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Regional LCA in a global perspective

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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

* 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 (Joliet *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 (Joliet *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 disproportionately 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 EC₅₀ or ED₅₀ (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 ecotoxicity by calculations on a test substance.
5. Creating an updated, global LCA normalisation system.

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. *Chemosphere* **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, Hupperts 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 and monitoring approaches. *Environ Sci Technol* **38**: 5682-5693

Toose L, Woodfine DG, MacLeod M, Mackay D, Guoin 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

