

USEtox fate and ecotoxicity factors for comparative assessment of toxic emissions in life cycle analysis: sensitivity to key chemical properties

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Received: 30 November 2010 / Accepted: 28 March 2011 / Published online: 8 June 2011
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Abstract

Purpose The USEtox model was developed in a scientific consensus process involving comparison of and harmonization between existing environmental multimedia fate models. USEtox quantitatively models the continuum from chemical emission to freshwater ecosystem toxicity via chemical-specific characterization factors (CFs) for Life Cycle Impact Assessment (LCIA). This work provides understanding of the key mechanisms and chemical parameters influencing fate in the environment and impact on aquatic ecosystems.

Materials and method USEtox incorporates a matrix framework for multimedia modeling, allowing separation of fate, exposure, and ecotoxicity effects in the determi-

nation of an overall CF. Current best practices, such as incorporation of intermittent rain and effect factors (EF) based on substance toxicity across species, are implemented in the model. The USEtox database provides a dataset of over 3,000 organic chemicals, of which approximately 2,500 have freshwater EFs. Freshwater characterization factors for these substances, with a special focus on a subset of chemicals with characteristic properties, were analyzed to understand the contributions of fate, exposure, and effect on the overall CFs. The approach was based on theoretical interpretation of the multimedia model components as well as multidimensional graphical analysis.

Electronic supplementary material The online version of this article (doi:10.1007/s11367-011-0294-6) contains supplementary material, which is available to authorized users.

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Results and discussion For direct emission of a substance to water, the EF strongly controls freshwater ecotoxicity, with a range of up to 10 orders of magnitude. In this release scenario, chemical-specific differences in environmental fate influence the CF for freshwater emissions by less than 2 orders of magnitude. However, for an emission to air or soil, the influence of the fate is more pronounced. Chemical partitioning properties between water, air, and soil may drive intermedia transfer, which may be limited by the often uncertain, media-specific degradation half-life. Intermedia transfer may be a function of landscape parameters as well; for example, direct transfer from air to freshwater is limited by the surface area of freshwater. Overall, these altered fate factors may decrease the CF up to 8 orders of magnitude.

Conclusions This work brings new clarity to the relative contributions of fate and freshwater ecotoxicity to the calculation of CFs. In concert with the USEtox database, which provides the most extensive compilation of CFs to date, these findings enable those undertaking LCIA to understand and contextualize existing and newly calculated CFs.

Keywords Characterization factors · Fate modeling · Freshwater ecotoxicity · Life Cycle Impact Assessment · Model comparison · USEtox

1 Introduction

In Life Cycle Impact Assessment (LCIA), the emissions that occur from the processes involved in the life cycle of a product are translated (characterized) into their potential impacts on the environment. This characterization of impact addresses a diverse set of environmental impacts at a range of scales (Hauschild 2005). Characterization factors for chemical emissions are calculated with the use of environmental multimedia models, and several such models exist for use in LCIA (e.g., McKone et al. 2001; Pennington et al. 2005, 2006; van Zelm et al. 2009). The models vary on central points in their scope and modeling principles, and hence also in terms of the characterization factors they produce (Dreyer et al. 2003; Pant et al. 2004). An emission inventory for the life cycle of a product can easily contain several hundred different substances, many of which have the potential to cause toxicity to humans or ecosystems when released to the environment. However, the existing characterization models for use in LCIA typically have CFs published for less than 1,000 substances. The LCA practitioner who wishes to include the chemical-related impacts in the environmental evaluation of products thus faces the situation of having large variation in available CFs and finding that many substances lack CFs altogether.

To support a more robust inclusion of freshwater toxicological impacts in LCA, a scientific consensus model

for characterization modeling of these impacts was developed under the UNEP-SETAC Life Cycle Initiative¹ (<http://lcinitiative.unep.fr>). The model, USEtox™, was developed based on comparisons of existing models and on recommendations from a series of workshops (Jolliet et al. 2006; Ligthart et al. 2004; McKone et al. 2006). It offers a parsimonious, robust, and transparent approach to deriving chemical-specific freshwater ecotoxicological impacts per unit mass released. The process leading to USEtox is described in Hauschild et al. (2008), and the characterization factors for several thousand substances are documented in Rosenbaum et al. (2008). The main advantages of USEtox™ are that it provides CFs for a larger chemical coverage than previous models, including for substances that have not been previously calculated, and a framework in which users may calculate new CFs.

Several efforts have been made to understand chemical fate in multimedia models (e.g., Fenner et al. 2005; Margni et al. 2004), and to predict intake fractions and human exposure (Bennett et al. 2002; Pennington et al. 2005). However, freshwater ecotoxicity has received less attention, and there is a need to explore how chemical properties affect fate and hence the resulting characterization factors in this domain. This paper identifies critical mechanisms for these CFs, covering the continuum from chemical emission to ecotox effect. While the effect factor has a clear role in determining characterization factors, identifying situations in which the fate factor may mitigate or exacerbate a chemical impact is less clear. Therefore, this paper addresses the following:

1. provide details on the basis of calculations for fate, exposure, and freshwater ecotoxicological factors in USEtox; and
2. discuss the relative influences of the fate, including intermedia transfer, and effect factors on overall freshwater ecotoxicity and the final characterization factor.

These issues will be illustrated through examination of approximately 2,500 substances, with specific examples from five chemicals with very different properties. The

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findings presented herein are relevant to LCA or other comparative chemical assessments, for they provide a means to understand the interplay between chemical properties, emission compartment, and ultimate impacts.

2 Materials and methods

2.1 Framework

USEtox™ adopts the principles of multimedia mass balance modeling (Mackay 2002), simulating the behavior of chemicals released from the technosphere, e.g., from a manufacturing facility or waste treatment plant, to the environment as the net result of mass flows between a suite of well-mixed, homogeneous compartments. The model accounts for direct exposure of freshwater and marine ecosystems at various spatial scales by applying the concept of spatial scale nesting (Brandes et al. 1996). USEtox distinguishes emissions in six main urban and continental environmental compartments (Fig. S1 and Table S1 of the supporting information) and accounts for possible feedback of a chemical from the global scale as described by Margni et al. (2004).

USEtox is structured in a matrix framework composed of a series of matrices combining fate with exposure and effect (Rosenbaum et al. 2007). Characterization factors ($CF_i^{\text{freshwater ecotox}}$, [PAF m³ day/kg_{emitted}]) represent the freshwater ecotoxicological impacts of chemicals per mass unit of chemical emitted, where the impact is quantified as the potentially affected fraction (PAF) of species. The characterization factors can be expressed as the multiplication of four factors. The first three terms describe the transport and exposure of a substance: the fraction transferred from emission compartment i to freshwater ($f_{i,w}$, [-]), the environmental fate factor in freshwater ($FF_{w,w}$ [kg_{in water}/(kg_{emitted}/day)=day]), and the exposure factor, i.e., the dissolved and bioavailable fraction (XF_w , [-]). The final term, the effect factor, describes the ecotoxicological impact for freshwater ecosystems (EF_w , [PAF m³/kg_{in water}]):

$$CF_i^{\text{freshwater ecotox}} = f_{i,w} \times FF_{w,w} \times XF_w \times EF_w \quad (1)$$

For ecosystem damage, the characterization factor CF thus links an emission to the temporally and spatially integrated increase in the affected fraction of species due to an emission into a specific compartment, expressed as [PAF m³ day/kg_{emitted}].

In the matrix framework of Rosenbaum et al. (2007), fate factors express the resident mass [kilogram] per unit of emission [kilogram day⁻¹], yielding an overall dimension of [day]. Persistence of a substance in water, for an emission to

the water compartment, is indicated by the fate factor $FF_{w,w}$. The tendency of a chemical to be transported into freshwater after an emission into compartment i is represented $FF_{w,i}$. The latter type of fate factor can be viewed as the product of an intercompartment transfer fraction [$f_{i,w}$, the transfer from compartment i to freshwater] and the residence time in water, $FF_{w,w}$. Exposure factors, XF_w [-], represent the bioavailability of the chemicals to aquatic organisms. For aquatic systems, the XF is calculated as the truly dissolved fraction of a substance.

2.1.1 Air compartment and rain

Chemicals in the urban air compartment are either removed via degradation or transfer to rural air via advection, to rural soil via deposition, and to rural surface water via deposition or runoff from the surface, which is considered to be 100% paved. Most existing multimedia fate models treat wet deposition as a continuous process (constant drizzle). Several studies have shown that this approach may seriously underestimate exposure via air for chemicals with small air-water partition coefficients (Hertwich 2001). This problem was solved in USEtox by implementing the routine published by Jolliet and Hauschild (2005) to describe intermittent wet atmospheric deposition.

2.2 Freshwater ecotoxicity effect factors

The effect factor expresses the ability of a substance to cause toxic effects to the exposed freshwater ecosystems. The elements of the effect factor matrix for ecotoxicity (EF_w) directly relate the dissolved concentration in the freshwater compartment of the environment to the species response, represented as the fraction of the species which are potentially affected.

These elements are calculated from effect concentrations obtained by laboratory testing of the toxicity of the substance with respect to different species in different phyla of the aquatic ecosystem. Historically, the characterization modeling of freshwater ecotoxicity has used the reciprocal of the predicted no effect concentration (PNEC) as the effect factor. While the conservative nature of the PNEC concept suits the purpose of chemical risk assessment, recent expert workshops (Diamond et al. 2010; Jolliet et al. 2006; Ligthart et al. 2004) have recommended that the purpose of LCIA is served better with more robust and less conservative effect parameters. The average toxicity, the HC50, based on the geometric mean of the EC50s of the species measured, showing the potentially affected fraction of species exposed above their chronic EC50 value, was found suitable (Larsen and Hauschild 2007a; Payet 2004; Payet and Jolliet 2004; Pennington et al. 2004, 2006).

Figure 1 illustrates the HC50 approach to toxicity using the example of malathion, an insecticide. This figure is based on chronic ecotoxicity data (EC50s) from 16 species covering five different phyla and compares several approaches to characterizing ecotoxicity (see Annex S2.1 of the supporting information). In Fig. 1, the left column shows the EC50s at the species level, and the second column shows the HC50s at the phyla level. The last three columns show PNECs and HC50s for three subdatasets, calculated by applying a safety factor of 10 to the EC50s for the most sensitive species. The PNEC is strongly dependent on the species tested: depending on whether *Daphnia magna* (the most sensitive species) and *Hesperoperla pacifica* (the second most sensitive species) are included in the data, the PNEC data can vary by 1 or 2 orders of magnitude. In contrast, the HC50 for these subsets varies only by a factor of 1.5. Using HC50 in LCA enables a more robust derivation of freshwater ecotoxicological effect factors because it is less dependent on the species tested than the PNEC or on safety factors.

In keeping with the recommendations to use a more robust effect parameter, an effect-based chronic PAF approach has been retained as best practice for comparative assessment, leading to the adoption of the following definition of freshwater ecotoxicological effect factor (EF) in USEtox:

$$EF = \frac{0.5}{HC50_{EC50}} \quad (2)$$

Species selection for calculation of HC50s should in general aim for the highest physiological variability, for as many species as possible, representing as many taxonomic

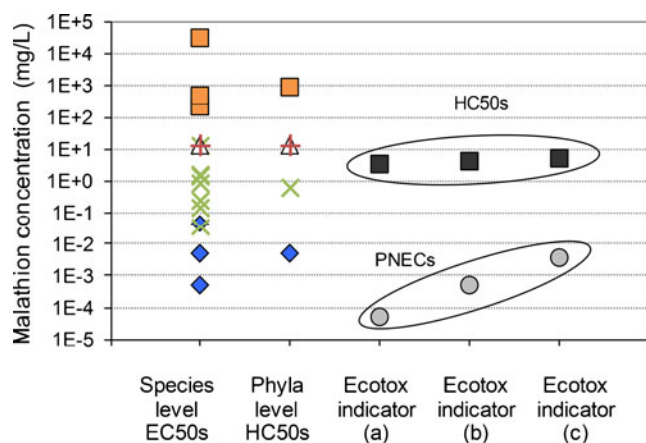


Fig. 1 EC50s, HC50s, and PNECs for the insecticide malathion, illustrating the robustness of the HC50 to individual species testing. In the left two columns of the figure, EC50s from 16 species are reported, and HC50s among 5 phyla are shown (red + Plant; open triangle Nematoda; orange square Mollusca; green × Chordata; blue diamond Arthropod). The most sensitive species are *D. magna* and *H. pacifica*. In the right three columns, HC50s and PNECs are reported for **a** all species tested, **b** all species with *D. magna* removed, and **c** all species with *H. pacifica* and *D. magna* removed. The PNEC is highly sensitive to testing of individual species, while the HC50 remains stable

groups as possible. In practice, USEtox draws on two main sources: van Zelm et al. (2007) use all species available, grouped into four taxa. In the AMI method, Payet (2004) also uses all species available and requires at least three EC50s from three different phyla to reflect the variability of the physiology and ensure a minimum diversity of biological responses. The factor 0.5 derives from the working point on the PAF curve corresponding to the HC50 value, which indicates that the potentially affected fraction of species is 50% (Annex S2.2 of supporting information).

A study by Larsen and Hauschild (2007b) indicates that unequal representation of data points (i.e., EC50 values) from different taxonomy groups at three trophic levels (represented by algae, crustacean, and fish) may introduce a bias in the estimation of the effect factor (also see, e.g., Aldenberg et al. 2002 and Forbes and Calow 2002). In its aim for best estimates suited for the comparative framework of LCIA, it might be argued that USEtox should make a conscious choice to first calculate separate averages for each taxonomic group. Currently, HC50 values are calculated on a species level, taking the geometric mean of all available species, mainly because chemicals have only been tested on a limited number of species (Rosenbaum et al. 2008). In addition, the USEtox aquatic ecotoxicological characterization factors have been specified as interim if the corresponding effect factors were based on species toxicity data covering less than three different taxa. If desired, geometric means on the various taxonomic groups can be used for sensitivity studies.

2.3 Chemical-specific input data

To illustrate the functioning of the model, different sets of data have been used. First, the USEtox model results have been analyzed for substances in the USEtox database, which provides data that (a) are consistent, (b) are drawn from recognized datasets, and (c) cover as many chemicals as possible for which characterization factors can be computed (Huijbregts et al. 2010). This database contains information on over 3,000 substances, with approximately 2,500 substances having freshwater ecotox characterization factors (e.g., Fig. 2). Second, a set of five well-known substances with widely different properties has been selected to illustrate quantitatively the main factors influencing fate, exposure, effect, and final characterization factors (Table 1). (Corresponding fate and characterization factors are tabulated in Annex S3 of the supporting information.)

3 Results and discussion

Results are first presented for direct emissions to freshwater. Emissions to other environmental compartments can also

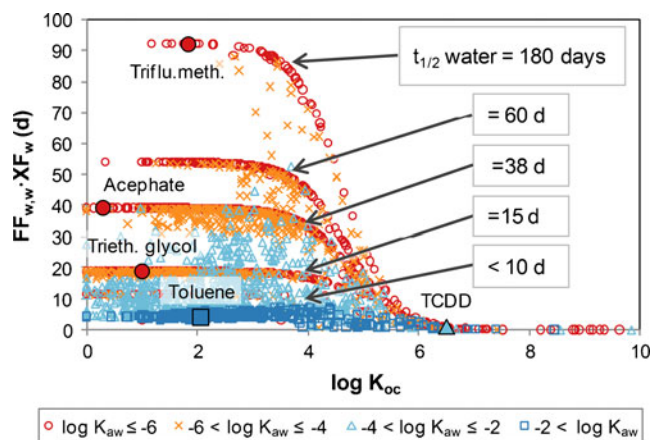


Fig. 2 Product of fate factor and exposure factor in the freshwater compartment ($FF_{w,w} \cdot XF_w$) as a function of $\log K_{oc}$ for 3,073 organic substances. Data are grouped according to the substance air–water partitioning coefficient ($\log K_{aw}$), and half-life regimes in water are indicated

contribute to the exposure of aquatic ecosystems; therefore, the fraction of an emission to soil that finds its way to freshwater via soil runoff is considered next, followed by emissions to air that enter water via atmospheric deposition to soil and water. Finally, the overall characterization factors are presented.

3.1 Fate and exposure in water

In the model, the bioavailable mass of chemical dissolved in water per unit of emission (expressed as the residence time of chemical dissolved in water) is the product of the fate factor in water for an emission to water, $FF_{w,w}$, and the dissolved fraction, XF_w (see Fig. 2).

Four removal processes affect the dissolved mass of a chemical in water: adsorption/sedimentation, volatilization, degradation, and advective transport out of the water compartment. Figure 2 shows how the fate factor of a chemical in the dissolved phase of the freshwater compartment is reduced at high K_{oc} , due to adsorption to particulates which removes the chemical from the dissolved phase (e.g., TCDD). Chemicals with high air–water partition coefficients also have low residence times and thus a

low fate factor in water, due to rapid volatilization (e.g., toluene: $K_{aw}=0.28$). The combined fate and exposure factor is further limited by a combination of substance-specific degradation half-life and the hydraulic residence time in the freshwater compartment (143 days), which is determined by the default landscape factors used in USEtox (Table S1, supporting information). Note that the strong influence of the chemical's hydrophobicity on the combined fate and exposure factor (resulting in near-zero values for $\log K_{oc}>6$) in Fig. 2 is caused by the equilibrium partitioning from water to suspended matter, followed by the subsequent removal to the sediment by deposition of particles.

Provided that $\log K_{oc}$ is <5 , the variation of the fate and exposure factor in the dissolved phase of the water compartment lies within 2 orders of magnitude. For substances with very high $\log K_{oc}$, the fate factor could be further reduced by several orders of magnitude, a variation that propagates to the characterization factor (Fig. S3 of the supporting information). The supporting information also details the residence time ($FF_{w,w}$) and the dissolved fraction (XF_w) separately, illustrating the factors which most strongly influence them (Figs. S4 and S5).

3.2 Fate in soil and transfer to water

The extent of transfer from soil to surface water is the net result of competition between the four main removal mechanisms from soil: degradation, volatilization, leaching to deeper layers of soil, and runoff to surface water. For surface water, only the chemical mass dissolved in (pore) water is modeled as available for taking part in physical and chemical processes. The more hydrophobic chemicals like TCDD partition to the immobile particulate phase, which results in a decreased tendency to be removed from the soil compartment by degradation, volatilization, or leaching. An exception to this is the runoff process, which in this model includes soil erosion. In this case, hydrophobic, sorbed chemicals are transferred from soil to water with eroding particles.

Figure 3 presents the transfer fraction from soil to water ($f_{s,w}$) as a function of the $\log K_{oc}$, showing that only nonsorbing, mobile chemicals ($\log K_{oc}<4$) are transferred from soil to water in significant amounts. Degradation in the

Table 1 Environmentally relevant chemical properties of selected substances: partition coefficients for octanol–water, octanol–carbon, and air–water; half-lives in air, soil, and water; and aquatic ecotox effect factor (Huijbregts et al. 2010)

Substance	K_{ow} (–)	K_{oc} (L kg ⁻¹)	K_{aw} (–)	$t_{1/2}$ air (day)	$t_{1/2}$ soil (day)	$t_{1/2}$ water (day)	EF (PAF m ³ kg ⁻¹)
Acephate	1.4E–01	2.0E+00	2.1E–11	0.96	75	38	1.6E+01
TCDD	6.3E+06	3.2E+06	2.1E–03	8.3	360	180	5.6E+06
Toluene	5.4E+02	1.2E+02	2.8E–01	1.8	30	15	1.4E+01
Triethylene glycol	1.8E–02	1.0E+01	1.1E–08	0.29	30	15	2.1E–02
Triflurosulfuron methyl	8.7E+03	6.9E+01	1.7E–11	2.8	360	180	4.5E+02

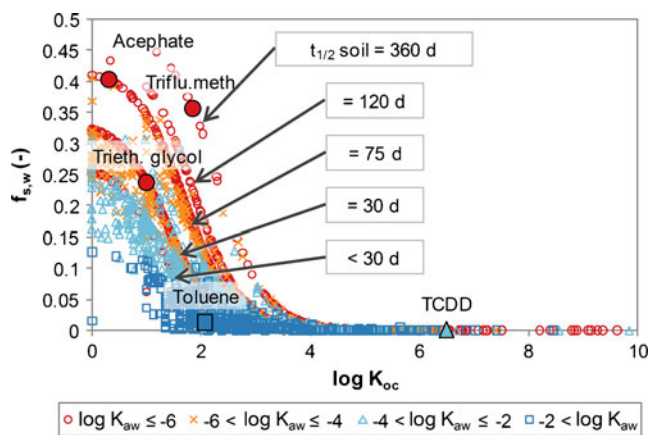


Fig. 3 Transfer fraction from soil to water ($f_{s,w}$) as a function of $\log K_{oc}$ for 3,073 organic substances. Data are grouped according to the substance air–water partitioning coefficient ($\log K_{aw}$), and the soil half-life regimes are indicated

soil competes with the transfer to the water such that only chemicals with the highest high half lives in soil have a high soil to water transfer fraction (e.g., triflusulfuron methyl or acephate). Chemicals with high K_{aw} , such as toluene, are volatilized from the soil. As a result, their soil fate factors, as well as their transfer fraction to water, are reduced. Based on typical values for a temperate climate, USEtox assumes that half of net precipitation onto soils is evaporated, with the remaining half being split equally between water runoff and water infiltration. The latter implies that the overall fraction transferred from soil to water is limited to 50%, as nonvolatile, hydrophilic chemicals are transported to freshwater via surface runoff, but there is a competition with removal via leaching to deep soil or groundwater, which removes mobile chemicals from the upper soil compartment.

Figure S6 (supporting information) provides the resulting fate and exposure factor from soil to freshwater, i.e., the multiplication of the transfer factor from soil to water by the fate and exposure factor in water from Fig. 2.

3.3 Fate in air and transfer to soil and water

The extent of transfer from air to soil is determined by a competition between three main removal mechanisms in the air compartment: degradation in air, advection to the air in the global box (where the soil surface is limited), and deposition either to soil or to surface water and oceanic water bodies.

The transfer rate between air and soil primarily depends on deposition and degradation in air (Fig. 4). At $\log K_{aw} > -4$, chemicals tend to remain in air (e.g., toluene), and removal by precipitation is low, such that only a very limited fraction of the chemicals are deposited to soil. At low K_{aw} , the fraction deposited increases as the half-life in air increases (e.g., triflusulfuron methyl). The upper bound of the overall

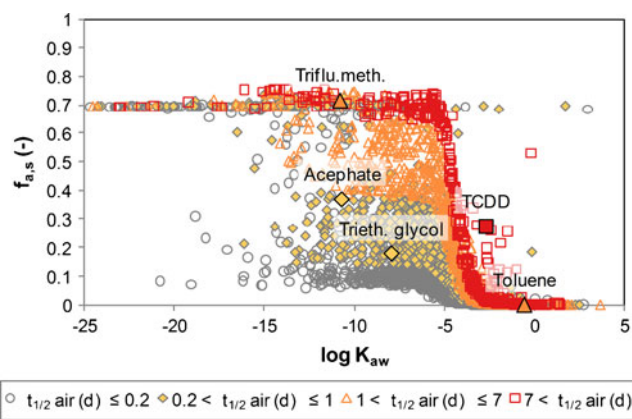


Fig. 4 Transfer fraction from air to soil ($f_{a,s}$) as a function of $\log K_{aw}$ for 3,073 organic substances. Data are grouped according to the half-life of the substance in air (days)

deposited fraction is set by the share of soil in the total surface area (11% of the continental box is ocean and freshwater: Table S1 in supporting information), and the fraction advected to the global box, which increases with the chemical residence time in air. Deposition to soil and fresh water in the global box is restricted by the fact that two thirds of the area in the global box is ocean. Wet removal by intermittent rain is responsible for the high fraction transferred at low K_{aw} . Fig. S7 shows the overestimation of the deposition rate from air to soil for hydrophilic chemicals when precipitation is modeled as a continuous (e.g., acephate and triethylene glycol).

The direct transfer from air to surface freshwater ($f_{a,w}$) also depends on K_{aw} , as was the case for $f_{a,s}$, but deposition is limited by the fact that freshwater covers only 2.7% of the area in the continental box, and 0.9% in the global box. Therefore, the transfer from air to freshwater will mainly occur via the soil compartment to water. This will only be important for substances with a high transfer to soil ($\log K_{aw} < -4$ and $t_{1/2}(\text{air}) > 1$ day), and a high transfer fraction from soil to water ($\log K_{oc} < 4$). As a result, only a small subset of substances has an air to surface water transfer fraction higher than 20% (Fig. S8, supporting information).

Comparing results in Fig. 2 to Figs. 3 and 4, it is clear that the possible range of the transfer fractions, $f_{i,w}$ (see Figs. 3 and 4) is as wide as the range of the fate factors in water, $FF_{w,w} \cdot XF_w$ (see Fig. 2). Hence, intermedia transfer strongly enhances the variation of characterization factors between substances.

3.4 Freshwater ecotoxicity effect and characterization factors

In comparison to the other factors in Eq. 1, the effect factor (EF) shows a very large variation among the substances covered by the USEtox database, with up to 10 orders of

magnitude, as visible from Fig. 5. The variation in EF therefore explains a large part of the variation in CFs among the substances for freshwater ecotoxicity after emission to freshwater.

The characterization factors in Fig. 5a have been calculated as the product of the effect factor on the x-axis and the combined fate and exposure factors (different colors) according to Eq. 1. In most cases, the fate factor changes the characterization factor by a maximum of 2

orders of magnitude, except for a few substances with high K_{oc} (Fig. S3, supporting information).

When considering a transfer to water from an emission to soil (see Fig. 5b) or air (see Fig. 5c), the characterization factor is reduced, and the combined exposure and fate factor plays a larger role. In this case, the fate and exposure factors generate, for a given EF, up to 8 orders of magnitude variation among the substances, which is similar to the variation that can be caused by the effect factors themselves. Overall, the 2,498 substances in Fig. 5 show a variation of 10–12 orders of magnitude in their $CF_i^{freshwater\ ecotox}$ for emissions to air or water.

4 Conclusions

With the development of the USEtox consensus model and publication of the USEtox characterization factors, a step forward has been made in addressing the challenges facing the LCA practitioner who wishes to include impacts from chemical emissions in a study. Freshwater ecotox characterization factors are available for close to 2,500 substances (www.usetox.org), a coverage exceeding that of any of the previous models. This article helps USEtox users understand the main characteristics of substances that drive the characterization factors for freshwater ecotoxicity. Specifically, the practitioner should focus on substances with high characterization and/or high effect factors. Classically, substances with high emission volume and high EF have been prioritized in the inventory stage. USEtox thus allows users to improve data collection efforts by focusing on the most important chemicals. If necessary, practitioners can calculate, check, and understand characterization factors for new chemicals.

These results show the influence of partition properties between water, air, and soil, the degradation half-life in various media, and the treatment of intermittent rain in the modeling of freshwater ecotoxicological effect. Among the influential input data, half-lives in water, air, and soil, as well as ecotoxicological effect factors, have high uncertainty. If uncertainties in life cycle impact assessments are to be reduced, improving the quality of these data is a priority. With the aim of introducing more ecosystem relevance (reflecting structure and function) in the averaging approach of the HC50, and thus improving the effect factor, the trophic level approach of Larsen and Hauschild (2007b) may be further investigated. This approach could be coupled with analysis and modeling of bioaccumulation in the food chain, e.g., building on the work of Arnot and Gobas (2004). As discussed below, consideration of spatial variation may also be important. In the ongoing development of USEtox, a number of areas for improvement have been identified for the modeling of fate and ecotox exposure and effect.

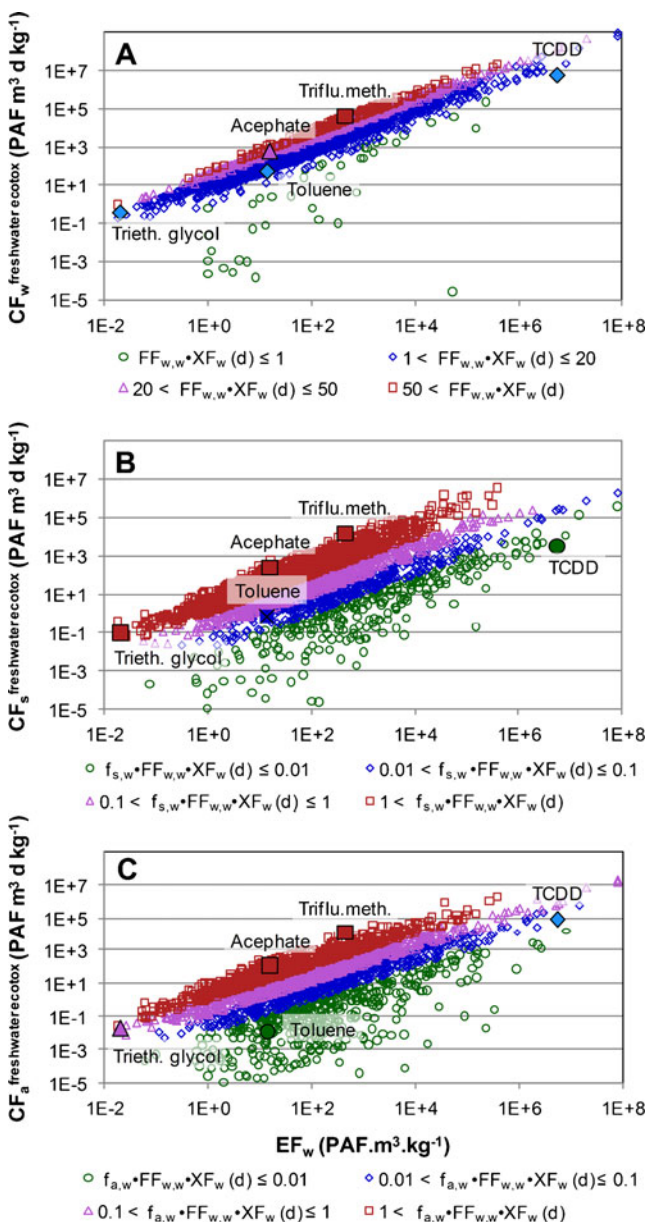


Fig. 5 Freshwater ecotox characterization factor for **a** emissions to water ($CF_w^{freshwater\ ecotox}$), **b** emissions to soil ($CF_s^{freshwater\ ecotox} = f_{s,w} \cdot CF_w^{freshwater\ ecotox}$), and **c** emissions to air ($CF_a^{freshwater\ ecotox} = f_{a,w} \cdot CF_w^{freshwater\ ecotox}$) as a function of the effect factor (EF_w) in water. Data are grouped according to the combined fate and exposure factor

4.1 Better factors for metals, ionizing compounds, and amphiphilics

All USEtox characterization factors provided for metals, ionizing compounds, and amphiphilics are presently classified as interim. Acephate, a weak acid, has been included in this manuscript as an example of a compound for which results should be interpreted with care. The fate and exposure parts of the USEtox model are considered insufficient to model the environmental behavior of metals (Diamond et al. 2010) and ionizing compounds; work is ongoing for both groups of compounds (Franco and Trapp 2010; Gandhi et al. 2010). For surfactants and detergents, focus will be on providing measured partitioning coefficients to avoid the use of questionable estimated values.

4.2 Marine and soil compartments

The fate modeling needed for determination of characterization factors for ecotox impacts in the marine and terrestrial compartment is already part of USEtox. However, the exposure and effect modeling in these compartments was considered immature for inclusion, due to the lack of specific data for chemical behavior and effects on organisms in these domains. Therefore, characterization factors are not yet provided for marine and terrestrial compartments, although their inclusion is one of the upcoming activities in the further development of USEtox. For exposure in soil, Haye et al. (2007) provided a first approach for metals that needs to be extended to cover the other substance groups.

4.3 Spatial differentiation

Since parsimony was one of the main goals in the development of the USEtox model, the model was set up to represent a global average continent within a global box, and with an urban zone nested within the continent. No spatial differentiation of location of the emission was considered. Since emissions in a life cycle can occur in many different parts of the world, and since the location may influence impact, a first improvement is to develop regional versions of USEtox. As is the case with the current version of USEtox, such regional models would model “typical” environmental conditions. An important issue is the determination of which level of spatial differentiation is relevant for ecotoxicity, including sensitivity studies on the influence of climate, e.g., testing the influence of temperature on half-lives. This can be investigated by comparing the output of the USEtox model to the output of multimedia models with a high degree of spatial resolution like the MAPPE model (Pistocchi 2008; Pistocchi et al. 2010) or the model developed by Jolliet and coworkers for investigation of human exposure to POPs (Humbert et al. 2009; Jolliet et al. 2008).

Acknowledgments Most of the work for this project was carried out on a voluntary basis and financed by in-kind contributions from the authors’ home institutions which are therefore gratefully acknowledged. The work was performed under the auspices of the UNEP-SETAC Life Cycle Initiative, which also provided logistic and financial support and facilitated stakeholder consultations. Financial support from American Chemical Council (ACC) and International Council on Mining and Metals (ICMM) is also gratefully acknowledged.

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