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Priority Assessment of Toxic Substances in the frame of LCA

**Time horizon dependency in toxicity potentials
calculated with the multi-media fate, exposure and
effects model USES-LCA**

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Abstract

Up till now, in the calculation of toxicity potentials (TPs) used in life cycle assessment (LCA) potential effects are taken into account using an infinite time horizon. However, by including potential effects which may occur over a very long time period, potential effects in the relatively short term may be dominated by effects due to persistent chemicals in the impact assessment of product systems. Furthermore, knowledge about the time dependence of impacts allows for assessing to what extent impacts are 'exported' to future generations. In this study the effect of using different time horizons (20, 100, 500 years) on TPs of 181 substances was assessed by using level IV multi-media fate calculations. Time horizon dependent TPs are calculated with the global nested multi-media fate, exposure and effects model USES-LCA for the impact categories human toxicity, marine aquatic ecotoxicity, fresh water aquatic ecotoxicity, marine sediment ecotoxicity, fresh water sediment ecotoxicity, and terrestrial ecotoxicity after initial emission to the compartments air, fresh water, sea water, industrial soil and agricultural soil, respectively. Time horizon dependent differences of several orders of magnitude are found for the metal TPs, while for TPs of other inorganics than metals and organic substances under study time horizon dependent differences remain within 0.5 order of magnitude. As metals may substantially contribute to the potential impact of product systems, the results of this study indicate that the choice of a time horizon in the LCA impact assessment of toxic substances is an important one.

Keywords: Toxicity potential, LCA, Time horizon, Dynamic calculations, Priority assessment, Ecotoxicity, Human toxicity, Environmental fate model

1. Introduction

Characterisation factors, also called ‘potentials’, are used in life cycle assessment (LCA) to represent substance-specific, quantitative representations of potential impacts for environmental problems, such as global warming and human toxicity. For global warming, it is possible to assess potential impacts over different time horizons (Albritton et al., 1996). For toxic impact categories, however, potential impacts are generally taken into account over an infinite time horizon (Guinee et al., 1996; Hertwich et al., 1998; Huijbregts et al., 2000a). One of the drawbacks of including exposure which may occur after a very long time is that potential impacts occurring over a shorter period of time may be dominated by effects due to persistent chemicals in the impact assessment of product systems. Furthermore, knowledge about the time dependence of impacts allows for assessing to what extent impacts are ‘exported’ to future generations.

This paper concentrates on the calculation of toxicity potentials (TPs) for LCA purposes using different time horizons. It builds on the work of Huijbregts et al. (2000a) that calculated, using an infinite time horizon, TPs of 181 substances for the impact categories (1) fresh water aquatic ecotoxicity, (2) marine aquatic ecotoxicity, (3) fresh water sediment ecotoxicity, (4) marine sediment ecotoxicity, (5) terrestrial ecotoxicity and (6) human toxicity with the globally nested multi-media fate, exposure and effects model USES-LCA. The same impact categories will be used here. TPs for the six impact categories were calculated after emission to air, fresh water, seawater, agricultural soil and industrial soil in West Europe, respectively.

The use of time horizon specific TPs in LCAs is relatively straightforward. Scores for a specified toxic impact category and time horizon can be calculated by

$$IS_{p,g,t} = \sum_e \sum_x TP_{g,t,x,e} \times E_{p,x,e} \quad (1)$$

$IS_{p,g,t}$ = Impact score of product system p related to impact category g for time horizon t (kg);

$TP_{g,t,x,e}$ = Toxicity potential related to impact category g for time horizon t of substance x due to an emission to compartment e (dimensionless);

$E_{p,x,e}$ = Emission due to product system p of substance x to compartment e (kg);

A dynamic version of USES-LCA is developed for the calculation of time horizon dependent TPs (Section 2). It is chosen to recalculate TPs for the 181 substances analysed by Huijbregts et al. (2000a), but now using time horizons of 20, 100 and 500 years. For 11 substances also a comparison is made with the TPs for an infinite time horizon (Section 3).

2. Method

2.1 Dynamic calculations

In LCA one is interested in assessing the potential impact of mass loadings (emission pulses) rather than emission fluxes. Although steady state models are in principle designed to assess the environmental impact of emission fluxes, it is possible to calculate the infinite time-integrated exposure $\gamma(\infty)$ to an emission pulse, shown in Figure 1, with a steady state model based on first-order linear differential equations (Heijungs, 1995, 1997). However, for the calculation of time horizon-dependent TPs, the time-integrated exposure over an infinite time horizon $\gamma(\infty)$ is not of interest, but the time-integrated exposure over time period $t=0$ up to $t=T$ (Figure 2). It will be shown below that environmental concentrations at time T , $c(T)$, calculated by a dynamic multi media fate model, can be used directly in the calculation of time horizon-dependent TPs.

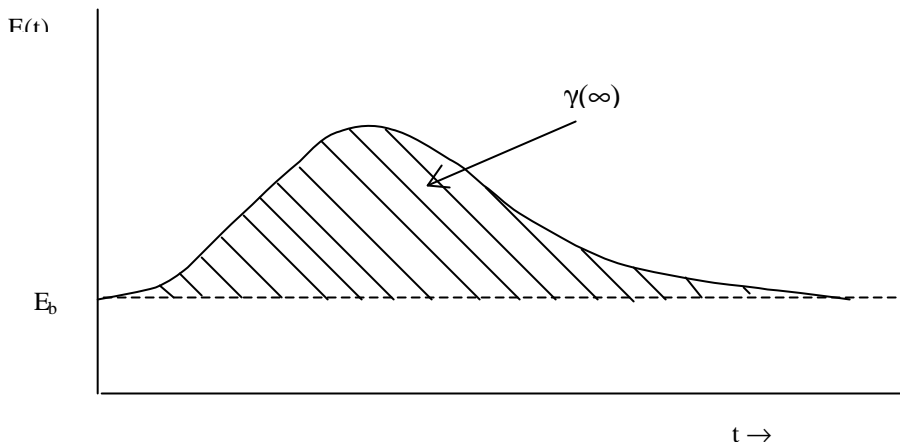


Figure 1: Graphical interpretation for the time-integrated exposure γ over an infinite time horizon in compartment j after an emission pulse ΔE released to compartment e at $t = 0$, superimposed to a background level E_b (derived from Heijungs, 1997).

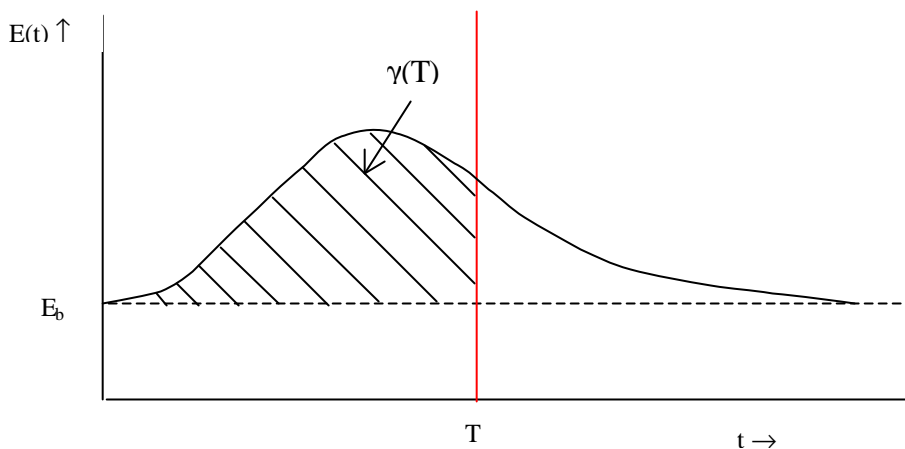


Figure 2: Graphical interpretation for the time-integrated exposure γ over time horizon T in compartment j after an emission pulse ΔE released to compartment e at $t = 0$, superimposed to a background level E_b .

The equation which describes the time-dependency of the concentrations c in the environment, can be written in matrix notation as

$$\frac{dc(t)}{dt} = \mathbf{A} \cdot \mathbf{c}(t) + \mathbf{f} \quad (2)$$

Equation 2 can be solved to yield (Heijungs, 1995; Brandes et al., 1996)

$$\mathbf{c}(t) = e^{t\mathbf{A}} \cdot \mathbf{c}(0) + (e^{t\mathbf{A}} - \mathbf{I}) \cdot \mathbf{A}^{-1} \cdot \mathbf{f} \quad (3)$$

where,

- $c(t)$ = vector of environmental concentrations at time t ($\text{kg}\cdot\text{m}^3$);
- $c(0)$ = vector of environmental concentrations at time $t=0$ ($\text{kg}\cdot\text{m}^3$);
- \mathbf{A} = matrix of coefficients which determines the fate of a substance (hr^{-1});
- \mathbf{I} = identity matrix (dimensionless);
- \mathbf{f} = vector of emission fluxes ($\text{kg}\cdot\text{m}^3\cdot\text{hr}^{-1}$).

According to Heijungs (1995), the time-integrated exposure at time T to a pulse emission ΔE , released at time $t = 0$ and added to the steady state situation E_b at $t = 0$, is

$$\gamma(T) = \int_0^T (\mathbf{E}(t) - \mathbf{E}_b) dt \quad (4)$$

Because

$$\mathbf{E}(t) = \mathbf{E}_b + e^{t\mathbf{A}} \cdot \Delta \mathbf{E} \quad (5)$$

equation 4 can be rewritten as

$$\gamma(T) = \int_0^T (e^{t\mathbf{A}} \cdot \Delta \mathbf{E}) dt \quad (6)$$

which is equal to

$$\gamma(T) = (e^{T\mathbf{A}} - \mathbf{I}) \cdot \mathbf{A}^{-1} \cdot \Delta \mathbf{E} \quad (7)$$

where,

- $\gamma(T)$ = vector of time-integrated exposure at time T ($\text{hr}\cdot\text{kg}$);
- ΔE = vector of emission pulse E at $t=0$ (kg).

It turns out that the time-integrated exposure $\gamma(T)$ is given in terms of $(e^{T\mathbf{A}} - \mathbf{I})\mathbf{A}^{-1}$ which is the same term used in the calculation of $c(t)$, under the condition that $c(0) = 0$ in

the dynamic flux model. As a consequence, outcomes of dynamic flux models can be used in the assessment of the time-integrated potential impact at time t of an emission pulse Δm_i , released at $t = 0$.

Dynamic calculations in USES-LCA are established by implementing a separate routine that numerically solves the mass balance equations of the fate part of USES-LCA. The dynamic module of the flux model Simblebox 2.0 is used for this purpose (Brandes et al., 1996).

2.2 Time horizon dependent toxicity potentials

For humans, the TP for time horizon t is characterised by the outcomes of the human exposure assessment at time t and the effects assessment after a unit emission to an environmental compartment. For marine aquatic ecosystems, fresh water aquatic ecosystems, marine sediment ecosystems, fresh water sediment ecosystems and terrestrial ecosystems, the ratio of the predicted environmental concentration at time t and the outcome of the effects assessment are taken as the TP for time horizon t . For each of the six impact categories, five different TPs were calculated, related to the five initial emission compartments considered (air, fresh water, seawater, agricultural soil, and industrial soil in West Europe). Thus, for one substance 30 TPs can be calculated.

It is chosen to calculate TPs 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. Relatively short time horizons are appropriate if one is more concerned with potential toxic impacts during the next few decades. Longer time horizons are more appropriate if one is more concerned about potential impacts of toxic emissions during the next centuries. Substance-specific data needed in the USES-LCA calculations are taken from Huijbregts (1999).

3. Results & discussion

3.1 Potentials

Annexes I, II and III list the TPs of all 181 substances for the time horizons 20, 100 and 500 years, respectively. Table 1 gives for 11 substances the relative differences between TPs calculated for an infinite time horizon (Huijbregts, 1999) and the respective time horizons 20 years, 100 years and 500 years.

As can be derived from Table 1 and Annex I, II and III, the time-integrated exposure of inorganics other than metals and organic substances under study is in most cases virtually completed within 20 years. For persistent organic substances, such as endrin, the relative difference between TPs 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 years and 500 years relative differences with an infinite time horizon are negligible. Compared to the influence of parameter uncertainty on TPs

(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 TPs can be up to several orders of magnitude (Annexes and Table 1), indicating that there may be a large export of impacts to future generations. It also shows that the choice of a particular time horizon is important in the impact assessment of heavy metal emissions. TPs 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 (up to 10^8 years). The very long modelled residence times of the metals in the marine environment follow from the fact that burial in deep sediment is the only important removal process for metals in USES-LCA. If the metal is emitted to one of the soil compartments, time horizon dependent differences of the marine TPs further increase (Table 1). The reason is that complete 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., 1992; Van de Meent, 1990; 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 TPs markedly increase, as metal run-off from the soil may cause exposure in the fresh water environment over a very long time (see above). The slow run-off to the aquatic environment and leaching to deeper soil layers from the upper soil compartment of metals also cause significant time horizon dependent differences in terrestrial ecotoxicity potentials of metals.

Finally, human toxicity potentials (HTPs) of metals show substantial time horizon dependent differences. The 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 human exposure routes, 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.

Table 1: Comparison of TPs for an infinite time horizon with TPs for the time horizons 20 years, 100 years, and 500 years, respectively. Values are given as ratios. FAETP = Fresh water Aquatic EcoToxicity Potential; MAETP = Marine Aquatic EcoToxicity Potential; FSETP = Fresh water Sediment EcoToxicity Potential; MSETP = Marine Sediment EcoToxicity Potential; TETP = Terrestrial EcoToxicity Potential; HTP = Human Toxicity Potential; - = toxicity potential is negligible ($< 1 \cdot 10^{-15}$ 1,4-DCB-eq.).

Substance	CAS No.	Type	Initial emission compartments														
			Air			Fresh water			Seawater			Agricultural soil			Industrial soil		
			20y/∞	100y/∞	500y/∞	20y/∞	100y/∞	500y/∞	20y/∞	100y/∞	500y/∞	20y/∞	100y/∞	500y/∞	20y/∞	100y/∞	500y/∞
Cadmium	7439-92-1	FAETP	$6.4 \cdot 10^{-2}$	$1.8 \cdot 10^{-1}$	$5.6 \cdot 10^{-1}$	$8.7 \cdot 10^{-1}$	1.0	1.0	-	-	-	$1.8 \cdot 10^{-2}$	$1.3 \cdot 10^{-1}$	$5.3 \cdot 10^{-1}$	$1.8 \cdot 10^{-2}$	$1.3 \cdot 10^{-1}$	$5.3 \cdot 10^{-1}$
		MAETP	$3.4 \cdot 10^{-3}$	$2.0 \cdot 10^{-2}$	$1.2 \cdot 10^{-1}$	$1.9 \cdot 10^{-3}$	$1.9 \cdot 10^{-2}$	$1.2 \cdot 10^{-1}$	$3.2 \cdot 10^{-3}$	$2.2 \cdot 10^{-2}$	$1.3 \cdot 10^{-1}$	$2.3 \cdot 10^{-5}$	$1.2 \cdot 10^{-3}$	$3.7 \cdot 10^{-2}$	$2.3 \cdot 10^{-5}$	$1.2 \cdot 10^{-3}$	$3.7 \cdot 10^{-2}$
		FSETP	$6.3 \cdot 10^{-2}$	$1.8 \cdot 10^{-1}$	$5.6 \cdot 10^{-1}$	$8.6 \cdot 10^{-1}$	1.0	1.0	-	-	-	$1.7 \cdot 10^{-2}$	$1.3 \cdot 10^{-1}$	$5.3 \cdot 10^{-1}$	$1.7 \cdot 10^{-2}$	$1.3 \cdot 10^{-1}$	$5.3 \cdot 10^{-1}$
		MSETP	$6.0 \cdot 10^{-3}$	$2.7 \cdot 10^{-2}$	$1.2 \cdot 10^{-1}$	$4.6 \cdot 10^{-3}$	$3.1 \cdot 10^{-2}$	$1.4 \cdot 10^{-1}$	$7.8 \cdot 10^{-3}$	$3.3 \cdot 10^{-2}$	$1.4 \cdot 10^{-1}$	$5.6 \cdot 10^{-5}$	$2.2 \cdot 10^{-3}$	$4.3 \cdot 10^{-2}$	$5.6 \cdot 10^{-5}$	$2.2 \cdot 10^{-3}$	$4.3 \cdot 10^{-2}$
		TETP	$3.0 \cdot 10^{-2}$	$1.4 \cdot 10^{-1}$	$5.4 \cdot 10^{-1}$	-	-	-	-	-	-	$3.1 \cdot 10^{-2}$	$1.4 \cdot 10^{-1}$	$5.4 \cdot 10^{-1}$	$3.1 \cdot 10^{-2}$	$1.4 \cdot 10^{-1}$	$5.4 \cdot 10^{-1}$
		HTP	1.0	1.0	1.0	$4.1 \cdot 10^{-1}$	$4.9 \cdot 10^{-1}$	$5.5 \cdot 10^{-1}$	$2.3 \cdot 10^{-2}$	$6.7 \cdot 10^{-2}$	$1.7 \cdot 10^{-1}$	$3.1 \cdot 10^{-2}$	$1.5 \cdot 10^{-1}$	$5.4 \cdot 10^{-1}$	$2.7 \cdot 10^{-2}$	$1.3 \cdot 10^{-1}$	$5.0 \cdot 10^{-1}$
Lead	7439-92-1	FAETP	$3.7 \cdot 10^{-2}$	$4.9 \cdot 10^{-2}$	$8.0 \cdot 10^{-2}$	$8.6 \cdot 10^{-1}$	1.0	1.0	-	-	-	$9.8 \cdot 10^{-4}$	$7.5 \cdot 10^{-3}$	$4.0 \cdot 10^{-2}$	$9.8 \cdot 10^{-4}$	$7.5 \cdot 10^{-3}$	$4.0 \cdot 10^{-2}$
		MAETP	$3.8 \cdot 10^{-3}$	$2.1 \cdot 10^{-2}$	$1.3 \cdot 10^{-1}$	$1.9 \cdot 10^{-3}$	$2.0 \cdot 10^{-2}$	$1.5 \cdot 10^{-1}$	$3.3 \cdot 10^{-3}$	$2.3 \cdot 10^{-2}$	$1.5 \cdot 10^{-1}$	$1.3 \cdot 10^{-6}$	$6.9 \cdot 10^{-5}$	$2.8 \cdot 10^{-3}$	$1.3 \cdot 10^{-6}$	$6.9 \cdot 10^{-5}$	$2.8 \cdot 10^{-3}$
		FSETP	$3.6 \cdot 10^{-2}$	$4.9 \cdot 10^{-2}$	$8.0 \cdot 10^{-2}$	$8.5 \cdot 10^{-1}$	1.0	1.0	-	-	-	$9.3 \cdot 10^{-4}$	$7.5 \cdot 10^{-3}$	$4.0 \cdot 10^{-2}$	$9.3 \cdot 10^{-4}$	$7.5 \cdot 10^{-3}$	$4.0 \cdot 10^{-2}$
		MSETP	$6.8 \cdot 10^{-3}$	$3.2 \cdot 10^{-2}$	$1.4 \cdot 10^{-1}$	$5.3 \cdot 10^{-3}$	$3.8 \cdot 10^{-2}$	$1.7 \cdot 10^{-1}$	$9.0 \cdot 10^{-3}$	$4.1 \cdot 10^{-2}$	$1.7 \cdot 10^{-1}$	$3.4 \cdot 10^{-6}$	$1.5 \cdot 10^{-4}$	$3.7 \cdot 10^{-3}$	$3.4 \cdot 10^{-6}$	$1.5 \cdot 10^{-4}$	$3.7 \cdot 10^{-3}$
		TETP	$1.8 \cdot 10^{-3}$	$9.2 \cdot 10^{-3}$	$4.5 \cdot 10^{-2}$	-	-	-	-	-	-	$1.7 \cdot 10^{-3}$	$8.4 \cdot 10^{-3}$	$4.1 \cdot 10^{-2}$	$1.7 \cdot 10^{-3}$	$8.4 \cdot 10^{-3}$	$4.1 \cdot 10^{-2}$
		HTP	$5.2 \cdot 10^{-2}$	$6.2 \cdot 10^{-2}$	$1.0 \cdot 10^{-1}$	$3.3 \cdot 10^{-1}$	$4.2 \cdot 10^{-1}$	$5.1 \cdot 10^{-1}$	$2.7 \cdot 10^{-2}$	$9.0 \cdot 10^{-2}$	$2.3 \cdot 10^{-1}$	$1.7 \cdot 10^{-3}$	$8.3 \cdot 10^{-3}$	$4.1 \cdot 10^{-2}$	$1.6 \cdot 10^{-3}$	$8.2 \cdot 10^{-3}$	$4.0 \cdot 10^{-2}$
Chromium III	7440-47-3	FAETP	$3.3 \cdot 10^{-2}$	$4.2 \cdot 10^{-2}$	$6.4 \cdot 10^{-2}$	$8.6 \cdot 10^{-1}$	1.0	1.0	-	-	-	$6.7 \cdot 10^{-4}$	$5.2 \cdot 10^{-3}$	$2.8 \cdot 10^{-2}$	$6.7 \cdot 10^{-4}$	$5.2 \cdot 10^{-3}$	$2.8 \cdot 10^{-2}$
		MAETP	$3.5 \cdot 10^{-3}$	$2.0 \cdot 10^{-2}$	$1.1 \cdot 10^{-1}$	$1.9 \cdot 10^{-3}$	$2.0 \cdot 10^{-2}$	$1.4 \cdot 10^{-1}$	$3.3 \cdot 10^{-3}$	$2.3 \cdot 10^{-2}$	$1.4 \cdot 10^{-1}$	$9.1 \cdot 10^{-7}$	$4.8 \cdot 10^{-5}$	$1.9 \cdot 10^{-3}$	$9.1 \cdot 10^{-7}$	$4.8 \cdot 10^{-5}$	$1.9 \cdot 10^{-3}$
		FSETP	$3.3 \cdot 10^{-2}$	$4.2 \cdot 10^{-2}$	$6.4 \cdot 10^{-2}$	$8.6 \cdot 10^{-1}$	1.0	1.0	-	-	-	$6.4 \cdot 10^{-4}$	$5.1 \cdot 10^{-3}$	$2.8 \cdot 10^{-2}$	$6.4 \cdot 10^{-4}$	$5.1 \cdot 10^{-3}$	$2.8 \cdot 10^{-2}$
		MSETP	$6.2 \cdot 10^{-3}$	$2.9 \cdot 10^{-2}$	$1.2 \cdot 10^{-1}$	$5.1 \cdot 10^{-3}$	$3.5 \cdot 10^{-2}$	$1.6 \cdot 10^{-1}$	$8.6 \cdot 10^{-3}$	$3.9 \cdot 10^{-2}$	$1.6 \cdot 10^{-1}$	$2.3 \cdot 10^{-6}$	$9.7 \cdot 10^{-5}$	$2.4 \cdot 10^{-3}$	$2.3 \cdot 10^{-6}$	$9.7 \cdot 10^{-5}$	$2.4 \cdot 10^{-3}$
		TETP	$1.4 \cdot 10^{-3}$	$6.8 \cdot 10^{-3}$	$3.3 \cdot 10^{-2}$	-	-	-	-	-	-	$1.2 \cdot 10^{-3}$	$5.8 \cdot 10^{-3}$	$2.8 \cdot 10^{-2}$	$1.2 \cdot 10^{-3}$	$5.8 \cdot 10^{-3}$	$2.8 \cdot 10^{-2}$
		HTP	$5.2 \cdot 10^{-2}$	$5.7 \cdot 10^{-2}$	$8.1 \cdot 10^{-2}$	$4.3 \cdot 10^{-1}$	$5.3 \cdot 10^{-1}$	$5.9 \cdot 10^{-1}$	$2.6 \cdot 10^{-2}$	$8.2 \cdot 10^{-2}$	$2.1 \cdot 10^{-1}$	$1.2 \cdot 10^{-3}$	$5.8 \cdot 10^{-3}$	$2.8 \cdot 10^{-2}$	$1.1 \cdot 10^{-3}$	$5.7 \cdot 10^{-3}$	$2.8 \cdot 10^{-2}$
Benzene	71-43-2	FAETP	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0
		MAETP	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0
		FSETP	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0
		MSETP	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0
		TETP	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0
		HTP	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0
2,3,7,8-TCDD	1746-01-6	FAETP	$9.7 \cdot 10^{-1}$	1.0	1.0	$9.7 \cdot 10^{-1}$	1.0	1.0	$8.4 \cdot 10^{-1}$	1.0	1.0	$9.2 \cdot 10^{-1}$	1.0	1.0	$9.2 \cdot 10^{-1}$	1.0	1.0
		MAETP	$8.6 \cdot 10^{-1}$	1.0	1.0	$7.7 \cdot 10^{-1}$	1.0	1.0	$8.7 \cdot 10^{-1}$	1.0	1.0	$6.9 \cdot 10^{-1}$	1.0	1.0	$6.9 \cdot 10^{-1}$	1.0	1.0
		FSETP	$9.7 \cdot 10^{-1}$	1.0	1.0	$9.7 \cdot 10^{-1}$	1.0	1.0	$8.3 \cdot 10^{-1}$	1.0	1.0	$9.1 \cdot 10^{-1}$	1.0	1.0	$9.1 \cdot 10^{-1}$	1.0	1.0
		MSETP	$8.7 \cdot 10^{-1}$	1.0	1.0	$7.6 \cdot 10^{-1}$	1.0	1.0	$8.8 \cdot 10^{-1}$	1.0	1.0	$6.7 \cdot 10^{-1}$	1.0	1.0	$6.7 \cdot 10^{-1}$	1.0	1.0
		TETP	$9.7 \cdot 10^{-1}$	1.0	1.0	$8.8 \cdot 10^{-1}$	1.0	1.0	$8.2 \cdot 10^{-1}$	1.0	1.0	$9.9 \cdot 10^{-1}$	1.0	1.0	$9.9 \cdot 10^{-1}$	1.0	1.0
		HTP	$9.9 \cdot 10^{-1}$	1.0	1.0	$9.7 \cdot 10^{-1}$	1.0	1.0	$9.2 \cdot 10^{-1}$	1.0	1.0	$9.9 \cdot 10^{-1}$	1.0	1.0	$9.7 \cdot 10^{-1}$	1.0	1.0

Table 1 continued

Substance	CAS No.	Type	Initial emission compartments																	
			Air			Fresh water			Seawater			Agricultural soil			Industrial soil					
			20y/∞	100y/∞	500y/∞	20y/∞	100y/∞	500y/∞	20y/∞	100y/∞	500y/∞	20y/∞	100y/∞	500y/∞	20y/∞	100y/∞	500y/∞			
Atrazine	1912-24-9	FAETP	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0		
		MAETP	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	
		FSETP	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0
		MSETP	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0
		TETP	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0
		HTP	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0
Endrin	72-20-8	FAETP	8.1·10 ⁻¹	1.0	1.0	1.0	1.0	1.0	1.0	7.4·10 ⁻¹	1.0	1.0	6.6·10 ⁻¹	1.0	1.0	7.2·10 ⁻¹	1.0	1.0	1.0	
		MAETP	7.5·10 ⁻¹	1.0	1.0	7.5·10 ⁻¹	1.0	1.0	7.6·10 ⁻¹	1.0	1.0	3.6·10 ⁻¹	1.0	1.0	4.0·10 ⁻¹	1.0	1.0	1.0	1.0	
		FSETP	8.1·10 ⁻¹	1.0	1.0	1.0	1.0	1.0	7.5·10 ⁻¹	1.0	1.0	6.6·10 ⁻¹	9.9·10 ⁻¹	1.0	7.2·10 ⁻¹	1.0	1.0	1.0	1.0	
		MSETP	7.9·10 ⁻¹	1.0	1.0	7.9·10 ⁻¹	1.0	1.0	8.0·10 ⁻¹	1.0	1.0	4.1·10 ⁻¹	9.8·10 ⁻¹	1.0	4.5·10 ⁻¹	1.0	1.0	1.0	1.0	
		TETP	7.1·10 ⁻¹	1.0	1.0	6.8·10 ⁻¹	1.0	1.0	5.4·10 ⁻¹	9.8·10 ⁻¹	1.0	6.7·10 ⁻¹	1.0	1.0	7.3·10 ⁻¹	1.0	1.0	1.0	1.0	
		HTP	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0
Hexachlorobenzene	118-74-1	FAETP	9.6·10 ⁻¹	1.0	1.0	1.0	1.0	1.0	9.7·10 ⁻¹	1.0	1.0	9.4·10 ⁻¹	1.0	1.0	9.6·10 ⁻¹	1.0	1.0	1.0	1.0	
		MAETP	8.2·10 ⁻¹	1.0	1.0	8.2·10 ⁻¹	1.0	1.0	8.2·10 ⁻¹	1.0	1.0	6.5·10 ⁻¹	1.0	1.0	6.8·10 ⁻¹	1.0	1.0	1.0	1.0	
		FSETP	9.7·10 ⁻¹	1.0	1.0	1.0	1.0	1.0	9.6·10 ⁻¹	1.0	1.0	9.3·10 ⁻¹	1.0	1.0	9.6·10 ⁻¹	1.0	1.0	1.0	1.0	
		MSETP	7.9·10 ⁻¹	1.0	1.0	7.9·10 ⁻¹	1.0	1.0	8.3·10 ⁻¹	1.0	1.0	6.0·10 ⁻¹	1.0	1.0	6.3·10 ⁻¹	1.0	1.0	1.0	1.0	
		TETP	5.5·10 ⁻¹	1.0	1.0	5.5·10 ⁻¹	9.8·10 ⁻¹	1.0	5.5·10 ⁻¹	9.8·10 ⁻¹	1.0	9.4·10 ⁻¹	1.0	1.0	9.5·10 ⁻¹	1.0	1.0	1.0	1.0	
		HTP	9.0·10 ⁻¹	1.0	1.0	9.4·10 ⁻¹	1.0	1.0	9.1·10 ⁻¹	1.0	1.0	9.5·10 ⁻¹	1.0	1.0	8.2·10 ⁻¹	1.0	1.0	1.0	1.0	
1,2-Dichloroethane	107-06-2	FAETP	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	
		MAETP	9.9·10 ⁻¹	1.0	1.0	9.9·10 ⁻¹	1.0	1.0	9.9·10 ⁻¹	1.0	1.0	9.9·10 ⁻¹	1.0	1.0	9.9·10 ⁻¹	1.0	1.0	1.0	1.0	
		FSETP	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0
		MSETP	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0
		TETP	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0
		HTP	1.0	1.0	1.0	1.0	1.0	1.0	9.9·10 ⁻¹	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0
Carcinogenic PAHs		FAETP	9.6·10 ⁻¹	1.0	1.0	1.0	1.0	1.0	9.1·10 ⁻¹	1.0	1.0	9.1·10 ⁻¹	1.0	1.0	9.1·10 ⁻¹	1.0	1.0	1.0	1.0	
		MAETP	9.3·10 ⁻¹	1.0	1.0	8.5·10 ⁻¹	1.0	1.0	9.3·10 ⁻¹	1.0	1.0	7.1·10 ⁻¹	1.0	1.0	7.1·10 ⁻¹	1.0	1.0	1.0	1.0	
		FSETP	9.6·10 ⁻¹	1.0	1.0	8.8·10 ⁻¹	1.0	1.0	9.1·10 ⁻¹	1.0	1.0	9.0·10 ⁻¹	1.0	1.0	9.0·10 ⁻¹	1.0	1.0	1.0	1.0	
		MSETP	9.5·10 ⁻¹	1.0	1.0	8.6·10 ⁻¹	1.0	1.0	9.5·10 ⁻¹	1.0	1.0	7.0·10 ⁻¹	1.0	1.0	7.0·10 ⁻¹	1.0	1.0	1.0	1.0	
		TETP	9.8·10 ⁻¹	1.0	1.0	9.0·10 ⁻¹	1.0	1.0	8.9·10 ⁻¹	1.0	1.0	9.8·10 ⁻¹	1.0	1.0	9.8·10 ⁻¹	1.0	1.0	1.0	1.0	
		HTP	1.0	1.0	1.0	9.8·10 ⁻¹	1.0	1.0	9.8·10 ⁻¹	1.0	1.0	9.8·10 ⁻¹	1.0	1.0	9.2·10 ⁻¹	1.0	1.0	1.0	1.0	
Nitrogen dioxide	7783-06-4	HTP	1.0	1.0	1.0	x	x	x	x	x	x	x	x	x	x	x	x	x	x	

3.2 USES-LCA

Although the model calculations may give a first impression of the relative impact of organic and inorganic pollutants for the time horizons 20, 100 and 500 years, both dynamic and steady state USES-LCA calculations may suffer from many uncertainties. In this respect, model uncertainties related to the application of USES-LCA for metals are particularly important. Important model uncertainties and possible model improvement options for metals will be discussed below.

First of all, a terrestrial vegetation compartment is not implemented in USES-LCA. Although it is expected that the lack of a terrestrial vegetation compartment does not change the fate of organic substances to large extent (Severinsen & Jager 1998; Huijbregts, 1999), this may not be the case for all metals. Removal of metals by harvesting may be a significant removal process for agricultural and natural soils (Moolenaar & Lexmond, 1998; Cleven et al., 1992; Fraters & Van Beurden, 1993; De Vries & Bakker, 1998). A first indication of the influence of removal of metals from agricultural soils on the TPs of Cd, Cu, and Zn is given by implementing biological uptake rate constants for these metals in the agricultural soil compartment (Moolenaar & Lexmond, 1998; Moolenaar & Beltrami, 1998). Changes in the TPs of Cd, Cu and Zn are up to a factor 3 for all time horizons involved. Compared to the influence of parameter uncertainty related to the application of USES-LCA (Huijbregts et al., 2000b), metal removal by harvesting does not strongly alter the TPs.

Another example of model uncertainty in the current metal calculations is that the subcompartmental differences in fate and corresponding effects are not taken into account in USES-LCA. 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 partitioning of metals is an important source of uncertainty for metal TPs (Huijbregts et al., 2000b). Partitioning in turn strongly depends on differences in environmental characteristics. As it is extremely difficult to derive 'representative' K_p -values for metals in generic box models, moving to spatially explicit models may be a useful exercise in the fate, exposure and effect assessment of metals (e.g. Fraters & Van Beurden, 1993; Van den Hout et al., 1998; Stolwijk et al., 1998; De Vries & Bakker, 1998; De Vries et al., 1998). For some metals, such as Pb, Cd, Zn, Ni, Cu and Cr, it appears that for this purpose enough site-specific information on the European scale is available (De Vries & Bakker, 1998; De Vries et al., 1998). 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 irreversibly adsorbed forms to the soil matrix (Harmsen, 1992; De Vries & Bakker, 1998; Otte et al., 1999) and the site dependent uptake of metals by organisms¹ (Peijnenburg et al., 1997, 1999). Further research in LCA context is strongly recommended here.

Finally, the fate analysis of geochemically reactive metals in the marine environment needs improvement. For the majority of the metals involved, oceanic residence times calculated by Goldberg (1965), are in the same order of magnitude as residence times

¹ If (differences in) bioavailability of metals is to be taken into account in the model calculations, no-effect concentrations should not be specified as soil concentrations but rather as internal body concentrations.

calculated by USES-LCA. However, Goldberg (1965) calculated substantial higher oceanic residence times for Cd, Sn and Zn than USES-LCA (up to 2.5 orders of magnitude). A reason for the differences found may be the use of a different set of input parameters by Goldberg (1965) compared to USES-LCA, such as metal-specific suspended matter K_p -values. Secondly, Goldberg (1965) calculates a much lower residence time for Be than USES-LCA (Table 2). As Be ions are expected to be rapidly hydrolysed at the pH of seawater and incorporated into minerals, such as ferro-manganese nodules (Riley, 1971), and this removal route is not included in USES-LCA, it is likely that current marine toxicity potentials of Be are largely overestimated. Caution is thus needed, if in LCA case studies Be appear to be important for potential toxic impacts in the marine environment.

Table 2: Residence times of metals in the marine aquatic compartment calculated with USES-LCA and given in Goldberg (1965)

Metal	Residence time (τ) in years	
	USES-LCA	Goldberg (1965)
Antimony	$3.5 \cdot 10^4$	$3.5 \cdot 10^5$
Arsene	$1.3 \cdot 10^4$?
Barium	$9.8 \cdot 10^4$	$8.4 \cdot 10^4$
Beryllium	$1.6 \cdot 10^5$	$1.5 \cdot 10^2$
Cadmium	$1.6 \cdot 10^3$	$5.0 \cdot 10^5$
Chroom	$1.1 \cdot 10^3$	$3.5 \cdot 10^2$
Cobalt	$3.3 \cdot 10^4$	$1.8 \cdot 10^4$
Copper	$3.1 \cdot 10^3$	$5.0 \cdot 10^4$
Lead	$8.1 \cdot 10^2$	$2.0 \cdot 10^3$
Mercury	$1.2 \cdot 10^3$	$4.2 \cdot 10^4$
Molybdenum	$1.2 \cdot 10^5$	$5.0 \cdot 10^5$
Nickel	$1.7 \cdot 10^4$	$1.8 \cdot 10^4$
Selenium	$2.4 \cdot 10^5$?
Thallium	$8.8 \cdot 10^4$?
Tin	$9.5 \cdot 10^2$	$1.0 \cdot 10^5$
Vanadium	$2.4 \cdot 10^4$	$1.0 \cdot 10^4$
Zinc	$1.8 \cdot 10^3$	$1.8 \cdot 10^5$

? = residence time not given in Goldberg (1965)

4. Conclusions

Dynamic USES-LCA calculations may give a first impression about the relative importance of organic and inorganic pollutants for 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 TPs, while time horizon dependent differences remain within 0.5 order of magnitude for TPs of other inorganics than metals and organic substances under study. 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 geochemically reactive chemicals, such as Be, in the marine environment and inclusion of spatial dependency of metal behaviour needs major improvement.

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