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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® is developed since 2003 under the auspices of the UNEP-SETAC Life Cycle Initiative as a harmonized approach for characterizing human and freshwater toxicity in life cycle assessment (LCA) 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 multi-pathway 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 U.S. Environmental Protection Agency. However, since the development of the original USEtox® substance databases, new chemical regulations have been enforced in Europe such as the 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 end-points are now available for thousands of chemical substances. The aim of the present study is to explore to which extent 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 exposure factor for freshwater ecotoxicity impacts particularly for persistent highly adsorbing and bio-accumulating substances. This article is protected by copyright. All rights reserved

Keywords: USEtox®; Environmental fate; Freshwater toxicology; Chemical regulation; Environmental Footprint; Chemical substances

INTRODUCTION

The calculation of impacts on humans and the environment associated with the use and release of chemical substances is of increasing importance in a number of 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 1980's, 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 UNEP-SETAC Life Cycle Initiative that started in 2003 and resulted in the scientific consensus model USEtox® [4–7]. USEtox® aims to characterize toxicity-related impacts of chemical emissions by combining multimedia modelling to estimate chemical fate in various environmental compartments, subsequent exposure of humans and freshwater ecosystems to those emitted chemicals, and finally toxicity-related effects. USEtox® 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 (ILCD)[8] and in the context of the European Commission's Environmental Footprint (EF) pilot project [9,10].

Traditionally, in LCA, the list of chemicals emitted into the different environmental compartments is compiled in the life cycle inventory (LCI) phase. The LCI 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 characterisation factors (CF). CFs represent the potential impact associated with a chemical emission unit to a particular environmental compartment. In USEtox®, CFs 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 CF is calculated in USEtox® using a combination of matrices containing substance-specific fate factors (FF), exposure factors (XF) and effect factors (EF), with CF = FF × XF × EF. For human toxicity CFs, fate and exposure factors are combined into the intake fraction with iF = FF × XF. Exposure and effect factors are calculated differently for the human toxicity and ecotoxicity impact categories as 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 version 1.01 and 2.0) to calculate fate and exposure factors and that are compiled in the USEtox® substance databases are, currently, mainly coming from the United States Environmental Protection Agency's (USEPA) Estimation Program Interface Suite (EPI Suite™) [11]. EPI Suite™ contains both experimental data and data estimated from various quantitative structure-property/activity-relationships models (QSPRs and/or QSARs). 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 REACH [13] or the Plant Protection Products (PPPs) [14] regulations require that a chemical risk assessment for humans and the environment is performed before the chemicals are placed on the market. One of the aims 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 PPPs, 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, need to be aligned with the life cycle impact assessment (LCIA) toxicity characterization framework.

The first aim of the present study toward the potential use of new data sources for LCA toxicity characterization with USEtox® is, 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 at reducing the environmental burden associated to a product, particularly in the context of Environmental Footprint (EF) 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 analyse and discuss the methodology followed in USEtox® to calculate chemical effect factors in the context of EF. The data for the selected pesticides are also included in the USEtox® organic substances database for comparison. In the present paper, using the same list of pesticides as in our complementary study [16], we evaluate the relevance and implications of using different physicochemical properties than those currently implemented in USEtox® to estimate fate and exposure factors.

The second aim of the present study is to highlight the implications that the exposure factor (XF) 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, we describe our analysis and the case study designed to illustrate the differences between applying different data sources for substance properties in USEtox®. As results, 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 EF.

In our conclusions, we finally highlighted some key elements requiring for further discussion and development to increase the acceptance and applicability of USEtox® and toxicity characterization in comparative assessments.

MATERIALS AND METHODS

In order 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, six pesticides have been selected based on [16] that are being used in PPPs as active substances and that are available in the current USEtox® organic substances database, namely clomazone (CAS 81777-89-1), fludioxonil (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 six pesticides included in USEtox® (versions 1.01 and 2.0 and both using USEPA EPI Suite™ as source of physicochemical properties) were compared to the

properties extracted from the corresponding individual EFSA 'Conclusions on Pesticides' reports [15] (from now on referred to as '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 to 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 DISCUSION

The result of our analysis are reported in the following, 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 six selected pesticides are summarized in the following:

- 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 Table S1 for all considered original values). For some substance parameters, there is a perfect match between the two data sources. However, for other substance parameters, there can be several orders of magnitude difference, namely 9 orders of magnitude for K_{ow} of

fenbutatin oxide as an extreme case. Input data between USEtox® 1.01 and 2.0 are identical for all parameters except K_{ow} for Halosulfuron, Prosulfocarb and Teflubenzuron are slightly different. Those differences do not change the observations made through the paper (see Table S1).

- Important input parameter for the fate model in the USEtox® is K_{ow}, which is currently taken for all six selected pesticides from EPI Suite™. For four of these pesticides the K_{ow} value as currently used in USEtox® comes from an experimental source in EPI Suite™. However, for fenbutatin oxide and halosulfuron methyl, the used K_{ow} is based on an estimated value thus, these data need to be applied with caution as they show higher uncertainty.
- Fate factors calculated from input data as currently used in USEtox® and those calculated with data from the EFSA database differ up to four orders of magnitudes for five of the six selected pesticides and differ thirteen orders of magnitude for fenbutatin oxide for an emission to continental seawater (Figure 1 and Table S2). Again, both fate factor results for fenbutatin oxide need to be interpreted with caution due to the interim model behind for organometallics in USEtox®.
- The ecosystem exposure factors for continental freshwater (Table 2 and 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, dissolved organic carbon in freshwater, and 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 (iF), 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 two orders of magnitude for five out of six considered pesticides and up to twelve orders of magnitude for fenbutatin oxide (Figure 2 and Table S4), where again the intake fraction results for fenbutatin oxide must be interpreted with caution due to 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 two 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 EF, i.e. representing meaningful average, best practice, and realistic situations.

Furthermore, while no chemical or product safety-related decision is being made in the context of LCA or EF, there may still be a shift from the focus on one chemical to another in terms of their human toxicity and/or ecotoxicity profiles.

Concerning the six selected pesticides, the exposure factors were not affected by the source of input data mainly due to the fact that for those pesticides sorption on suspended matter, on dissolved organic carbon, and the fraction bio-accumulated in freshwater biota are all estimated from the K_{ow} and, generally, very small differences exist between the two 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 EPI Suite™ is currently used that is nine orders of magnitude higher compared to the K_{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 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 EF.

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 ($K_{susp} \times C_{susp}$), on dissolved organic matter ($K_{doc} \times C_{doc}$), and the fraction that is bio-accumulated in aquatic biota ($BAF_{fish} \times C_{biota}$) (see Equation 1 and [12]).

$$XF_{freshwater} = (1 + K_{susp} \times C_{susp} + K_{doc} \times C_{doc} + BAF_{fish} \times C_{biota})^{-1} \quad (1)$$

with:

K_{susp}: Suspended solids/water partitioning coefficient [L/kg],

C_{susp}: Concentration of suspended matter in freshwater [kg/m^3],

K_{doc}: Dissolved (colloidal) organic carbon/water partition coefficient [L/kg],

C_{doc}: Concentration of dissolved (colloidal) organic carbon in freshwater [kg/m^3],

BAF_{fish}: Bioaccumulation factor for freshwater fish [L/kg], and

C_{biota}: Concentration of biota in freshwater [kg/m^3]

In practice, when performing the LCIA 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 $K_{doc} \times C_{doc}$ 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 chealculation 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 (PEC), which is composed of the sum of concentration at point of release and 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 bio-concentrated in the freshwater organisms, which usually drives the related chemical ecotoxicity if the concentration in freshwater reaches a certain level.

By considering all three 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 at estimating the toxicity of the chemical still present in the environment in truly dissolved form, as equivalent to the 'background concentration' in Environmental Risk Assessment (ERA). 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 around 1, meaning that approximately 100% of the mass entering the aquatic environment is in 'true' dissolved form (Figure 3). However, for some chemicals, 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 due to the limited availability of ecotoxicity data for many chemicals towards 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 CF.

Out 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 EC_{50} effect concentration of $HC_{50} < 1$ mg/L. When 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 [20] versus the fraction of substances in freshwater that is not 'truly' dissolved expressed as 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, more than 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 ECHA Guidance for the assessment assessment persistent, bioaccumulative and toxic or very persistent/very bioaccumulative (PBT/vPvB) substances would be applied [21]. In Figure 5, the exposure factors representing the 'true' dissolved substance fraction in freshwater are plotted against the bioaccumulation factors (BAF) 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 ECHA 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 due to 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 as these aspects are not considered as 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, our results emphasize that it is important to improve the current acute-to-chronic

ratio, taking potential bioaccumulation into account and aim for including data from additional chronic endpoints (EC10, NOEC, LOEC, 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. USEtox® therefore aims at assessing and comparing the potential overall impact of substances on humans and ecosystems and not at the identification of the chemicals of concerns 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 a no effect'. USEtox® (and LCA in general) does not address safety, but aims at estimating 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 modelling aspects contribute to the fact that while 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 for the identification of the chemical of concerns according to current risk assessment criteria (PBT, Substance of very high concern - SVHC, etc.). Capitalising on the supply chain-oriented approach of LCA for the application in EF, a complementary method could be proposed to identify and quantify the mass of those chemicals of concerns in products, before they are even released into the environment. It will help to identify products using and emitting less of

those substances of concern through their entire life cycle, when conducting LCA and EF studies. To achieve this goal, the list of elementary flows as currently published in the ILCD database and being used to construct inventory input-output files of an EF (or any LCA) could be complemented with the information on chemical classification according to EU Regulation on classification, labelling and packaging of substances and mixtures (CLP) [20]

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 LCA or EF. The recent enforcement of chemical policies, such as the REACH and the Plant Protection Product regulations, constitute 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 LCIA 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 bio-accumulative substances to the overall product toxicity score needs to be further assessed to ensure that the long term impact of bio-accumulative substance on aquatic food chain as well as the toxicity to sediment living organisms is duly considered in the ecotoxicity impact assessment.

For bio-accumulative substances, two options could be envisaged: either acting on the BAF, avoiding that high BAF results in unrealistically low XFs, or 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 EF context as a first proxy be set higher compared to the extrapolation factor used for non-bioaccumulative 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 bio-accumulate.

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 a foreseeable future.

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

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Data availability—All data used and model are free available on public websites. URL of those are directly provided in the paper.

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Figure 1. Ratios of Fate Factors for 6 pesticides for urban and continental compartments using the USEtox® 1.01 and EFSA database.

Figure 2. Ratios of Fate Factors for 6 pesticides for urban and continental compartments using the USEtox® 1.01 and EFSA database.

Figure 3. Exposure Factors (XF) for freshwater ecotoxicity impact category extracted from the USEtox® 1.01 organic database.

Figure 4. Cumulated number to chemicals present in the USEtox® organic database with an estimated Effect Factor which could be classified as very toxic (E(L)C50 < 1 $mg.L^{-1}$) according to (24).

Figure 5. Exposure Factors (XF) versus bioaccumulation factors (BAF) extracted from the 'USEtox® 1.01 organic database. The horizontal red line indicates the limits between bio accumulative and very bio accumulative chemicals according to (13 and 21).

Table 1: Ratios of USEtox® physico-chemical properties and half-life data extracted from USEtox 1.01 organic database and used by EFSA to perform environmental risk assessments.

	CAS		Kow	Koc (L/kg)	Kh (Pa.m3/mol)	Pvap (Pa)	Solubility (mg/L)	kdegA	KdegW	kdegSd	KdegS
Clomazone	81777-89-1	USEtox 1.01/EFSA	1	1	1	1	1	1	1	1.20E-01	1[a]
Fludioxonil	131341-86-1	USEtox 1.01/EFSA	1	1.00E-02	1	1	1	1	17	2	2[a]
Halosulfuron methyl	100784-20-1	USEtox 1.01/EFSA	3[a]	9.00E-02	3.00E-03	3.00E-05	1	1	1.00E-01	2.00E-02	2.00E-01[a]
Prosulfocarb	52888-80-9	USEtox 1.01/EFSA	1[a]	2	9.00E-02	9.00E-02	1	5.00E-01	27	1	1.60E-01[a]
Teflubenzuron	83121-18-0	USEtox 1.01/EFSA	2[a]	8.00E-02	2.00E-03	1.00E-03	2	3.00E-04	4.00E-02	9.00E-03	2.60E-01[a]
Fenbutatin oxide	13356-08-6	USEtox 1.01/EFSA	3.16E+09	2E+14*	7.00E-02	6.00E-02	1	1	6	9.00E-02	1[a]

**: Based on a USEtox 1.01 value of 7.4E+15 compared to 4.5E+1 from EFSA BD. In USEtox 2.0, this high value has been deleted.*

a: Ratios are different when using USEtox 2.0 DB (see TS.2 in supplementary material)

Table 2: Exposure Factors (XF) and percentage adsorbed on suspended matter (Kp*SUSP), dissolved organic matter (Kdoc*DOC) and bio-concentrated for 6 commonly used pesticides using the USEtox® 1.01 or EFSA database. See equation 1 in text for detail on how the XF is calculated.

Pesticides	CAS	Database	Exposure Factor (XF)	Kp*SUSP	Kdoc*DOC	Bio-concentrated
Clomazone USEtox	81777-89-1	USEtox 1.01	0.999	73%	22%	5%
		EFSA	0.999	73%	24%	3%
Fludioxonil USEtox	131341-86-1	USEtox 1.01	0.992	22%	67%	11%
		EFSA	0.817	97%	2%	0%
Halosulfuron methyl	100784-20-1	USEtox 1.01	1.000	89%	6%	6%
		EFSA	1.000	100%	0%	0%
Prosulfocarb	52888-80-9	USEtox 1.01	0.978	22%	78%	0%
		EFSA	0.984	16%	75%	9%
Teflubenzuron	83121-18-0	USEtox 1.01	0.982	17%	81%	1%
		EFSA	0.954	81%	17%	2%
Fenbutatin	13356-08-6	USEtox 1.01	9.03E-11	100%	0%	0%
		EFSA	0.946	0%	99%	1%

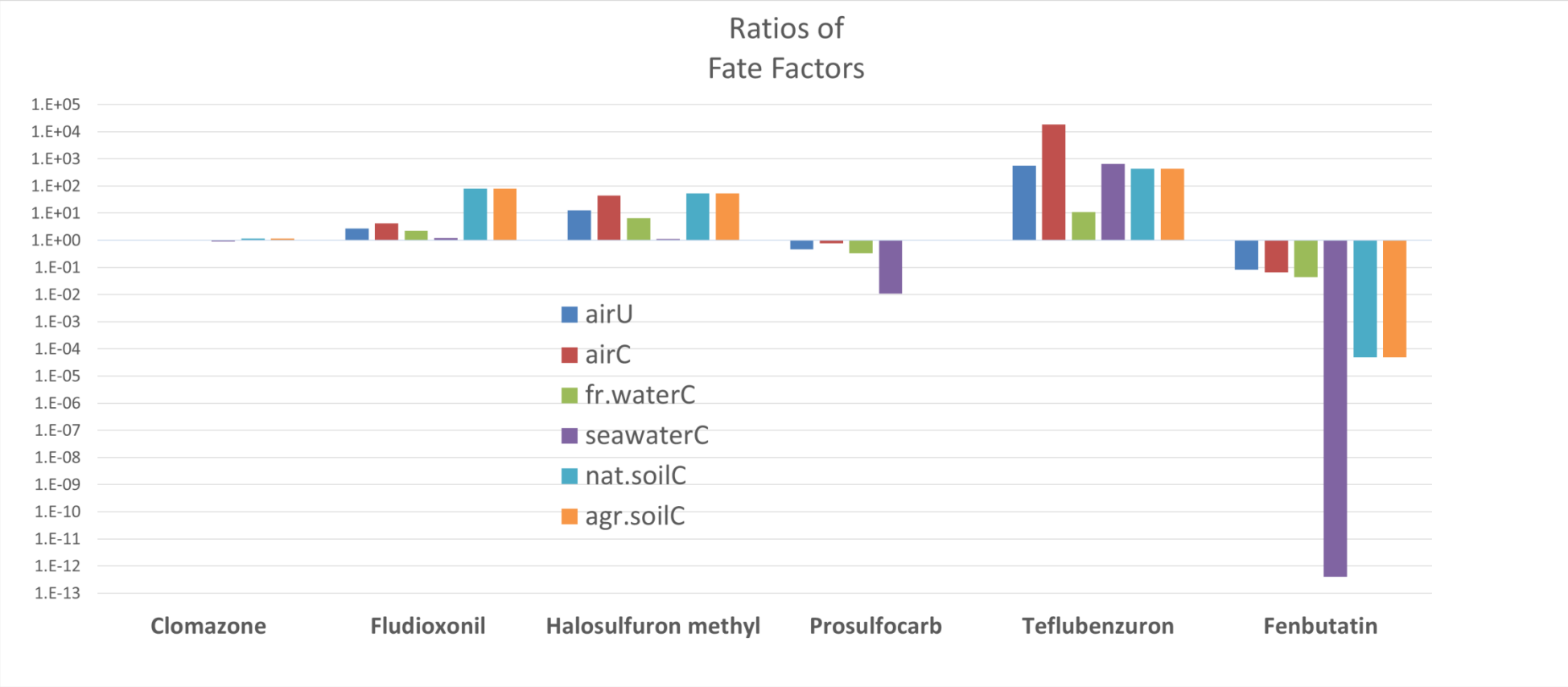

Figure 1: Ratios of Fate Factors for 6 pesticides for urban and continental compartments using the USEtox® 1.01 and EFSA database.

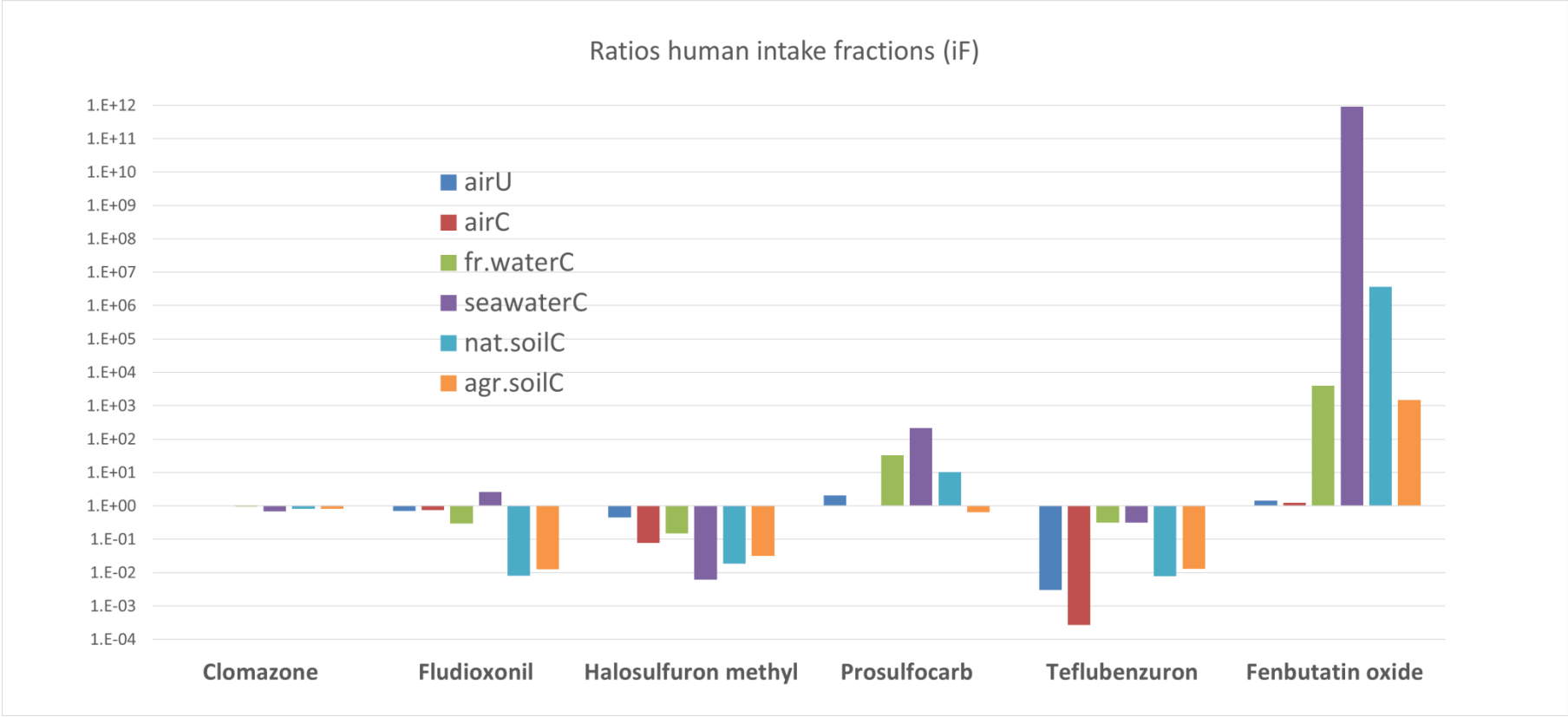

Figure 2: Ratios of Fate Factors for 6 pesticides for urban and continental compartments using the USEtox® 1.01 and EFSA database.

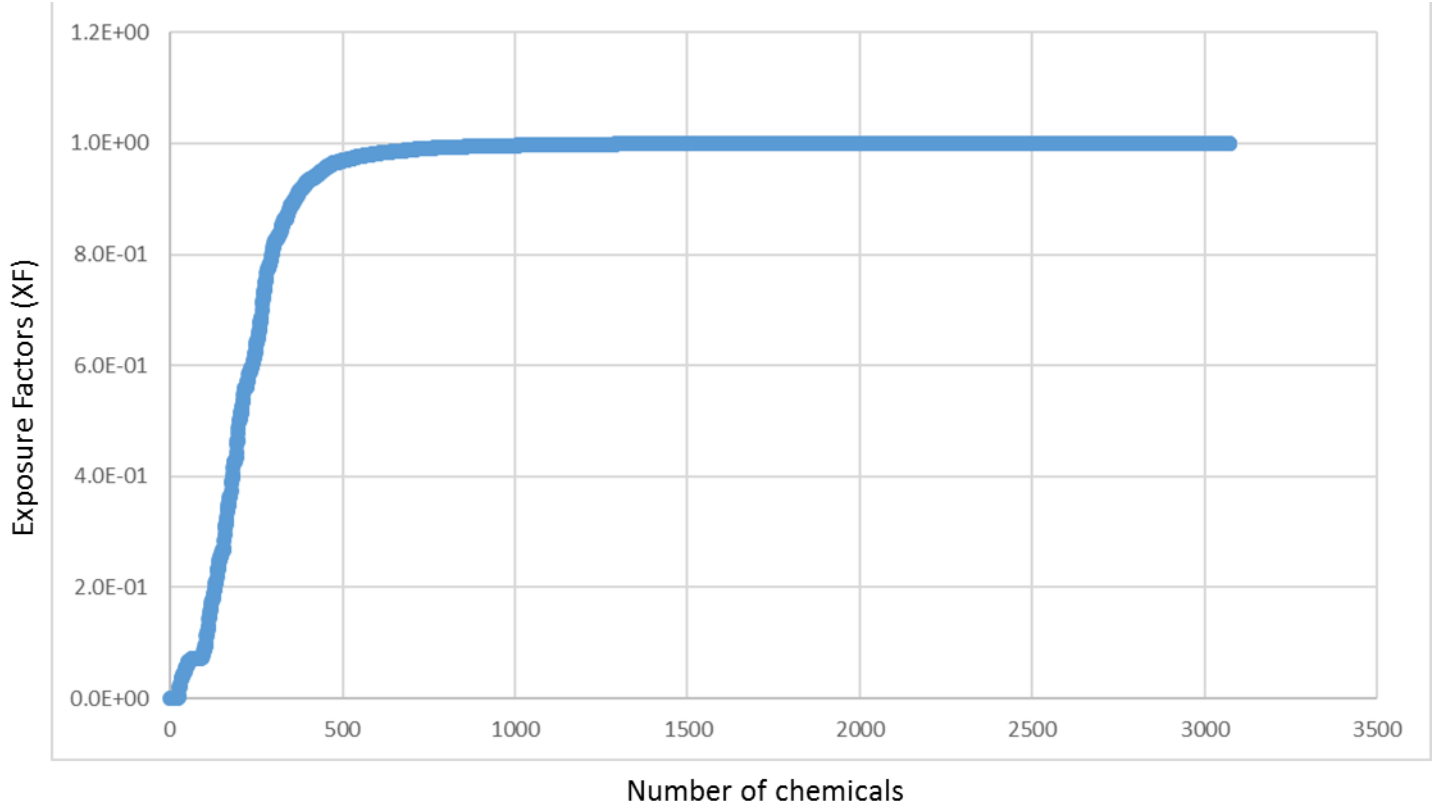

Figure 3: Exposure Factors (XF) for freshwater ecotoxicity impact category extracted from the USEtox® 1.01 organic database.

Figure 4 : Percentage of mass adsorbed (100-EX*100) and cumulated number of chemicals present in the USEtox® organic database with an estimated Effect Factor which could be classified as very toxic (E(L)C50 < 1 mg.L^{-1}) according to (24).

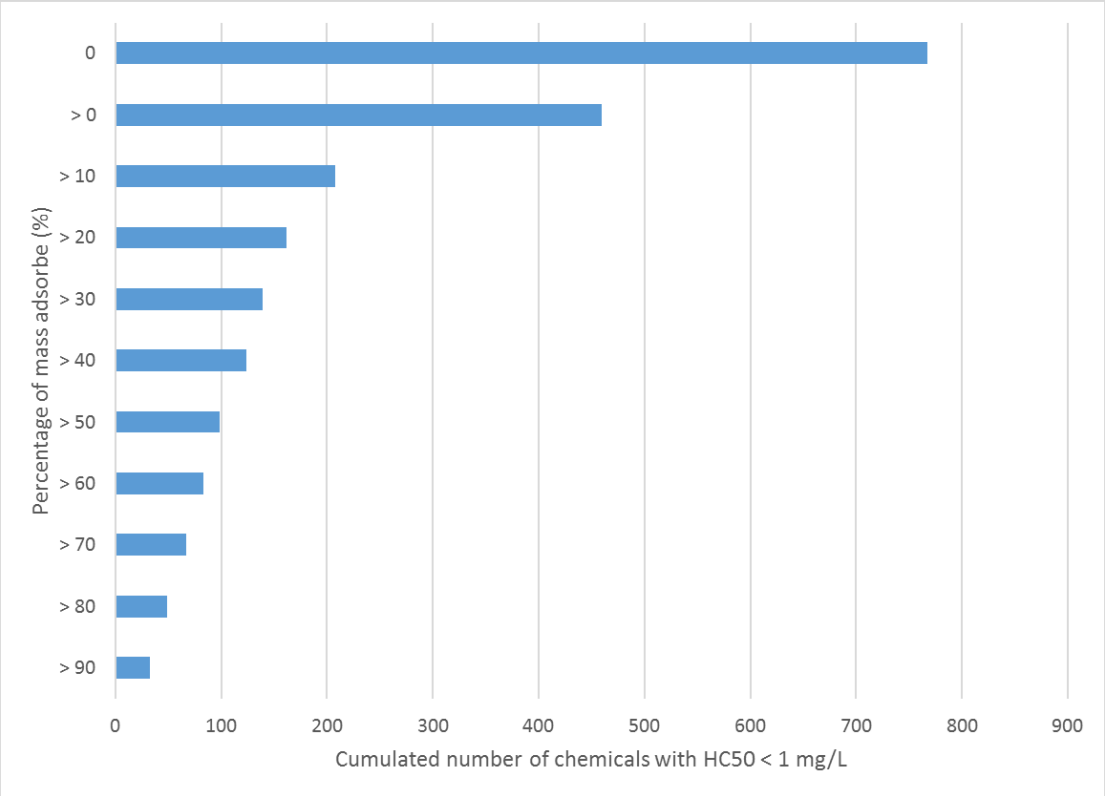

Figure 5: Exposure Factors (XF) versus bioaccumulation factors (BAF) extracted from the 'USEtox® 1.01 organic database. The horizontal red line indicates the limits between bio accumulative and very bio accumulative chemicals according to (13 and 21)