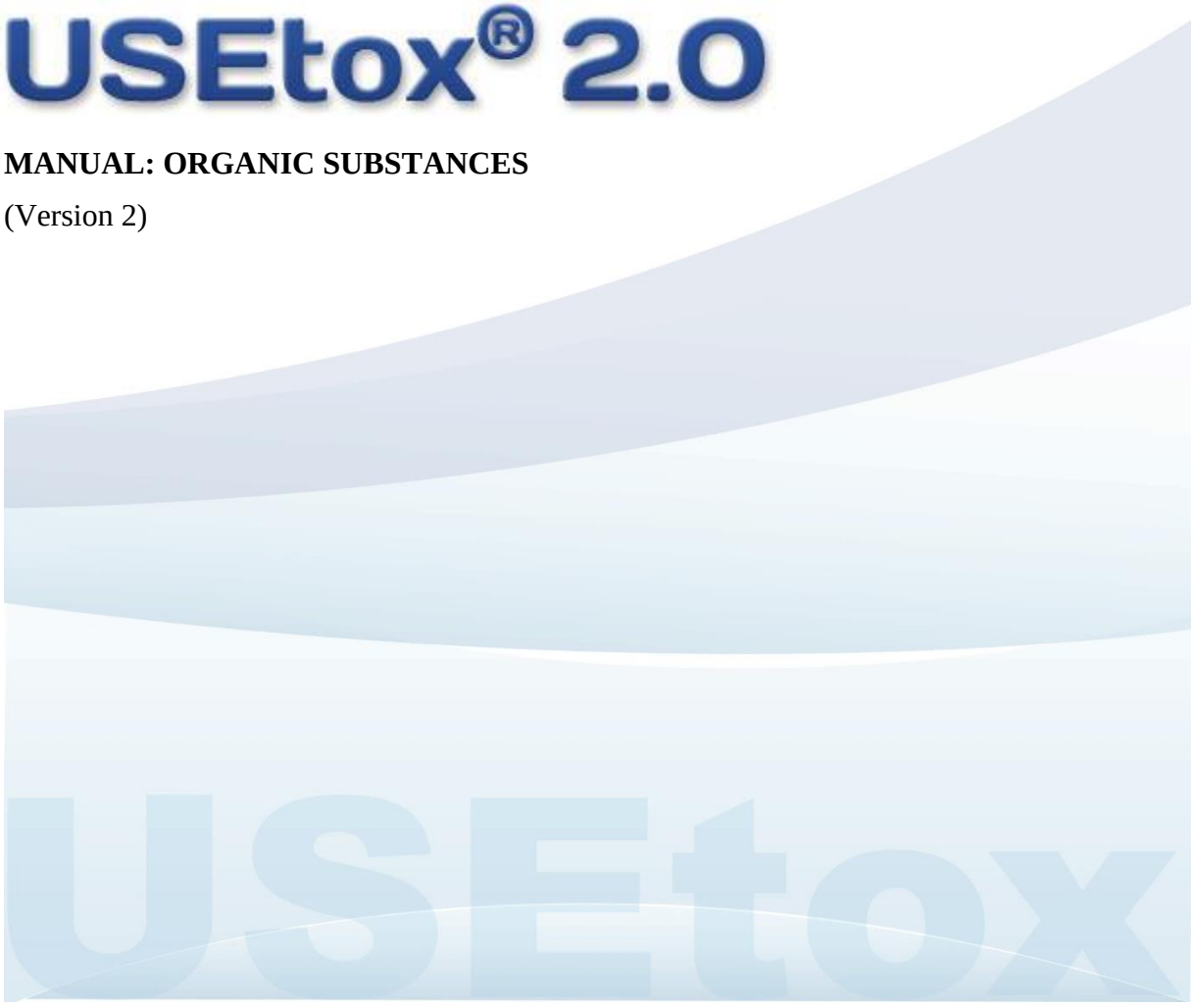
UNEP/SETAC scientific consensus model for characterizing human toxicological and ecotoxicological impacts of chemical emissions in life cycle assessment

USEtox® 2.0

MANUAL: ORGANIC SUBSTANCES

(Version 2)



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USEtox® 2.0 Manual: Organic Substances (Version 2)

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PREFACE

This document represents the official **manual for the organic substances database of USEtox**, the United Nations Environment Programme (UNEP) / Society of Environmental Toxicology and Chemistry (SETAC) scientific consensus model for characterizing human and ecotoxicological impacts of chemical emissions in life cycle assessment. Main output of USEtox is a database of **«recommended» and «indicative» characterization factors** for human toxicity and freshwater ecotoxicity, based on modelling of environmental fate, exposure, and effect parameters for the substances. Due to deficiencies in the model or the available substance data, the «indicative» factors are accompanied by a higher uncertainty than the «recommended» factors, and this should be considered when applying the factors and interpreting the results.

USEtox is officially endorsed by the UNEP/SETAC Life Cycle Initiative, and recommended as assessment method by the European Commission (EC) in the Recommendations on the Use of Common Methods to Measure and Communicate the Life Cycle Environmental Performance of Products and Organisations, 2013/179/EU, by the European Commission's Joint Research Centre – Institute for Environment and Sustainability (JRC-IES) in the International Reference Life Cycle Data System (ILCD) Handbook – Recommendations for Life Cycle Impact Assessment in the European context, EUR 24571 EN, by the World Business Council for Sustainable Development (WBCSD) in the Life Cycle Metrics for Chemical Products – A Guideline by the Chemical Sector to Assess and Report on the Environmental Footprint of Products, Based on Life Cycle Assessment, and by the United States Environmental Protection Agency in the Tool for the Reduction and Assessment of Chemical and other Environmental Impacts (TRACI) User's Manual, S-10637-OP-1-0.

The latest release version of USEtox is available at http://usetox.org.

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1. INTRODUCTION

The USEtox model is an environmental model for characterization of human toxicological and ecotoxicological impacts in life cycle assessment. It has been developed by a team of researchers from the Task Force on Toxic Impacts under the UNEP-SETAC Life Cycle Initiative (Hauschild et al. 2008, Rosenbaum et al. 2008). The mission is to improve understanding and management of chemicals in the global environment by further developing, evaluating, applying and disseminating the model USEtox that describes the fate, exposure and effects of chemicals (Westh et al. 2015).

The USEtox model has been implemented in Microsoft® Excel® and applied for 3077 organic substances to calculate characterization factors for human toxicity and freshwater aquatic ecotoxicity. The chemical-specific data selection for the calculations of the organic substances is described in the present manual. Further details can also be found in Henderson et al. (2011) and Rosenbaum et al. (2011). It should be stressed that the characterization factors are useful for a first tier assessment. In case an organic substance appears to dominantly contribute to the impact scores for toxicity, it is recommended to verify the reliability of the chemical-specific input data for this substance and to improve the data whenever possible.

A database of chemical-specific properties is available in Microsoft® Excel® format (file name «USEtox_substance_data_organics.xlsx») containing data aiming to (a) have a consistent set of data (b) of a certain minimum quality (c) for as many organic substances as possible for which characterization factors can be computed. This includes three types of datasets: (1) physicochemical properties, (2) toxicological effect data on laboratory animals as a surrogate to humans, and in rare cases effect data on humans, and (3) ecotoxicological effect data for freshwater organisms. We focused our effort on identifying and collecting existing reviewed databases for which scientific judgement was already made in selecting and recommending values from a large range of values collected from the literature. For each of the three types of datasets, we (1) identified the existing databases, (2) defined a selection scheme and criteria for data gathering and (3) compiled the database for all the organic substances for which partitioning coefficients and effect data for aquatic ecosystems or humans were found.

In USEtox, characterization factors can be specified as «indicative», reflecting the level of reliability of the calculations in a qualitative way. Due to the relatively high uncertainty of addressing environmental fate and human exposure, the following organic substance groups are classified as «indicative»:

- Dissociating substances: all organic substances, for which dissociation constants (pKa) could not be calculated with SPARC 6.0 (http://www.archemcalc.com/sparc.html), are flagged as «indicative».
- Amphiphilic substances: a list of marketed detergents received from Procter & Gamble has been used to specify these organic substances in the database as «indicative» (Pant 2008, personal communication).
- Organometallic substances.

Additionally, we flagged factors as «indicative» in the following cases:

- Aquatic ecotoxicological characterization factors are specified as «indicative», if effect factors are based on ecosystem species toxicity data covering less than three different trophic levels. This is to ensure a minimum variability of biological responses.

- For human health effects, characterization factors are specified as «indicative» if effect factors are based on sub-acute data. Furthermore, if route-to-route extrapolation is applied to obtain ingestion or inhalation human health effect factors, a subdivision should be made between recommended and «indicative» characterization factors. First, human health characterization factors based on route-to-route extrapolation should be considered «indicative» when the primary target site is specifically related to the route of entry. In addition, characterization factors based on extrapolation from the ingestion to inhalation route of entry should be considered «indicative» if the expected fraction absorbed via inhalation is much higher than the fraction absorbed via ingestion, e.g. a factor of 1,000. This factor of 1,000 is rare but indicates that exposure by inhalation may be far more toxic than by ingestion. With the Kow-based QSARs applied to calculate the expected fraction absorbed via inhalation, it appears that this factor of 1,000 applies for organic substances with Kow smaller than 2.5×10^{-2} or Kow larger than 4.5×10^{9}. In these cases, the «indicative» characterization factor can underestimate the potential impact by inhalation.

In Table 1, an overview of chemical-specific data used by USEtox for organic substances is given. These data along with their main sources and how to apply them in USEtox are detailed in the following chapters.

Table 1. Chemical-specific data in USEtox for organic substances

Parameter	**Symbol**	**Unit**	**Remarks**
Chemical abstract service registry number	CAS RN	-	-
Chemical common name	Name	-	-
Target class for pesticides	PesticideTargetClass	-	New in USEtox 2.0
Chemical class for pesticides	PesticideChemClass	-	New in USEtox 2.0
Molar mass	MW	g/mol	-
pKa chemical class	pKaChemClass	-	New in USEtox 2.0
pKa base reaction	pKa.gain	-	New in USEtox 2.0
pKa acid reaction	pKa.loss	-	New in USEtox 2.0
Partitioning coefficient between *n*-octanol and water	K_{OW}	L/L	-
Partitioning coefficient between organic carbon and water	K_{OC}	L/kg	-
Henry's law constant (at 25°C)	K_{H25C}	$Pa\cdot m^3/mol$	-
Vapor pressure (at 25°C)	P_{vap25}	Pa	-
Solubility (at 25°C)	Sol_{25}	mg/L	-
Partitioning coefficient between dissolved organic carbon and water	K_{DOC}	L/kg	-
Rate constant degradation in air	k_{degA}	1/s	-
Rate constant degradation in water	k_{degW}	1/s	-
Rate constant degradation in sediment	k_{degSd}	1/s	-
Rate constant degradation in soil	k_{degSl}	1/s	Updated in USEtox 2.0

Parameter	Symbol	Unit	Remarks
Rate constant dissipation in above-ground plant tissues	k_{dissP}	1/s	Updated in USEtox 2.0
Rate constant dissipation in wheat	$k_{dissWheat}$	1/s	New in USEtox 2.0
Rate constant dissipation in rice	$k_{dissRice}$	1/s	New in USEtox 2.0
Rate constant dissipation in tomato	$k_{dissTomato}$	1/s	New in USEtox 2.0
Rate constant dissipation in apple	$k_{dissApple}$	1/s	New in USEtox 2.0
Rate constant dissipation in lettuce	$k_{dissLettuce}$	1/s	New in USEtox 2.0
Rate constant dissipation in potato	$k_{dissPotato}$	1/s	New in USEtox 2.0
Bioaccumulation factor in plant roots	BAF_{root}	kg_{veg}/kg_{soil}	-
Bioaccumulation factor in plant leaves	BAF_{leaf}	kg_{veg}/kg_{soil}	-
Biotransfer factor in meat	BTF_{meat}	d/kg_{meat}	-
Biotransfer factor in milk	BTF_{milk}	d/kg_{milk}	-
Bioaccumulation factor in fish	BAF_{fish}	L/kg_{fish}	-
Average of the log of the species-specific geometric means of concentrations affecting 50% of the exposed species population for a defined endpoint	$avlog_{EC50}$	mg/L	-
Human-equivalent lifetime dose per person that causes a non-cancer disease probability of 50% via inhalation	$ED50_{inh,noncanc}$	kg/lifetime	-
Human-equivalent lifetime dose per person that causes a non-cancer disease probability of 50% via ingestion	$ED50_{ing,noncanc}$	kg/lifetime	-
Human-equivalent lifetime dose per person that causes a cancer disease probability of 50% via inhalation	$ED50_{inh,canc}$	kg/lifetime	-
Human-equivalent lifetime dose per person that causes a cancer disease probability of 50% via ingestion	$ED50_{ing,canc}$	kg/lifetime	-

2. ENVIRONMENTAL FATE AND EXPOSURE DATA

Physicochemical properties and bioaccumulation factors of organic substances were derived in the following way:

Generally, the Estimation Programs Interface (EPI) Suite™ for Microsoft® Windows®, version 4.11 (http://www.epa.gov/oppt/exposure/pubs/episuite.htm) has been selected as the default database for the derivation of physicochemical properties for the USEtox fate calculations of organic substances. The EPI Suite is a Windows-based suite of physical/chemical property and environmental fate estimation programs developed by the United States – Environmental Protection Agency's Office of Pollution Prevention Toxics and Syracuse Research Corporation. Experimental data are also provided in EPI Suite and as a general rule, these experimental data were favored over any estimated data provided by EPI Suite or elsewhere. If experimental data were not available, USEtox internal estimation routines are applied (e.g. for Koc) as implemented in the sheet «Fate» of the main USEtox model file. In case that no USEtox internal estimation routines are available, the following estimation routines in EPI Suite were applied:

- Molar mass (MW in g/mol): no estimation routine required.
- pKa: dissociation constants for organic acids ('pKa.loss' of the acid dissociation reaction) or bases ('pKa.gain' of the dissociation reaction of the base's conjugated acid), and amphoters (both pKa.loss and pKa.gain) are calculated with SPARC 6.0 (http://www.archemcalc.com/sparc.html), taking the lowest reported pKa across acid reactions as 'pKa.loss' and the highest reported pKa across base reactions as 'pKa.gain'. When no acid pKa is reported by SPARC, the value 14 is taken for 'pKa.loss'; when no base pKa is reported by SPARC, 'pKa.gain' is set to the value 0, effectively predicting no significant net ionization of the parent substance. For substances containing metal ions and some other organic substances, dissociation constants could not be derived in SPARC, which means that currently, these substances are assumed to follow environmental fate behavior of neutral substances.
- Octanol-water partitioning coefficient (Kow in L/L): A 'fragment constant' methodology to predict log Kow has been applied. In a 'fragment constant' method, a structure is divided into fragments (atoms or larger functional groups).
- Organic carbon-water partitioning coefficient (Koc in L/kg): logKow-based regression equations from the sub-routine KOCWIN are provided in the substance database, but not currently used as QSAR estimates based on Franco and Trapp (2008) are always preferred.
- Vapor pressure (Pvap25 in Pa): For solids, the modified Grain estimate is the suggested VP. For liquids and gases, the suggested VP is the average of the Antoine and the modified Grain estimates. Both methods use the boiling point to estimate vapor pressure.
- Solubility (Sol25 in mg/L): The water solubility is estimated with regression equations using the octanol-water partition coefficient (Kow) and the melting point of an organic substance.
- Henry constant (KH25C in $Pa.m^3/mol$): In case experimental information is lacking, KH25C is calculated by Pvap25*MW/ Sol25.
- Partitioning coefficient between dissolved and organic carbon (Kdoc in L/kg): no experimental data were implemented in the database and no estimation routine in EPI Suite™ was available. In USEtox, the Kdoc is estimated by Kdoc = 0.08 * Kow in the log Kow range up to 7.5, based on Burkhard (2000).

Degradation rates in air, water, soil and sediment are required for the USEtox calculations for organic substances. For air degradation rates, experimental values for the k_{OH} (the hydroxyl radical rate constant in units of cm^3/molecule/sec) are for some organic substances available in EPI Suite. To derive the degradation rate in air (kdegA in 1/s), the k_{OH} is multiplied with the [OH] (the hydroxyl radical concentration in units of molecules (or radicals) per cm^3). The default [OH] is set at 1.5×10^6 molecules (radicals)/cm^3 per 12 hours of daylight. For dioxins and PCBs, experimental degradation data in air, water, soil and sediments are taken from Sinkkonen and Paasivirta (2000). For pesticides, degradation data in soil are based on experimental data reported from field studies in the Pesticide Properties Database (DT50 in days) of the Footprint project (Footprint 2015), from which the degradation rate constant kdegSl (1/s) is obtained as kdegSl = ln(2)/(DT50×86400) with 86400 seconds per day as unit conversion factor.

If experimental data were not available or not provided by Sinkkonen and Paasivirta (2000) or Footprint (2015), the following estimation routines in EPI Suite™ were applied:

- Degradation rates in air (kdegA in 1/s): The estimation methods for k_{OH} are based upon structure-activity relationship (SAR) methods using 'fragment constants'.
- Degradation rates in water, soil and sediment (kdegW, kdegSl, kdegSd in 1/s): specifically for estimating biodegradation half-lives with EPI Suite, the Biowin3 model is used for USEtox input to convert the ultimate biodegradation probability in half-lives for all chemicals in the database (Figure 2).

Table 2. Relation between Biowin3 output and default biodegradation half-lives and biodegradation rate constants.

Biowin3 Output	**Assigned half-life (days)**	**Rate constant (1/s)**
Hours	0.17	4.7×10^{-5}
Hours to Days	1.25	6.4×10^{-6}
Days	2.33	3.4×10^{-6}
Days to Weeks	8.67	9.3×10^{-7}
Weeks	15	5.3×10^{-7}
Weeks to Months	37.5	2.1×10^{-7}
Months	60	1.3×10^{-7}
Recalcitrant	180	4.5×10^{-8}

In addition, division factors of 1:2:9 are used to extrapolate biodegradation rates for water, soil and sediment compartments respectively, as suggested in EPI Suite. Other degradation mechanisms, such as direct photolysis and hydrolysis, were not included in the chemical database of USEtox. The user could of course adjust the specific degradation rates in any environmental compartment considering that generally:

$k_{degradation,total} = k_{biodegradation} + k_{hydrolysis} + k_{photolysis}$, etc.

Dissipation rates in above-ground plant tissues and for the specific plant archetypes wheat, (paddy) rice, tomato, apple, lettuce, and potato are not available in EPI Suite and are derived from Fantke et al. (2014). Dissipation rates for wheat, (paddy) rice, tomato, apple, lettuce, and potato are only calculated for pesticides.

Experimental data for the bioaccumulation in fish are provided in EPI Suite, which were favored over estimated data. For biotransfer factors for milk and meat, experimental data were taken from Rosenbaum et al. (2009) and implemented in the USEtox database.

If experimental data were not available, the following estimation routines were applied:

- Bioaccumulation factors for fish: the Arnot-Gobas model for the upper trophic level in EPI Suite is selected to estimate steady-state bioaccumulation factors (BAF; L/kg) for non-dissociating chemicals and chemicals with log Kow < 9 (Arnot & Gobas 2004). The model includes mechanistic processes for bioconcentration and bioaccumulation such as chemical uptake from the water at the gill surface and the diet, and chemical elimination at the gill surface, fecal egestion, growth dilution and metabolic biotransformation. The model requires the octanol-water partition coefficient (Kow) of the chemical and the estimated whole-body metabolic biotransformation rate constant (1/d) as input parameters to predict BAF values. In case the chemical is indicated as dissociating or the chemical has a log Kow larger than 9, the Arnot-Gobas model is not recommended. Instead, we applied the log Kow-based Bioconcentration factor (BCF; L/kg) estimation routine in EPI suite for these chemicals.
- Biotransfer factors (BTF in d/kg) for milk and meat are estimated based on the model by Travis and Arms (1988), truncated at the maximum and minimum Kow used in the underlying data. This results in a constant BTF outside the Kow range of their training set, as recommended in the Technical Guidance Document (TGD) on Risk Assessment (EC European Commission 2003).
- For bioaccumulation in plant roots and leaves, no experimental data are implemented in the USEtox database for organic substances. QSARs readily implemented in USEtox are applied for this purpose.

3. TOXICOLOGICAL EFFECT DATA

3.1 Human toxicity – cancer

The following order of preference in selecting human toxicity data has been used in the USEtox calculations of carcinogenic effect factors:

1. The carcinogenic effect factor takes as a point of departure the effect dose at 50% (ED_{50}) which is preferably estimated from the low-dose, slope factor (q*), based on human data (Crettaz et al. 2002). The slope factors for 1,3-butadiene, acrylonitrile, benzene and benzidine for humans after inhalation were available via the IRIS database (http://www.epa.gov/iris/). Low-dose slope factors for inhalation are reported in units of $m^3/\mu g$. Again, the ED_{50} is derived by 0.8/q* where 0.8 is a 1/q*-to-ED_{50} conversion factor. After that, the unit was converted from $\mu g/m^3$ to kg/person/lifetime, using a default lifetime of 70 years and a default inhalation rate of 13 m^3/day per person.
2. In case no quantitative effect information on humans was available from the IRIS database, ED_{50} values from the carcinogenic potency database were taken (CPDB; http://potency.berkeley.edu/). ED_{50} values for ingestion and inhalation are reported in units of mg/kg/day and converted to kg/person/lifetime, using a default lifetime of 70 years and a default body weight of 70 kg per person. For cancer, the harmonic mean of all positive ED_{50} in the CPDB is retained for the most sensitive species of animal cancer tests after application of an allometric interspecies conversion factor proportional to body weight to the power of 0.25. Table 3 (see next section) provides an overview of interspecies conversion factors applied in constructing the USEtox organic substances database (Huijbregts et al. 2005). Experimental data in the CPDB database are available for rats, mice, hamsters, dogs, monkeys.
3. In case no quantitative effect information was available from the CPDB, the carcinogenic ED_{50} has been estimated from the low-dose slope factor (q*) by a 1/q*-to-ED_{50} conversion factor of 0.8, based on animal data. The slope factors were again taken from the IRIS database (http://www.epa.gov/iris/).
4. In case no data was available for a specific exposure route, a route-to-route extrapolation has been carried out, assuming equal ED_{50} or slope factor between inhalation and ingestion route (Rosenbaum et al. 2011). Organic substances with all negative carcinogenic effect data were also included as true zero carcinogenic effect factors and distinguished from organic substances with missing data.

3.2 Human toxicity – non-cancer

In the case of effects other than cancer, for most of the organic substances insufficient data were available to recalculate an ED_{50} with dose–response models. In those cases the ED_{50} has been estimated from no-observed effect level (NOEL) by a NOEL-to-ED_{50} conversion factor of 9 (Huijbregts et al. 2005). In case only a LOEL was available, a LOEL-to-ED_{50} conversion factor of 2.25 has been applied (Huijbregts et al. 2005). NOELs and LOELs were derived from the IRIS database (http://www.epa.gov/iris/) and from the World Health Organisation (WHO) with priority for data from the WHO (Rosenbaum et al. 2011). If relevant, conversion factors to extrapolate from sub-chronic to chronic exposure were applied as well (see Huijbregts et al. (2005) for further details). Also for non-carcinogenic effects, the units were converted to kg/person/lifetime, using a default lifetime of 70 years and a default body

weight of 70 kg for ingestion and a default inhalation rate of 13 m^3/day and a default lifetime of 70 years for inhalation, all per person. An allometric interspecies conversion factor proportional to body weight to the power of 0.25 has been applied to the ED_{50} for ingestion (see Table 3). As for non-cancer effects for inhalation, the critical effect concentration is defined as the concentration in the air, the interspecies extrapolation factor for inhalation is in principle 1, assuming that inhalation rates between species scale proportionally to metabolic rates. For some toxicity data after inhalation, however, substance-specific interspecies differences were derived by the US-EPA via pharmacokinetic modelling. In these specific cases, the interspecies conversion factors reported by the US-EPA were applied. As for carcinogenic effects, in case no data is available for a specific exposure route, a route-to-route extrapolation has been carried out, assuming equal ED_{50} between inhalation and ingestion route.

Table 3. Interspecies conversion factors (CF) to humans for various animal species.

Type	**CF interspecies (-)**	**Average body weight (kg)**
human	1.0	70
pig	1.1	48
dog	1.5	15
monkey	1.9	5
cat	1.9	5
rabbit	2.4	2
mink	2.9	1
guinea pig	3.1	0.750
rat	4.1	0.250
hamster	4.9	0.125
gerbil	5.5	0.075
mouse	7.3	0.025

In summary, the following calculation steps of the human-equivalent ED_{50} for organic substances are identified:

1. Gather experimental (i) carcinogenic oral (ingestion exposure) ED_{50} data, (ii) carcinogenic inhalation exposure ED_{50} data, (iii) non-carcinogenic oral (ingestion exposure) ED_{50} data, and (iv) non-carcinogenic inhalation exposure ED_{50} data;
2. Specify for every ED_{50} value whether it is chronic, subchronic or subacute exposure;
3. In case of subchronic or subacute ED_{50} data, derive the chronic-equivalent ED_{50} by respectively dividing by a factor of 2 and a factor of 5 (subchronic-to-chronic extrapolation factor and subacute-to-chronic extrapolation factor);
4. In case of non-human ED_{50} data, derive the human-equivalent ED_{50} by dividing by an extrapolation factor for interspecies differences (see Table 3);
5. In case only carcinogenic, low-dose, slope factors are available, derive the carcinogenic ED_{50} via multiplication of 1/q* with the extrapolation factor for 1/q* to ED_{50}, which is a factor of 0.8;
6. In case only NOAEL-data or NOAEC-data are available, derive the non-carcinogenic ED_{50} via multiplication with the extrapolation factor for NOAEL to ED_{50}, which is a factor of 9;
7. In case only LOAEL-data or LOAEC-data are available, derive the non-carcinogenic ED_{50} via division by the extrapolation factor for LOAEL to NOAEL, which is a factor

of 4, and multiply with the extrapolation factor for NOAEL to ED_{50}, which is a factor of 9;
8. Implement the human-equivalent ED_{50} values (maximum 4 values) in columns AE:AH of the sheet «Substance data» of USEtox model file or of the USEtox organic substances database file.
9. Always be careful with the units!

3.3 Freshwater ecosystem toxicity

Two databases with aquatic ecotoxicity effect data on average EC_{50} values (i.e. HC_{50}) were available, covering, respectively, 3,498 (van Zelm et al. 2007, van Zelm et al. 2009) and 1,408 (Payet 2004) organic substances, the first one being based on acute EC_{50} values from the e-toxBase database of the National Institute for Public Health and the Environment, RIVM (http://ru.nl/environmentalscience/research/themes-0/risk-assessment/e-toxbase/) and the second one being based on chronic and acute EC_{50} data mainly from ECOTOX (http://www.epa.gov/ecotox) and IUCLID International Uniform Chemical Information Database (2000). We prioritize chronic values from Payet (2004) as long as they represent measured EC_{50} values. Second priority is given to acute data from Payet (2004), applying a best estimate extrapolation factor as an acute-to-chronic ratio (ACR), e.g. 1.9 for organic substances and 2.2 for pesticides. In case Payet (2004) does not provide ecotoxicity information for a chemical, acute toxicity data from the RIVM e-toxBase was used, applying an acute-to-chronic ratio (ACR) of 2.

The following calculation steps of the HC_{50} for organic substances are identified:
1. Gather experimental or estimated EC_{50} data for the chemical of interest;
2. Specify for every EC_{50}-value whether it is based on chronic or acute exposure;
3. For acute EC_{50}-data, derive the chronic-equivalent EC_{50} per species by dividing by a chronic-to-acute ratio (ACR) of 2 (Payet 2004);
4. Calculate the geometric mean of EC_{50} (mg/L) for every individual species (this can e.g. be done with the function =GEOMEAN() in Excel);
5. Take the log of the geometric mean EC_{50} per species and calculate the average of the log-values. This average equals the $logHC_{50}$ (log mg/L);
6. Implement this value in column AD of the sheet «Substance data» of USEtox model file or of the USEtox organic substances database file.
7. Always be careful with the units!

4. SUBSTANCES DATABASE IMPORT

The organic substances database, which can be downloaded from http://usetox.org, will be independently updated from the USEtox model itself. To ensure a proper connection between substance database and USEtox model, we provide a step-by-step procedure to import the substance database into the model file below. The proposed procedure assures that the substance database will be fully imported and correctly functional within the USEtox model:

1. Open the USEtox model file «USEtox2.0.xls»
2. Select the worksheet named «Substance data» in the USEtox model file
3. Click on the button «Import a database» in cell C3 (see Figure 1)
4. Select a substance database file to import and confirm

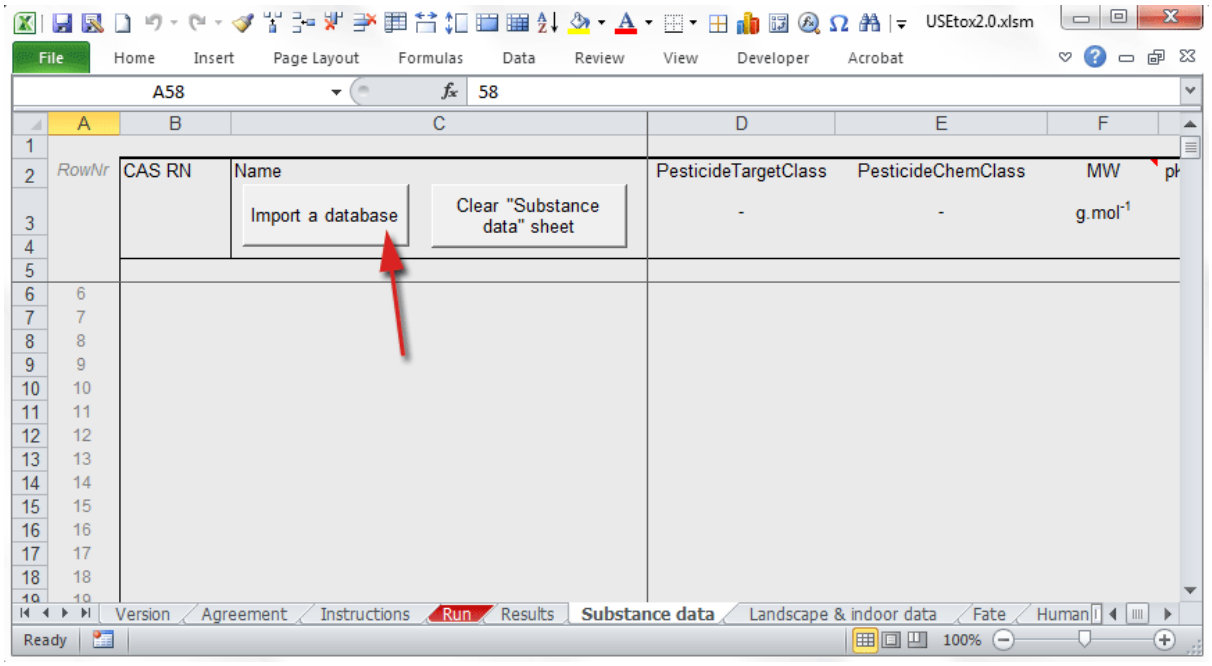

Figure 1. Importing substances database into the USEtox model file.

You have now successfully imported the substances database into your USEtox model file which is ready to calculate factors (e.g. characterization factors) for the imported substances. See the «USEtox 2.0 Manual» for further information on the calculation procedure.

Substance data can also be imported via the USEtox user interface wizard (new in USEtox 2.0). The interface wizard can be opened by clicking in the USEtox model file in sheet «Version» on the button «Launch the USEtox user interface». Then, click in the interface wizard start page (see Figure 2) on the button «Set up calculations with USEtox», where you can either calculate different factors (e.g. characterization factors) for up to 10 selected substances or for all substances available in USEtox. On the next screen, the interface wizard database import page (see Figure 3), you can import the substance database via the button «Import a substance database». More information on how to use the USEtox user interface wizard can be found in the «Manual: User Interface Wizard» that can be found on http//usetox.org.

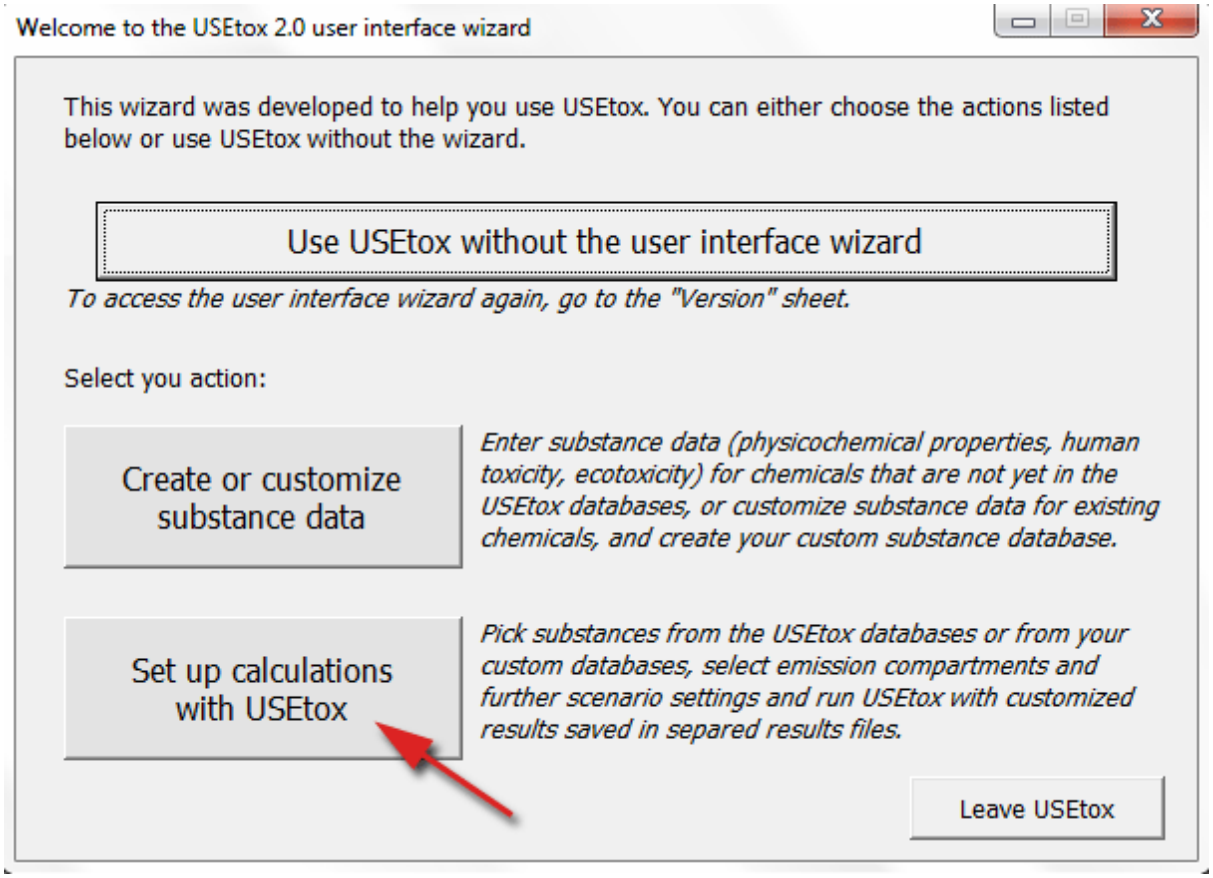

Figure 2. USEtox user interface wizard start screen.

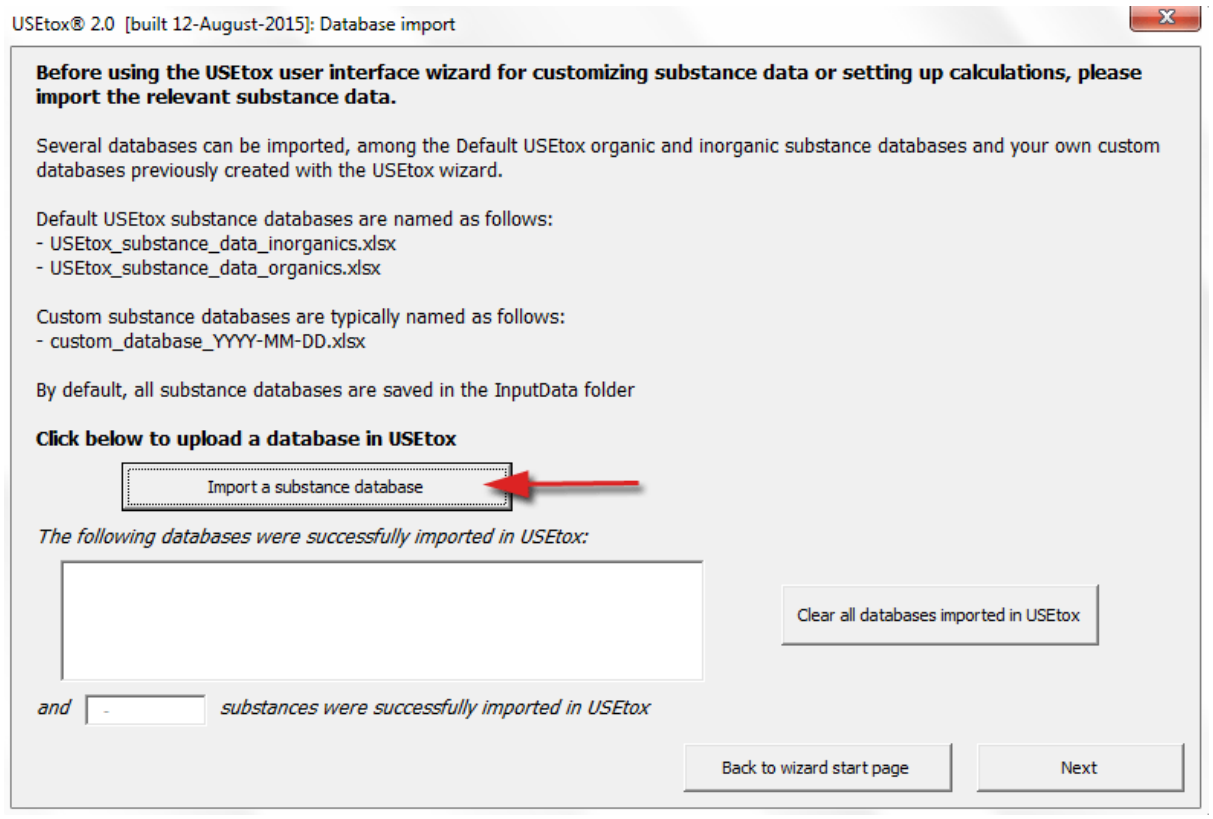

Figure 3. USEtox user interface wizard database import page.

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