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Priority assessment of toxic substances in life cycle assessment. III: Export of potential impact over time and space

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Abstract

Toxicity potentials are scaling factors used in life cycle assessment (LCA) indicating their relative importance in terms of potential toxic impacts. This paper presents the results of an uncertainty assessment of toxicity potentials for 181 substances that were calculated with the global nested multi-media fate, exposure and effects model USES-LCA. The variance in toxicity potentials resulting from choices in the modelling procedure was quantified by means of scenario analysis. A first scenario analysis showed to what extent potential impacts in the relatively short term are obscured by the inclusion of impacts on the very long term. Toxicity potentials representing potential impacts over time horizons of 20, 100 and 500 years were compared with toxicity potentials representing potential impacts over an infinite time horizon. Time horizon dependent differences up to 6.5 orders of magnitude were found for metal toxicity potentials, while for toxicity potentials of organic substances under study, differences remain within 0.5 orders of magnitude. The second scenario analysis addressed to what extent potential impacts on the continental scale are obscured by the inclusion of impacts on the global scale. Exclusion of potential impacts on the global scale changed the toxicity potentials of metals and volatile persistent halogenated organics up to 2.3 orders of magnitude. These scenario analyses also provide the basis for determining exports to future generations and outside the emission area.

Keywords: LCA; Type IV multi media model; Ecotoxicity and human toxicity; Environmental fate and exposure model

1. Introduction

Toxicity potentials are substance-specific, quantitative measures of potential impacts per unit emission of a toxic substance that can be used as weighting factors in the aggregation of emissions coming from life cycle inventories. Huijbregts et al. (2000a) calculated toxicity potentials for 181 substances with the global nested multi-media fate, exposure and effects model USES-LCA, which is based on the Uniform System for the Evaluation of Substances 2.0 (USES 2.0), developed by RIVM et al. (1998).

Although USES–LCA may be better suited for the calculation of toxicity potentials than methods previously used, the calculated toxicity potentials may still contain large uncertainties. For instance, the variance in toxicity potentials resulting from input parameter uncertainties and human variability for Atrazine, 2,3,7,8-TCDD and Lead, expressed by the ratio of the 97.5 percentile and the 2.5 percentile, ranges from about 1.5 to 6 orders of magnitude (Huijbregts et al., 2000b).

The relevance of (value) choices in the modelling procedure has, however, so far not been assessed in USES–LCA. In this respect an important choice in the

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calculations may be the choice for a certain time horizon. For instance, the global warming potential of a pollutant used in the impact assessment of greenhouse gases may differ more than one order of magnitude depending on the time horizon chosen (Albritton et al., 1996). In the calculation of toxicity potentials, an infinite time horizon is generally used (Guinée et al., 1996; Hertwich et al., 1998; Huijbregts et al., 2000a). However, by using an infinite time horizon potential impacts occurring over a shorter period of time may be obscured in the impact assessment of product systems.

Another important choice may be the decision whether or not to include potential impacts exported from the continental scale to the global scale. Huijbregts et al. (2000a) included potential impacts on the global scales in the calculation of toxicity potentials by way of scale-specific weighting factors. However, including exposure that occurs on the global scale may fully dominate the potential impacts, obscuring those on the continental scale.

This paper assesses the influence of export of potential impact over time and space in the calculation of toxicity potentials. Toxicity potentials using time horizons of 20, 100 and 500 years and toxicity potentials excluding impacts on the global scale are calculated. Then, these potentials are compared with toxicity potentials calculated by Huijbregts et al. (2000a,b), which relate to potential impacts over an infinite time horizon and the global scale.

2. Analysis of scenario uncertainty

2.1. Toxicity potentials

USES–LCA calculates toxicity potentials for the six impact categories fresh water aquatic ecotoxicity, marine aquatic ecotoxicity, fresh water sediment ecotoxicity, marine sediment ecotoxicity, terrestrial ecotoxicity and human toxicity, after initial emission to the compartments air, fresh water, seawater, industrial soil and agricultural soil, respectively. Thus, ultimately, 30 toxicity potentials can be calculated for each substance; one for each combination of six impact categories and five emission compartments.

2.2. Time horizon dependency

For the calculation of time horizon-dependent toxicity potentials the time-integrated exposure over the time period T considered is of interest (Fig. 1). The time-integrated exposure at time T to a pulse emission Δm, released at time $t = 0$ and added to the steady state situation m_b at $t = 0$, is (Heijungs, 1995)

$$\gamma_T = \int_0^T (m(t) - m_b)\,\mathrm{d}t, \tag{1}$$

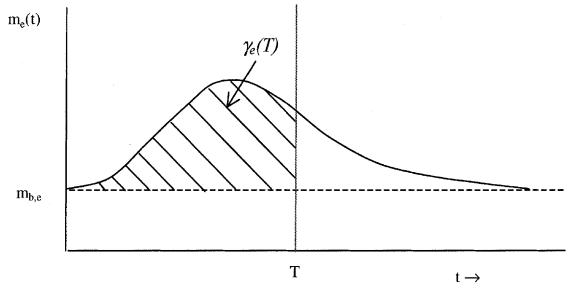

Fig. 1. Graphical interpretation of the time-integrated exposure γ_e over time horizon T in compartment e after an emission pulse Δm_i released to compartment i at $t = 0$, superimposed to a background level $m_{b,e}$ in compartment e.

Because

$$m(t) = m_b + \mathrm{e}^{tA} \cdot \Delta m. \tag{2}$$

Eq. (1) can be rewritten as

$$\gamma_T = \int_0^T \left(\mathrm{e}^{tA} \cdot \Delta m\right) \mathrm{d}t \tag{3}$$

which is equal to

$$\gamma_T = (\mathrm{e}^{TA} - I) \cdot A^{-1} \cdot \Delta m, \tag{4}$$

where γ_T is the vector of time-integrated exposure from 0 to T (h.kg), $m(t)$ the vector of mass m at time t (kg), m_b the vector of steady state mass situation m_b (kg), A the matrix of coefficients which determines the fate of a substance (h^{-1}), I the identity matrix (dimensionless) and Δm is the vector of emission pulse m at $t = 0$ (kg).

As the term $(\mathrm{e}^{TA} - I) \cdot A^{-1}$, needed in the integrated exposure calculations (Eq. (4)), is also applied in dynamic mass-balance models (Brandes et al., 1996; Heijungs, 1999), outcomes of dynamic mass-balance modelling can be used directly in the assessment of time horizon dependent toxicity potentials.

Dynamic calculations in USES–LCA are performed by implementing a routine that numerically solves the mass balance equations of the fate part of USES–LCA. The dynamic module of the fate model Simplebox 2.0 is used for this purpose (Brandes et al., 1996). It has been chosen to calculate toxicity potentials for the time horizons 20, 100 and 500 years, following the time horizons used in the calculation of global warming potentials (Albritton et al., 1996). It is believed that these three time horizons provide a practical range for policy applications.

2.3. Exclusion of the global scale

USES–LCA has two spatial scales (continental and global) and three climate zones, reflecting arctic, moderate and tropic climatic zones of the Northern hemi-

sphere. Huijbregts et al. (2000a,b) aggregated potential impacts on the continental scale and the global scale by way of scale-specific weighting factors. Potential impacts in the marine aquatic compartments were aggregated on the basis of the compartment's volume, and potential impacts in the marine sediment and terrestrial compartments were both aggregated on the basis of the compartment's mass. For humans, the human population present at a certain scale has been used as a weighting factor. For the impact categories related to the fresh water aquatic and sediment compartment no weighting factors were needed, as these compartments are only identified at the continental scale.

Excluding potential impacts on the global scale in the calculation of toxicity potentials can be done by setting the weighting factors for the arctic, tropic and moderate zone of the impact categories involved to zero. Similar to the assessment of export of potential impacts over time, inclusion or exclusion of potential impacts on the global scale can be seen as a (value) choice in the calculation of toxicity potentials.

3. Results and discussion

3.1. Export over time

Figs. 2–5 compare the toxicity potentials calculated for the time horizons 20, 100 and 500 years with the toxicity potentials calculated for an infinite time horizon.

The time-integrated exposure to organic substances is in most cases virtually completed within 20 years. For persistent organic substances, such as endrin, the relative difference between toxicity potentials calculated for an infinite time horizon (Huijbregts et al., 2000a) and a time horizon of 20 years is up to 0.5 orders of magnitude, while for the time horizons 100 and 500 years relative differences with an infinite time horizon are negligible. Compared to the influence of parameter uncertainty on toxicity potentials (Huijbregts et al., 2000b), time horizon dependent differences for these substances can be considered small.

On the other hand, time horizon dependent differences for metal toxicity potentials can be up to several orders of magnitude, indicating that there may be a large export of impacts to future generations. Therefore, the choice of a particular time horizon is important in the

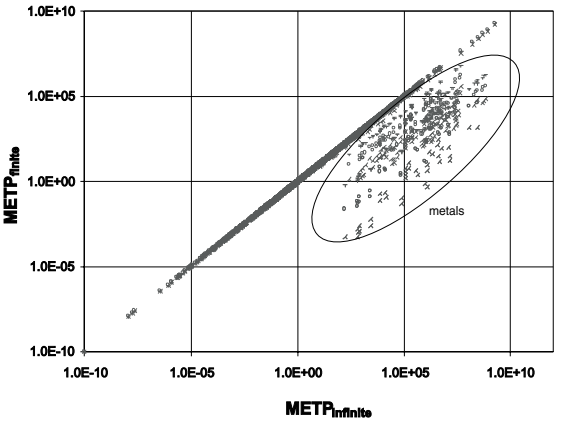

Fig. 2. Comparison of marine aquatic and sediment ecotoxicity potentials for an infinite time horizon ($METP_{infinite}$) with marine aquatic and sediment ecotoxicity potentials for the time horizons 20 years (×), 100 years (○), and 500 years (+) ($METP_{finite}$).

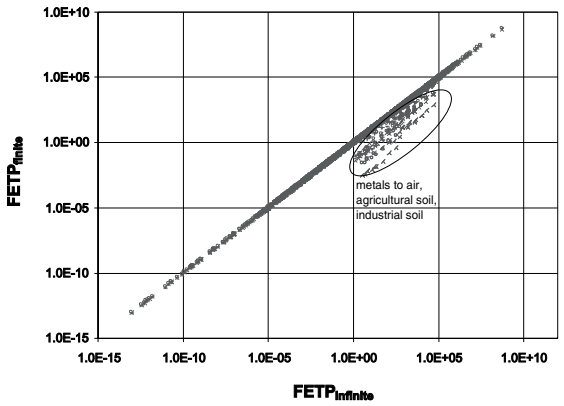

Fig. 3. Comparison of fresh water aquatic and sediment ecotoxicity potentials for an infinite time horizon ($FETP_{infinite}$) with fresh water aquatic and sediment ecotoxicity potentials for the time horizons 20 years (×), 100 years (○), and 500 years (+) ($FETP_{finite}$).

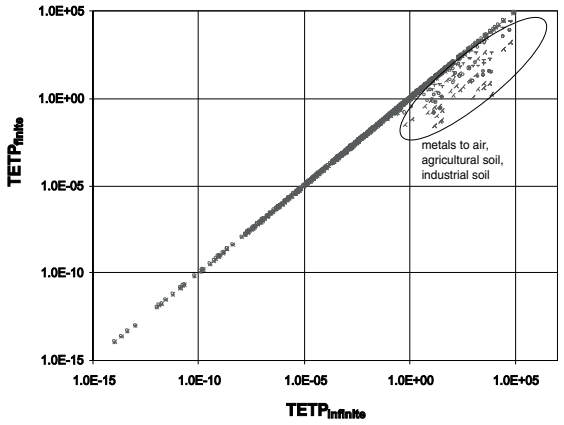

Fig. 4. Comparison of terrestrial ecotoxicity potentials for an infinite time horizon ($TETP_{infinite}$) with terrestrial ecotoxicity potentials for the time horizons 20 years (×), 100 years (○), and 500 years (+) ($TETP_{finite}$).

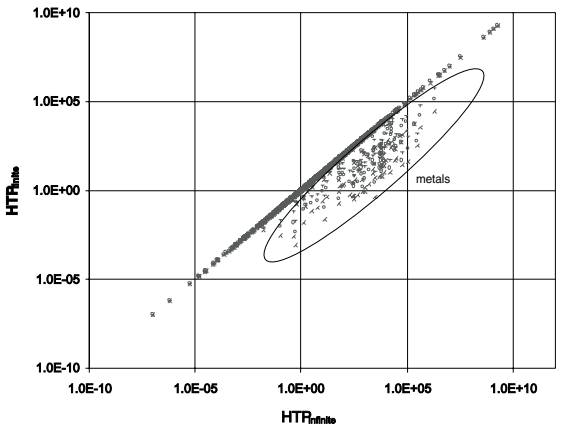

Fig. 5. Comparison of human toxicity potentials for an infinite time horizon ($HTP_{infinite}$) with human toxicity potentials for the time horizons 20 years (×), 100 years (○), and 500 years (+) (HTP_{finite}).

impact assessment of heavy metal emissions. Toxicity potentials related to the marine environment show a relatively high time horizon dependency due to the very long modelled residence times of most metals in the marine aquatic compartment and the upper layer of the marine sediment (Fig. 2). For most of the metals, residence times in USES–LCA are in the same order of magnitude as reported by Goldberg (1965), the major exception being Be (Huijbregts, 2000). If the metal is emitted to one of the soil compartments, time horizon dependent differences of the marine toxicity potentials further increase. The reason is that run-off from the soil to the aquatic environment may take a very long time (>1000 years) for metals strongly bound to the soil matrix (Cleven et al., 1993; Guinée et al., 1999).

Exposure to metals in the fresh water environment after emission to fresh water is almost completed in 20 years. This follows from efficient removal pathways, such as burial of metals in deep fresh water sediment and metal flow from the fresh water compartment to the sea water compartment. However, after emission to air and soil, fresh water toxicity potentials markedly increase over time, as metal run-off from the soil may cause exposure in the fresh water environment over a very long time (Fig. 3). The slow run-off of metals to the aquatic environment and leaching of metals to deeper soil layers from the upper soil compartment, which is also shown in other fate models (Van de Meent, 1990; Cleven et al., 1993; Moolenaar et al., 1997; Guinée et al., 1999), cause significant time horizon dependent differences in terrestrial ecotoxicity potentials (TETP) of metals (Fig. 4). In this respect it should also be noted that USES–LCA assumes a vertically mixed soil layer up to 1 m. If a smaller soil depth is assumed ecologically relevant, the modelled residence time of metals in the soil may decrease substantially (De Vries and Bakker, 1998). In turn, this will lower all metal TETPs, in particular for the longer time horizons. It also decreases the time horizon dependent differences between the metal TETPs. Finally, human toxicity potentials (HTPs) of metals may show substantial time horizon dependent differences (Fig. 5). The actual time horizon dependency of HTPs follows from the dominant exposure route. If exposure via air or fresh water is the dominant exposure route, no substantial time horizon dependent differences in HTPs are found. If, however, the marine environment (via fish consumption) or the soil compartments (e.g., via crop consumption or direct soil ingestion) are important, differences between HTPs for an infinite time horizon and the time horizons 20, 100 and 500 years can be up to several orders of magnitude.

3.2. Export to the global scale

Figs. 6–9 compare the toxicity potentials excluding and including impacts on the global scale. As can be seen in the Figs. 6–9, toxicity potentials of the majority of the substances are not affected by excluding potential impacts on the global scale. The reason is that organic substances which are not very persistent and volatile are not capable of moving from the continental to the global scale.

On the other hand, as shown in Figs. 6 and 7, exclusion of potential impacts on the global scale decrease the marine aquatic ecotoxicity potentials (MAETP) and marine sediment ccotoxicity potentials (MSETP) of metals and persistent volatile halogenated organic substances up to 2.3 and 1.6 orders of magnitude, respectively. This is true for all initial emission compartments. It shows that the marine toxicity potentials of these

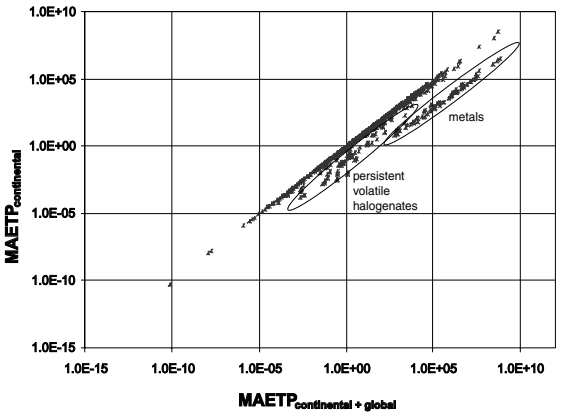

Fig. 6. Comparison of marine aquatic ecotoxicity potentials including the global scales ($MAETP_{continental+global}$) and marine aquatic ecotoxicity potentials excluding the global scales ($MAETP_{continental}$).

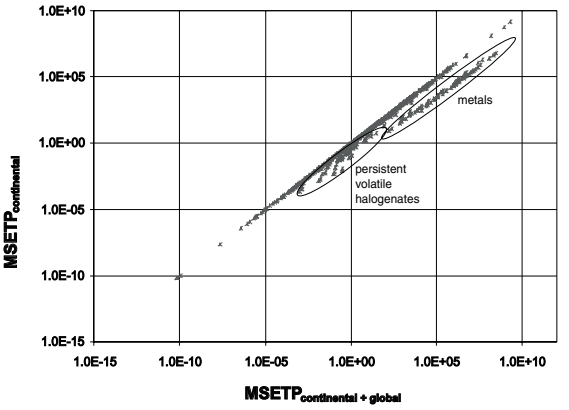

Fig. 7. Comparison of marine sediment ecotoxicity potentials including the global scales ($MSETP_{continental+global}$) and marine sediment ecotoxicity potentials excluding the global scales ($MSETP_{continental}$).

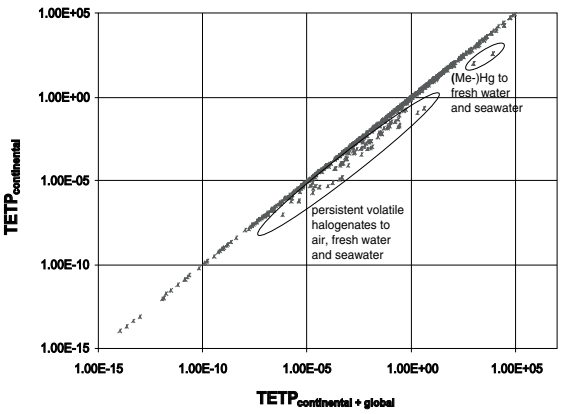

Fig. 8. Comparison of terrestrial ecotoxicity potentials including the global scales ($TETP_{continental+global}$) and terrestrial ecotoxicity potentials excluding the global scales ($TETP_{continental}$).

substances are dominated by the time-integrated exposure at the global scale, reflecting that the oceanic compartment acts as a major sink for these persistent pollutants.

Fig. 8 shows that potential impacts on the global scale substantially contribute to TETPs of persistent and volatile substances emitted to continental air, fresh water and seawater compartment. Exclusion of the global scale results for these substances in a decrease in TETPs up to 1.5 orders of magnitude. In contrast, TETPs of all direct emissions to agricultural and industrial soils are completely explained by potential impacts in the continental soil compartments. This means that after emission to continental soils transport of substances to soils on the global scale hardly occurs.

Finally, Fig. 9 indicates that the HTPs of metals and persistent volatile halogenated organic substances may

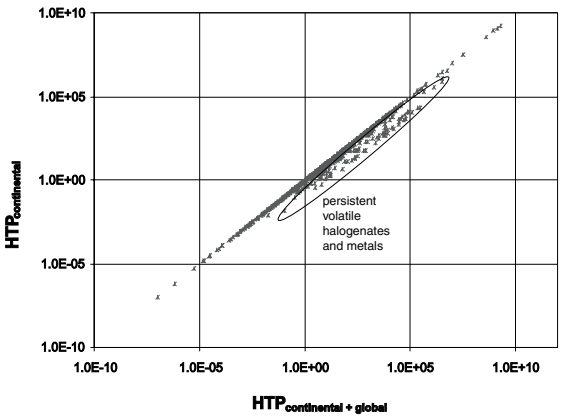

Fig. 9. Comparison of human toxicity potentials including the global scales ($HTP_{continental+global}$) and human toxicity potentials excluding the global scales ($HTP_{continental}$).

be up to 1.2 orders of magnitude lower compared to substances not persistent and/or mobile enough to enter the global scale. Compared to the ecotoxicity potentials, excluding the global scale has a less pronounced effect on the HTPs. The reason is that the weighting factors in the HTP calculation are based on population numbers instead of the compartment's mass or volume. Therefore, for instance, exclusion of the arctic zone hardly influences the HTP outcomes, while this is not the case for the ecotoxicity potentials of metals and persistent volatile halogenated organic substances involved.

3.3. USES–LCA

USES–LCA calculations may suffer from substantial model uncertainties (Ragas et al., 1999; Huijbregts et al., 2000a). In this respect, model uncertainties related to the application of USES–LCA for metals are particularly important. Two important examples of uncertainty in the model structure and possible improvement options will be discussed below.

A major drawback of using box models, such as USES–LCA, is that they do not account for subcompartimental differences in fate and corresponding effects. Although for organic substances spatial variability may not be very important in the assessment of fate and effects compared to the influence of parameter uncertainties (Hertwich et al., 1999), this may not be the case for metals. For instance, lack of reliable information about partition coefficients is an important source of uncertainty for toxicity potentials of lead (Huijbregts et al., 2000b). Metal partitioning in turn strongly depends on environmental characteristics and may have a large influence on the residence time of metals particularly in the soil compartment (De Vries and Bakker, 1998). Therefore, moving to spatially explicit models (e.g. Stolwijk et al., 1998; Klepper and Den Hollander, 1999;

Van den Hout et al., 1999) may be an improvement in the fate, exposure and effect assessment of metals. Moreover, in these spatially explicit models it may be easier to account for currently lacking site-dependent processes in USES-LCA, such as the site dependent slow conversion of reversibly adsorbed heavy metals into forms irreversibly adsorbed to the soil matrix (Harmsen, 1992; De Vries and Bakker, 1998) and corresponding uptake of metals by organisms (Peijnenburg et al., 1997, 1999). Including these processes may substantially decrease the metal toxicity potentials after emission to the soil and air compartments, and lower the time horizon dependent differences between these toxicity potentials. Further research in LCA context is recommended here.

The fate analysis of geochemically reactive metals in the marine environment, such as Be, also needs improvement. Goldberg (1965) reports an oceanic residence time of Be three orders of magnitude lower than calculated by USES–LCA (Huijbregts, 2000). The reason is that the ions of Be are expected to be rapidly hydrolysed at the pH of seawater and incorporated into minerals, such as ferro-mangenese nodules (Goldberg, 1965; Riley, 1971), giving rise to a removal mechanism which has not been included in USES–LCA.

4. Conclusions

The dynamic USES–LCA calculations may give a first impression about the time horizon dependence of organic and inorganic pollutants over the time horizons 20, 100 and 500 years. It is shown that time horizon dependent differences can be up to several orders of magnitude for the metal toxicity potentials, while time horizon dependent differences remain within 0.5 order of magnitude for organic substances. Exclusion of potential impacts on the global scale changed the toxicity potentials of metals and volatile persistent halogenated organics. Differences up to 2.3 orders of magnitude are found for these types of substances. As the latter substances may substantially contribute to the potential impact of product systems, the (value) choice of the time and spatial horizon in the LCA impact assessment of toxic substances is an important one. It should, however, be stressed that uncertainties in the model structure of USES–LCA may be large, as results have not been validated. In particular, modelling of geochemical reactive metals in the marine environment and spatial dependency of metal behaviour needs improvement.

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