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## Regional LCA in a global perspective

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# Synopsis

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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 ecotoxicity by calculations on a test substance.
5. Creating an updated, global LCA normalisation system.

Contrary to existing LCA multimedia fate and exposure models, that often implicitly 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 and 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 existing 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 hypothesised 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 calculated 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<sub>50</sub>), 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 and 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.