid met een verzameling parameters voor deelgebieden binnen de Verenigde Staten en Canada. Om de effectbeoordeling te volmaken is daarnaast een normalisatiemodel toegevoegd. Hiermee is het gegevensbestand van mondiale milieu- en blootstellingsparameters uitgebreid met een set mondiale emissie- en onttrekkingsgegevens. Met het GLOBOX-model kunnen specifieke karakterisatiefactoren voor toxische effecten worden berekend voor ieder land of territorium en iedere zee of oceaan op de wereld. Emissies die bijdragen aan actuele effecten of risico's zijn daarbij expliciet herkenbaar, als onderdeel van de voor LCA gebruikelijke potentiële effecten. Het model kan hiermee bijdragen aan de wereldwijde bruikbaarheid van

LCA en aan het terugdringen van de verontreiniging van het milieu, te beginnen bij de emissies met de hoogste risico's.

Bibliography

Wegener Sleeswijk A, Heijungs R (2010) GLOBOX: a spatially differentiated global fate, intake and effect model for toxicity assessment in LCA. *Sci Tot Env* **408**: 2817-2832

Wegener Sleeswijk A, Van Oers L, Guinée J, Struijs J, Huijbregts M (2008) Normalisation in product life cycle assessment: an LCA of the global and European economic systems in the year 2000. *Sci Tot Env* **390**: 227-240

Guinée JB, Heijungs R, Kleijn R, Van der Voet E, De Koning A, Van Oers L, Elshkaki A, Huele R, Huppes G, Suh S, Wegener Sleeswijk A (2006) Human and Ecological Life cycle tools for the Integrated Assessment of Systems (HELIAS) *Int J LCA* **11** (1): 19-28

Udo de Haes HA, Wegener Sleeswijk A, Heijungs R (2005) Similarities, differences and synergisms between HERA and LCA – An analysis at three levels. *Human and Ecological Risk Assessment* **12** (3): 431-449

Wegener Sleeswijk A (2005) *Metals in the ocean. An adapted LCA fate and exposure model.* In: Dubreuil A (ed.) *Life-cycle assessment of metals: issues and research directions.* Society of Environmental Toxicology and Chemistry (SETAC), Pensacola (FL), USA. p. 205-213

Wegener Sleeswijk A, Heijungs R, Erler ST (2003) Risk assessment and life-cycle assessment: fundamentally different yet reconcilable. *Greener Management International* **41**: 77-87

Wegener Sleeswijk A (2003) General prevention and risk minimization in LCA: a combined approach. *Environ Sci & Pollut Res* **10** (1): 69-77

Guinée JB, Gorrée M, Heijungs R, Huppes G, Kleijn R, De Koning A, Van Oers L, Wegener Sleeswijk A, Suh S, Udo de Haes HA, De Bruijn H, Van Duin R, Huijbregts MAJ (2002) *Handbook on Life Cycle Assessment. Operational Guide to the ISO Standards.* Kluwer Academic Publishers, Dordrecht [etc.], The Netherlands.

Wegener Sleeswijk A (2000) Recensie betreffende het proefschrift van Potting JMB, "Spatial Differentation in Life Cycle Impact Assessment" *Milieu* **15**: 214-216

Huijbregts MAJ, Thissen UMJ, Guinée JB, Jager T, Kalf D, Van de Meent D, Ragas AMJ, Wegener Sleeswijk A, Reijnders L (2000): Priority Assessment of Toxic Substances in Life Cycle Assessment. Part I: Calculation of Toxicity Potentials for

181 Substances with the Nested Multi-Media Fate, Exposure and Effects Model USES-LCA. *Chemosphere* **41**: 541-573

Heijungs R, Wegener Sleeswijk A (1999) The structure of impact assessment: mutually independent dimensions as a function of modifiers. Letters to the Editor: Comments and Reply. Comment. *Int J LCA* **4** (1): 2-3

Van Zeijts H, Lenenman H, Wegener Sleeswijk A (1999) Fitting fertilisation in LCA: allocation to crops in a cropping Plan. *J Cleaner Prod* **7**: 69-74

Wegener Sleeswijk A (1998) Participatie: een basis voor draagvlak? *Milieu* **13**: 107

Wegener Sleeswijk A (1997) *Product versus process in impact assessment.* In: Proceedings of Eco-Informa'97. October 6-9, 1997. Eco-Informa Press, Bayreuth, Germany.

Guinée J, Heijungs R, Van Oers L, Wegener Sleeswijk A, Van de Meent D, Vermeire Th, Rikken M (1996) USES – Uniform System for the Evaluation of Substances. Inclusion of fate in LCA characterisation of toxic releases applying USES 1.0. *Int J LCA* **1**: 133-138

Wegener Sleeswijk A, Heijungs R (1996) Modelling fate for LCA. *Int J LCA* **1** (4): 237-240

Wegener Sleeswijk A (1996) *LCA of agricultural products.* In: Ceuterick D (ed.) *International Conference on Application of Life Cycle Assessment in Agriculture, Food and Non-Food Agro-Industry and Forestry: Achievements and Prospects.* Preprints. 4-5 April 1996, Brussels, Belgium. VITO, Mol, Belgium.

De Snoo GR, Wegener Sleeswijk A (1995) Gebruik van bestrijdingsmiddelen langs akkerranden en slootkanten in de Haarlemmermeer. *H2O* **28**: 430-431

Wegener Sleeswijk A (1993) *Life cycle Assessment of Wheat Fertilization: Methodological Aspects and Results.* In: Pedersen Weidema B (ed.) *Life Cycle Assessment of Food Products. Proceedings of the 1st European Invitational Expert Seminar on Life Cycle Assessment of Food Products. 22d-23d of November 1993.* The Ecological Food Project, Interdisciplinary Centre, Technical University of Denmark, Lyngby, Denmark.

De Snoo GR, Wegener Sleeswijk A (1993) Use of pesticides along field margins and ditch banks in The Netherlands. *Med Fac Landbouww Univ* **58** (3A): 921-926

Curriculum Vitae

Anneke Wegener Sleeswijk was born in 1960 in Naarden, The Netherlands. She graduated from secondary school Sint Maartenscollege in Haren in 1979 (VWO). After her graduation, she lived in Cambridge (UK) for a short while, where she followed a course in English (Proficiency) at the Cambridge School of Languages. From 1980-1987, she studied biology at the Rijksuniversiteit Groningen. From 1983-1984, she interrupted her studies for a trip through India, where she worked as a volunteer at the Beatitudes Social Welfare Centre in Madras. She graduated from her biology study in 1987 in the fields of cell genetics and biological psychiatry, and acquired a teacher qualification as well. From 1987-1989, she worked in the Leiden University hospital AZL (now LUMC) as a nurse. From 1989-1990, she followed a post-graduate course on environmental science at P-HTS in Amsterdam. In 1991, she started to work as a volunteer at the Centre of Environmental Science (CML) of Leiden University, where she also started her work on toxicity and exposure assessment for the LCA manual and background documents of 1992, and produced the corresponding characterisation factors for the toxicity-related impact categories. From 1993-2006, she was appointed as a researcher and later as a PhD-student at CML. Apart from her thesis, she worked on several LCA studies, mainly on methodological issues. Besides spatially differentiated fate and exposure modelling, she has also specialised in the methodological complications of agricultural product assessment. In 2006, she was appointed as a researcher at the Radboud University Nijmegen, where she worked on the collection of region-specific environmental parameters for Canada and the United States, and on LCA normalisation, in collaboration with CML. By the end of 2006, Anneke started up her own business GLOBRIGHT. One of her jobs was to build an LCA web portal for RIVM, which she finished in the first half of 2007. Some smaller projects followed. From September 2009 to July 2010, Anneke was appointed at CE Delft, where she worked on the subject of chain management research. She then decided to change back to her own GLOBRIGHT business, to work as a freelancer again. In her leisure time, Anneke works on autism research. It is one of her passions to contribute to the integration of the many different disciplinary research results on this subject.