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IMPROVING SUBSTANCE INFORMATION IN USETOX®, PART 2: DATA FOR ESTIMATING FATE AND ECOSYSTEM EXPOSURE FACTORS

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Abstract: The scientific consensus model USEtox® has been developed since 2003 under the auspices of the United Nations Environment Programme–Society of Environmental Toxicology and Chemistry Life Cycle Initiative as a harmonized approach for characterizing human and freshwater toxicity in life cycle assessment and other comparative assessment frameworks. Using physicochemical substance properties, USEtox quantifies potential human toxicity and freshwater ecotoxicity impacts by combining environmental fate, exposure, and toxicity effects information, considering multimedia fate and multipathway exposure processes. The main source to obtain substance properties for USEtox 1.01 and 2.0 is the Estimation Program Interface (EPI Suite™) from the US Environmental Protection Agency. However, since the development of the original USEtox substance databases, new chemical regulations have been enforced in Europe, such as the Registration, Evaluation, Authorisation and Restriction of Chemicals (REACH) and the Plant Protection Products regulations. These regulations require that a chemical risk assessment for humans and the environment is performed before a chemical is placed on the European market. Consequently, additional physicochemical property data and new toxicological endpoints are now available for thousands of chemical substances. The aim of the present study was to explore the extent to which the new available data can be used as input for USEtox—especially for application in environmental footprint studies—and to discuss how this would influence the quantification of fate and exposure factors. Initial results show that the choice of data source and the parameters selected can greatly influence fate and exposure factors, leading to potentially different rankings and relative contributions of substances to overall human toxicity and ecotoxicity impacts. Moreover, it is crucial to discuss the relevance of the exposure factor for freshwater ecotoxicity impacts, particularly for persistent highly adsorbing and bioaccumulating substances. Environ Toxicol Chem 2017;36:3463–3470. © 2017 The Authors. Environmental Toxicology and Chemistry Published by Wiley Periodicals, Inc. on behalf of SETAC.

Keywords: USEtox® Environmental fate Freshwater toxicity Chemical regulation Environmental footprint

INTRODUCTION

The calculation of impacts on humans and the environment associated with the use and release of chemical substances is of increasing importance in numerous policies, including product policies. Chemical releases should be assessed along the entire value chain of a product, adopting a life cycle perspective, which embraces emissions into air, soil, and water from the extraction of raw materials to the end of life treatment of a product. In the context of the life cycle assessment (LCA) approach, since the late 1980s several models have been proposed to characterize potential ecotoxicity and human toxicity impacts associated with chemical emissions, such as CalTOX [1] and USES-LCA [2]. However, the fact that those models produced diverging characterization results spanning several orders of magnitude [3] led to a global consensus-building process under the auspices of the United Nations Environment Programme–Society of Environmental Toxicology and Chemistry (UNEP-SETAC) Life Cycle Initiative that started in 2003 and resulted in the scientific consensus model USEtox® [4–7]. The USEtox model aims to characterize toxicity-related impacts of chemical emissions by combining multimedia modeling to estimate chemical fate in various environmental compartments, subsequent exposure of humans and freshwater ecosystems to those emitted chemicals, and finally toxicity-related effects. The USEtox model is officially endorsed by the UNEP-SETAC Life Cycle Initiative, is now widely used in LCA and other comparative assessment frameworks, and has been included in the International Reference Life Cycle Data System recommendations [8] and in the context of the European Commission’s Environmental Footprint pilot project [9,10].

Traditionally, in LCA, the list of chemicals emitted into the different environmental compartments is compiled in the life cycle inventory phase. The life cycle inventory may contain up to thousands of chemicals emitted to water, soil, and/or air during the various life cycle stages of the considered products or services. To assess the overall human toxicity and freshwater aquatic ecotoxicity impacts of a product in LCA, the mass of each chemical emitted is multiplied by its associated characterization factors. Characterization factors represent the potential impact associated with a chemical emission unit to a particular environmental compartment. In USEtox, characterization factors are chemical-specific and represent the potency of a chemical with respect to causing human toxicity and/or freshwater ecotoxicity impacts. For each substance, a characterization
Factor is calculated in USEtox using a combination of matrices containing substance-specific fate factors, exposure factors, and effect factors, with characterization factor = fate factor × exposure factor × effect factor. For human toxicity characterization factors, fate and exposure factors are combined into the intake fraction, with intake fraction = fate factor × exposure factor. Exposure and effect factors are calculated differently for the human toxicity and ecotoxicity impact categories because the impact pathways differ between these categories.

Data for physicochemical properties and substance degradation half-lives that are used as input for USEtox (for both Ver 1.01 and Ver 2.0) to calculate fate and exposure factors and that are compiled in the USEtox substance databases are, currently, mainly coming from the US Environmental Protection Agency’s (USEPA’s) Estimation Program Interface Suite (EPI Suite™) [11]. The EPI Suite contains both experimental data and data estimated from various quantitative structure–property/activity relationship models. For the purpose of calculating fate and exposure factors in USEtox, experimental data contained in EPI Suite are always preferred over estimated data [12].

Chemical regulations in Europe, such as the Registration, Evaluation, Authorisation and Restriction of Chemicals (REACH) [13] and the Plant Protection Products [14] regulations, require that a chemical risk assessment for humans and the environment is performed before the chemical is placed on the market. One aim of these regulations is to guarantee a high level of human health and environmental health protection from the risks posed by exposures to chemicals. To reach this goal, all chemicals must be assessed against the risk they could pose for humans and the environment. Consequently, a significant effort has been made to improve and expand chemical properties databases, covering thousands of chemicals. For plant protection products, complete peer-reviewed risk-assessment reports (“Conclusions on Pesticides”) from the European Food Safety Authority (EFSA) are publicly available [15].

However, for potential application in LCA, the various relevant data from these new risk-assessment–related sources would need to be made freely available in tabular format for the thousands of chemicals that appear in life cycle inventories and, furthermore, would need to be aligned with the life cycle impact assessment toxicity characterization framework.

The first aim of the present study on the potential use of new data sources for LCA toxicity characterization with USEtox was, hence, to shed light on the differences between data sources, highlighting the implications of applying data from these sources in terms of decision support regarding the chemicals to be prioritized when aiming to reduce the environmental burden associated with a product, particularly in the context of environmental footprint studies. For that, we use an illustrative case study. In a complementary study [16], we used the physicochemical properties and ecotoxicity data of several pesticides whose risk was assessed by EFSA to analyze and discuss the methodology followed in USEtox to calculate chemical effect factors in the context of the environmental footprint. The data for the selected pesticides are also included in the USEtox organic substances database for comparison. In the present report, using the same list of pesticides as in our complementary study [16], we evaluate the relevance and implications of using different physicochemical properties from those currently implemented in USEtox to estimate fate and exposure factors.

The second aim of the present study was to highlight the implications that the exposure factor has on the contribution of some chemicals to the overall product toxicity score. For that, we first present the methodology adopted in USEtox to derive fate and exposure factors and corresponding intake fractions as well as the status of data availability and quality within the databases based on current European chemical regulations.

In the following sections, we describe our analysis and the case study designed to illustrate the differences between applying different data sources for substance properties in USEtox. In the Results and Discussion section, we compare currently implemented USEtox input data with data retrieved from EFSA risk-assessment reports for the same parameters, and we discuss how differences in input data could be reflected in the USEtox calculation of fate and exposure results. Furthermore, we discuss the meaning of the exposure factor and its influence on the toxicity score in the context of the environmental footprint.

In the Conclusions section, we highlight some key elements requiring further discussion and development to increase the acceptance and applicability of USEtox and toxicity characterization in comparative assessments.

**MATERIALS AND METHODS**

To illustrate the differences in resulting fate and exposure results as well as the implications for a possible LCA study outcome related to the selection of input data sources for physicochemical substance properties, 6 pesticides have been selected based on our complementary study [16] that are being used in plant protection products as active substances and that are available in the current USEtox organic substances database, namely clomazone (Chemical Abstracts Service [CAS] 81777-89-1), fluodioxonil (CAS 131341-86-1), halosulfuron methyl (CAS 100784-20-1), prosulfocarb (CAS 52888-80-9), teflubenzuron (CAS 83121-18-0), and fenbutatin oxide (CAS 13356-08-6). The physicochemical properties and chemical half-life data of these 6 pesticides included in USEtox (Ver 1.01 and Ver 2.0, both using the USEPA EPI Suite as a source of physicochemical properties) were compared with the properties extracted from the corresponding individual EFSA “Conclusions on Pesticides” reports [15] (hereafter referred to as the EFSA database). The physicochemical properties extracted from the EFSA database were then compiled to be used as input data for the USEtox model to calculate fate factors (for emissions to urban and rural continental air, continental freshwater and seawater, and continental natural and agricultural soil), exposure factors, and intake fractions. These results were then compared with the officially reported factors in the USEtox organic substances results database.

To illustrate and discuss the implications of the contribution of the ecosystem exposure factor to the overall freshwater ecotoxicity characterization results, substance data already reported in the USEtox organic substances database were used.

**RESULTS AND DISCUSSION**

The results of our analysis are reported in the following sections, focusing on the finding of the illustrative case study, highlighting the implication of input data selection and the parameters and equations used for calculating exposure factors.

*Illustrative case study to demonstrate the importance of data selection principles*

The main results from the illustrative case study for the 6 selected pesticides are summarized as follows:

Table 1 shows the ratio between the substance-related input data as currently used in USEtox 1.01 and those extracted from the EFSA database (see Supplemental Data, Table S1 for all
Table 1. Ratios of physicochemical properties and half-life data extracted from the USEtox 1.01 organic database and used by the European Food Safety Authority to perform environmental risk assessments

| CAS         | CAS          | K_{OW} | K_{OC} (L/kg) | K_{b} (Pa m²/m) | P_{vap} (Pa) | Solubility (mg/L) | k_{degA} | k_{degW} | k_{degSd} | K_{degS} |
|-------------|--------------|--------|---------------|-----------------|-------------|------------------|-----------|---------|-----------|---------|
| Clomazone   | USEtox 1.01/EFSA | 1      | 1             | 1               | 1           | 1                | 1         | 1       | 1         | 1.20E-01 |
| Fludioxonil | USEtox 1.01/EFSA | 1      | 1.00E-02      | 1               | 1           | 1                | 1         | 1       | 17        | 2       |
| Halosulfuron methyl | USEtox 1.01/EFSA | 3      | 9.00E-02      | 3.00E-03        | 3.00E-05    | 1                | 1         | 1       | 1.00E-01  | 2.00E-02 |
| Prosulfocarb| USEtox 1.01/EFSA | 1      | 2             | 9.00E-02        | 9.00E-02    | 1                | 5.00E-01  | 27      | 1         | 1.60E-01 |
| Teflubenzuron | USEtox 1.01/EFSA | 2      | 8.00E-02      | 2.00E-03        | 1.00E-03    | 2                | 3.00E-04  | 4.00E-02 | 9.00E-03  | 2.60E-01 |
| Fenbutatin oxide | USEtox 1.01/EFSA | 3.16E+09 | 2E+14         | 7.00E-02       | 6.00E-02    | 1                | 1         | 6       | 9.00E-02  | 1       |

*Based on a USEtox 1.01 value of 7.4E+15 compared to 4.5E+11 from the EFSA database. In USEtox 2.0, this high value has been deleted.

The ecosystem exposure factors for continental freshwater (Table 2; Supplemental Data, Table S3) are not significantly affected by the input database for this specific set of pesticides. The main contributing terms to the ecosystem exposure factor are the adsorption on both suspended matter in freshwater and dissolved organic carbon in freshwater as well as biota living in freshwater. However, for the pesticides fludioxonil, teflubenzuron, and fenbutatin oxide, the proportion adsorbed on suspended matter versus dissolved organic carbon is reversed depending on the source of the data.

The aggregated human intake fraction, which corresponds to the product of fate and human exposure factors aggregated over all considered human exposure routes (i.e., ingestion and inhalation only) varied by 2 orders of magnitude for 5 out of 6 considered pesticides and up to 12 orders of magnitude for fenbutatin oxide (Figure 2; Supplemental Data, Table S4), where again the intake fraction results for fenbutatin oxide must be interpreted with caution because of the interim fate and exposure model for organometallics in USEtox.

Overall, these initial observations highlight that the choice of the input data source can have an important impact on the model results. As demonstrated by Henderson et al. [17], chemical-specific differences influence the ecotoxicological characterization.
factors by less than 2 orders of magnitude across chemicals, while they may have a much stronger influence on the variability of fate factors. Consequently, using different sources for chemical-specific data can potentially lead to different rankings of chemicals in terms of their ecotoxicity potential. If the ranking of chemicals is influenced, this may potentially lead to different decisions regarding the overall toxicity characterization profile in cases where the considered chemicals dominate human toxicity or ecotoxicity. It is, therefore, crucial that USEtox builds on the best available data for all substance-related input parameters or on input data that are based on broad consensus and suitable for LCA and environmental footprint—that is, representing meaningful average, best practice, and realistic situations.

Furthermore, although no chemical or product safety-related decision is being made in the context of LCA or the environmental footprint, there may still be a shift from the focus on one chemical to another in terms of human toxicity or ecotoxicity profiles. Concerning the 6 selected pesticides, the exposure factors were not affected by the source of input data, mainly because those pesticides’ sorption on suspended matter, on dissolved organic carbon, and the fraction bioaccumulated in freshwater biota are all estimated from the K\textsubscript{OW} and, generally, very small differences exist between the 2 selected data sources for the considered pesticides (see Table 1). The only exception is, however, the organometallic compound fenbutatin oxide. For this pesticide, in USEtox an estimated value from the EPI Suite is currently used that is 9 orders of magnitude higher compared with the K\textsubscript{OW} value reported in the EFSA database. This again highlights the need to always check the applicability domain of property estimation models as used in the EPI Suite or elsewhere. On a broader perspective, it is clear that the choice of the data source for physicochemical properties can significantly influence the results related to the quantification of fate, exposure, and intake fractions for thousands of chemicals in LCA and the environmental footprint.

### Impact of the ecosystem exposure factor on ecotoxicity characterization results

The ecosystem exposure factor for freshwater ecotoxicity impacts is related to the “true” dissolved fraction of the chemical in the water column. It considers the fraction adsorbed on suspended matter in freshwater (K\textsubscript{susp} × C\textsubscript{susp}), on dissolved organic carbon (K\textsubscript{doc} × C\textsubscript{doc}), and the fraction that is bioaccumulated in aquatic biota (BAF\textsubscript{fish} × C\textsubscript{biota}) (see Equation 1 and Huijbregts et al. [12]).

$$\text{XF}_{\text{freshwater}} = \left(1 + K_{\text{susp}} \times C_{\text{susp}} + K_{\text{doc}} \times C_{\text{doc}} + BAF_{\text{fish}} \times C_{\text{biota}}\right)^{-1}$$  \hspace{1cm} (1)

In Equation 1, XF is the exposure fraction, K\textsubscript{susp} is the suspended solids/water partitioning coefficient (L/kg), C\textsubscript{susp} is the concentration of suspended matter in freshwater (kg/m\textsuperscript{3}), and C\textsubscript{doc} is the concentration of dissolved organic carbon in freshwater (mg/L), and BAF\textsubscript{fish} is the bioaccumulation factor for freshwater biota.
$K_{\text{doc}}$ is the dissolved (colloidal) organic carbon/water partition coefficient (L/kg), $C_{\text{doc}}$ is the concentration of dissolved (colloidal) organic carbon in freshwater (kg/m³), $\text{BAF}_{\text{fish}}$ is the bioaccumulation factor for freshwater fish (L/kg), and $C_{\text{biota}}$ is the concentration of biota in freshwater (kg/m³).

In practice, when performing the life cycle impact assessment ecotoxicity characterization, the quantity of a specific chemical mass emitted into or reaching the freshwater environment after multimedia fate processes is multiplied by its corresponding characterization factor, where in the ecosystem exposure factor component the “true” dissolved fraction of the chemical mass in freshwater is considered. As a consequence, an exposure factor of 0.1 means that only a fraction of 10% is truly dissolved in freshwater and that 90% of the mass emitted into or reaching the freshwater environment is not used for the calculation of the freshwater ecotoxicity potential for this chemical.

Sorption to suspended particles is, indeed, a clear toxicity mitigation process in natural aquatic environments, and this aspect is also used when assessing the risk of chemicals in the aquatic environment in an ecological risk assessment [18]. The ecosystem exposure equation (without the product term $K_{\text{doc}} \times C_{\text{doc}}$ in Equation 1) that is applied in USEtox is originally derived from the SimpleBox multimedia fate model [19]. In SimpleBox, this ecosystem exposure equation is used principally to estimate intermedia mass transfer between environmental compartments [19]. This mass transfer estimation allows the calculation of the “background concentration” of a chemical in the environment, where this background concentration is used to estimate what “remains” in dissolved form in the freshwater environment at steady state. In safety assessment of chemicals, the aquatic toxicity potential of a chemical is not directly compared to this background concentration but to a predicted environmental concentration, which is composed of the sum of concentrations at the point of release and the background concentration in freshwater. For the estimation of the concentration at point of release, the “bioavailable” fraction is considered using only the adsorption to suspended matter. This is done to assess risk to freshwater biota before a considered chemical is bioconcentrated in the freshwater organisms, which usually drives the related chemical ecotoxicity if the concentration in freshwater reaches a certain level.

By considering all 3 terms in the ecosystem exposure equation (i.e., adsorption to suspended matter in freshwater, adsorption to dissolved organic carbon in freshwater, and bioconcentration in freshwater organisms), USEtox aims to estimate the toxicity of the chemical still present in the environment in truly dissolved form as equivalent to the “background concentration” in environmental risk assessment. As a result, chemicals that are highly “bioaccumulative” and/or highly adsorptive on suspended matter and/or dissolved organic carbon will generally show a low exposure factor in USEtox.

Assessing the exposure factors provided within the USEtox organic substances results database, the large majority of chemicals (87%) have an ecosystem exposure factor of approximately 1, meaning that approximately 100% of the mass entering the aquatic environment is in “true” dissolved form (Figure 3). For some chemicals, however, the ecosystem exposure factor can be very low, leading to a quasi-complete elimination of chemicals that are assessed for their toxicity potential. This is because, in the current approach, the toxicity of chemicals that are adsorbed on suspended matter in freshwater and might ultimately accumulate in sediment is not included in the ecosystem toxicity impact score, which represents toxicity to organisms living in the freshwater column, not to those living in the sediment. The latter were excluded because of the limited availability of ecotoxicity data for many chemicals toward sediment-dwelling organisms.

The bioaccumulation potential of such substances is already considered in the ecotoxicity data underlying the effect factors for pelagic species to the extent that they are based on chronic ecotoxicity tests. In the cases where the effect factor for strongly bioaccumulative substances is based on extrapolation from acute ecotoxicity test data (which is the case for the majority of chemicals in USEtox), there could be a need to correct for the bioaccumulation potential in the calculation of the chemical characterization factor.

Of 2503 ecotoxicity effect factors provided by USEtox 1.01 and 2.0, 767 chemicals have an estimated hazardous concentration affecting 50% of all exposed freshwater ecosystem species above their median effect concentration of $<1\text{ mg/L}$. If the criteria of Regulation (EC) No 1272/2008 on Classification, Labelling and Packaging of Substances and Mixtures [20] would be applied on those 767 chemicals, they would be classified as very toxic for the environment. Figure 4 shows the cumulated number of those potentially very toxic chemicals according to the European Commission [20] versus the fraction

![Figure 3. Exposure factors for freshwater ecotoxicity impact category extracted from the USEtox 1.01 organic database.](image)

![Figure 4. Cumulated number of chemicals present in the USEtox organic database with an estimated effect factor that could be classified as very toxic (median effect or lethal concentration $<1\text{ mg/L}$) according to [20], plotted against percentage of mass adsorbed.](image)
of substances in freshwater that is not “truly” dissolved, expressed as a percentage and based directly on ecosystem exposure factors from the USEtox organic substances results database. This shows that for 33 chemicals present in the USEtox database, >90% of the substance mass emitted into or arriving in the freshwater environment will not be considered for the calculation of respective ecotoxicity characterization factors; for about 100 chemicals, it is 50% or more of the emitted or received mass in freshwater that does not contribute to the corresponding characterization results.

The same observation can be made with substances potentially classified as bioaccumulative or very bioaccumulative when the criteria of the European Chemicals Agency’s guidance for the assessment of persistent, bioaccumulative, and toxic or very persistent/very bioaccumulative characterization would be applied [21]. In Figure 5, the exposure factors representing the “true” dissolved substance fraction in freshwater are plotted against the BAFs for fish directly extracted from the USEtox organic substances input data and results databases. The horizontal red lines represent the set threshold between “bioaccumulative” and “very bioaccumulative” chemicals according to the European Chemicals Agency guidance [21]. Figure 5 shows that, for some bioaccumulative and very bioaccumulative substances (left upper part of the graph), the contribution to the overall ecotoxicity score is minimized because of a low exposure factor. As a consequence, the potentially high ecotoxicity of some of the worst chemicals (highly toxic and/or bioaccumulative) in terms of characterization results would exclusively rely on the assumption that high toxicity and/or high bioaccumulation is already captured in the corresponding data underlying the effect factor because these aspects are not considered to be contributors to high exposure when deriving the “true” dissolved chemical mass fraction in freshwater. However, the fact that higher toxicity and/or bioaccumulation potential is captured in the ecotoxicity effect factors would only be correct if the effect factors were exclusively based on chronic ecotoxicity data, which is unfortunately not the case today with the USEtox organic substances database. In fact, currently, in USEtox mostly acute data are used and extrapolated to a chronic effect by applying a fixed, substance-independent, acute-to-chronic ratio. Hence, the present results emphasize that it is important to improve the current acute-to-chronic ratio, taking potential bioaccumulation into account, and to aim for including data from additional chronic endpoints (10% effect concentration, no-observed-effect concentration, lowest-observed-effect concentration, etc.) for calculating ecotoxicity effect factors in USEtox.

The inclusion of an exposure factor is coherent with the objective of the impact assessment phase in LCA. Therefore, USEtox aims to assess and compare the potential overall impact of substances on humans and ecosystems and not to identify the chemicals of concern from a purely hazard-based point of view. In fact, USEtox provides an outcome in line with the risk-assessment concept in the sense that no exposure leads to no effect. The USEtox model (and LCA in general) does not address safety but aims to estimate the potential toxicity pressure of thousands of chemical substances still present in the aquatic environment at steady state that are emitted along the entire life cycle of a considered product or service. However, to provide a fair product-related comparison of freshwater ecotoxicity impacts, the potential toxicity to organisms living in the sediment compartment below the actual water column should additionally be considered in the freshwater toxicity score to take into account those chemicals with high sediment accumulation properties.

These modeling aspects contribute to the fact that although USEtox is a scientific consensus model to screen hundreds to thousands of substances for their potential human toxicity and freshwater ecotoxicity impacts in a life cycle perspective, it will not necessarily be able to help in the identification of the chemical of concern according to current risk-assessment criteria (persistent, bioaccumulative, and toxic; substance of very high concern; etc.). Capitalizing on the supply chain-oriented approach of LCA for application in the environmental footprint, a complementary method could be proposed to identify and quantify the mass of those chemicals of concern in products before they are even released into the environment. This will help to identify products using and emitting less of those substances of concern through their entire life cycle when conducting LCA and environmental footprint studies. To achieve this goal, the list of elementary flows as currently published in the International Reference Life Cycle Data System database and being used to construct inventory input–output files of an environmental footprint (or any LCA) could be complemented with the information on chemical classification according to the European Union’s Regulation on Classification, Labelling and Packaging of Substances and Mixtures [20].

Figure 5. Exposure factors versus bioaccumulation factors extracted from the USEtox 1.01 organic database. The horizontal red line indicates the limits between bioaccumulative and very bioaccumulative chemicals according to the European Commission [13] and the European Chemicals Agency [21].
CONCLUSIONS

Overall, our illustrative case study shows that the selection of appropriate, reliable, and consistent input data for physicochemical properties in USEtox is a critical component in the correct calculation of any product’s LCA or environmental footprint. The recent enforcement of chemical policies, such as REACH and the Plant Protection Product regulations, constitutes a unique opportunity to build a common database of physicochemical data, including chemical half-lives and toxicity information. Regarding the REACH database that contains both high- and low-quality data, a rigorous selection of the data needs to be performed first. Moreover, for potential application in LCA, data from this and potentially other new sources would need to be made freely available in tabular format for the numerous chemicals relevant for LCA and finally be aligned with the life cycle impact assessment toxicity characterization framework. Specific and detailed guidance and protocols should be developed in parallel to allow all users to follow the same methodology when extracting physicochemical properties from such databases.

The impact of the exposure factor by lowering the contribution of highly adsorptive and bioaccumulative substances to the overall product toxicity score needs to be further assessed to ensure that the long-term impact of a bioaccumulative substance on the aquatic food chain as well as the toxicity to sediment-living organisms is duly considered in the ecotoxicity impact assessment.

For bioaccumulative substances, 2 options could be envisaged: either acting on the BAF, avoiding a high BAF that results in unrealistically low exposure factors, or acting on the static extrapolation factors of 2 from acute to chronic ecotoxicity effects. This extrapolation factor, as currently used in USEtox to derive the effect factors, could in the environmental footprint context as a first proxy be set higher compared with the extrapolation factor used for nonbioaccumulative chemicals to reflect that the currently mainly used acute toxicity test results are less capable of capturing the increased toxicity of those chemicals that is caused by their ability to bioaccumulate.

Regarding chemicals absorbed on suspended particles, those chemicals will ultimately end up in sediment where organisms are exposed to chemicals via interstitial water or directly by ingestion of sediment [22]. However, the scarcity of toxicity data for sediment-dwelling organisms makes this option difficult to implement in a robust way in the foreseeable future.

Supplemental Data—The supplemental data are available on the Wiley Online Library at DOI: 10.1002/etc.3903.

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Data availability—All data used and the model are freely available on public websites (see URLs directly provided in the references).

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