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

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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 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.

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 article 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

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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 paper 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.

2. The GLOBOX model

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 exists 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