

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

USEtox[®] 2.0

MANUAL: INORGANIC SUBSTANCES

(Version 2)

USEtox

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USEtox[®] 2.0 Manual: Inorganic Substances (Version 2)

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PREFACE

This document represents the official **manual for the inorganic 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 27 inorganic substances (all cationic metals) to calculate characterization factors for human toxicity and freshwater aquatic ecotoxicity. The chemical-specific data selection for the calculations of the inorganic 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 inorganic 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_inorganics.xlsx») containing data aiming to (a) have a consistent set of data (b) of a certain minimum quality (c) for as many inorganic 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 inorganic substances for which partitioning coefficients and effect data for aquatic ecosystems or humans were found.

In USEtox, several characterization factors for inorganic substances are specified as «indicative» due to insufficient ecotoxicity effect data. Further, in contrast to organic substances, for which the substance-to-substance variations in transport properties can be attributable to basic physicochemical properties such as solubility ratios, variations in transport properties for inorganic substances depend in complex ways on a range of media properties. The solid/liquid partitioning of inorganic substances in soil can depend on several mineral components as well as the pH, redox potential (EH) and cation-exchange capacity, see e.g. Owsianiak et al. (2013). As a result, there can be significant variations of chemical mobility over very small geographic scales. So it is difficult to identify the appropriate regional *bulk* transport properties for inorganic substances, as is done for organic substances. In addition, inorganic substance species are not *removed* by chemical reactions in the same way that most organic substances are transformed by actions such as biodegradation, photolysis, and hydrolysis. The biodegradation of an organic substance in soil, water, or sediment effectively removes it from the system, but inorganic substance species such as lead, cadmium, and arsenic can only be truly removed from water, soil, or sediment by advection and tend to persist for very long time periods. However, many inorganic substances

species can be made inactive in terms of toxicity by sequestration in a chemical form that is chemically and biologically unavailable. The magnitude and variability of this process is often difficult to quantify, but can be very important for both fate and exposure assessment. Finally, relative to organic substances there are large uncertainties in determining how the variations in observed bioaccumulation and bioavailability come about (in both aquatic and terrestrial food webs). There have not been sufficient experiments to provide the data needed to address the nature and mechanism of the variations of these processes for inorganic substances species.

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.
- Human toxicological characterization factors based on route-to-route extrapolation were considered «indicative» when the primary target site is specifically related to the route of entry.
- Human toxicological characterization factors based on extrapolation from the ingestion to inhalation route of entry were 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. Fractions absorbed for inorganic substances were taken from Owen (1990). This factor of 1,000 indicates that exposure by inhalation may be far more toxic than by ingestion. In these cases, the «indicative» characterization factor can underestimate the potential impact by inhalation. This is the case for Hg(II).

In Table 1, an overview of chemical-specific data used by USEtox for inorganic 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 inorganic substances

Parameter	Symbol	Unit	Remarks
Chemical abstract service registry number	CAS RN	-	-
Chemical common name	Name	-	-
Molar mass	MW	g/mol	-
pKa chemical class	pKaChemClass	-	-
pKa base reaction	pKa.gain	-	-
pKa acid reaction	pKa.loss	-	-
Partitioning coefficient between <i>n</i> -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·m ³ /mol	-
Vapor pressure (at 25°C)	P _{vap25}	Pa	-
Solubility (at 25°C)	SO _{l25}	mg/L	-
Partitioning coefficient between dissolved organic carbon and water	K _{DOC}	L/kg	-

Parameter	Symbol	Unit	Remarks
Partitioning coefficient between suspended solids and water	K_{pSS}	L/kg	Updated in USEtox 2.0
Partitioning coefficient between sediment particles and water	K_{pSd}	L/kg	Updated in USEtox 2.0
Partitioning coefficient between soil particles and water	K_{pSI}	L/kg	Updated in USEtox 2.0
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_{degSI}	1/s	-
Rate constant dissipation in above-ground plant tissues	k_{dissP}	1/s	-
Rate constant dissipation in wheat	$k_{dissWheat}$	1/s	-
Rate constant dissipation in rice	$k_{dissRice}$	1/s	-
Rate constant dissipation in tomato	$k_{dissTomato}$	1/s	-
Rate constant dissipation in apple	$k_{dissApple}$	1/s	-
Rate constant dissipation in lettuce	$k_{dissLettuce}$	1/s	-
Rate constant dissipation in potato	$k_{dissPotato}$	1/s	-
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	Updated in USEtox 2.0
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 inorganic substances were derived in the following way:

- Molar mass (MW in g/mol) is taken from the periodic table.
- pKa: dissociation constants for inorganic substances are not used in case of cationic metals. Instead, the equilibrium-based metal speciation model WHAM 7.0 (Tipping et al. 2011) has been used to calculate below described partition coefficients based on archetype-specific water chemistry.
- The Henry constant (KH25C in Pa.m³/mol) is set at 1×10^{-20} Pa.m³/mol, indicating negligible transfer of inorganic substances species from soil and water to air via volatilization.
- Partition coefficients for water (Kp and Kdoc) were modelled using the speciation model WHAM (Tipping et al. 2011) to estimate the dissolved and the adsorbed fraction and then calculate the partition coefficient.
- Degradation rates in air, water, soil and sediment of inorganic substances are set at 1×10^{-20} s⁻¹, indicating no degradation of inorganic substances in the environment.
- Bioconcentration factors (BCF) for fish are preferably taken from IAEA International Atomic Energy Agency (2010). For Beryllium and Cadmium no BCF information was provided for fish by IAEA International Atomic Energy Agency (2010). For these two inorganic substances, BCFs for fish are taken from US-EPA United States - Environmental Protection Agency (2002).
- Biotransfer factors for milk and meat were taken from IAEA International Atomic Energy Agency (2010) and US-EPA United States - Environmental Protection Agency (2002) with a preference for the IAEA-data. For Copper, however, these two data sources did not provide a biotransfer factor for milk or meat. In this case, the biotransfer factor to milk and meat for Copper was taken from Ng (1982).
- Bioconcentration factors for root crops are derived from IAEA International Atomic Energy Agency (2010) and US-EPA United States - Environmental Protection Agency (2002) with a preference for the IAEA-data. Concerning the IAEA-data, information for temperate regions was used. The bioconcentration factors specified as *root crops* are taken from IAEA International Atomic Energy Agency (2010) and US-EPA United States - Environmental Protection Agency (2002) and converted from dry weight to wet weight by dividing with a factor of 5. For Copper, however, these two data sources did not provide a bioconcentration factor for root crops. In this case, the bioconcentration factor in roots for Copper was derived from Versluijs and Otte (2001), also using a conversion factor of 5 to extrapolate from dry weight to wet weight.
- Bioconcentration factors for leaf crops are derived from IAEA International Atomic Energy Agency (2010) and US-EPA United States - Environmental Protection Agency (2002) with a preference for the IAEA-data. For leaf crops, the bioconcentration factors specified for *cereals - grain* are taken from IAEA International Atomic Energy Agency (2010) and US-EPA United States - Environmental Protection Agency (2002), as cereals dominantly contribute to the food consumption by humans within this category. The dry weight to wet weight conversion was set at a factor of 1, indicating approximately equal water content in the grains of cereals and soils. For Copper, however, these two data sources did not provide a bioconcentration factor for leaf crops. In this case, the bioconcentration factor in leaf crops for Copper was derived from Versluijs and Otte (2001). The bioconcentration factor for leaf crops in the review of Versluijs and Otte

(2001) refer to *leafy vegetables*, using a factor of 10 for dry weight to wet weight conversion.

Note that for Tin – Sn(II) – no bioaccumulation factors were available, but also no human toxicological effect data were found, i.e. no human health characterization factors were calculated for this inorganic substance.

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 arsenic (inhalation and ingestion), beryllium (inhalation), cadmium (inhalation) chromium VI (inhalation) and nickel (inhalation) for humans were available via the IRIS database (<http://www.epa.gov/iris/>). Low-dose slope factors for ingestion are reported in units of day.kg/mg. First, the ED_{50} is derived by $0.8/q^*$ where 0.8 is a $1/q^*$ -to- ED_{50} conversion factor (Huijbregts et al. 2005). After that, the unit was converted from mg/kg/day to kg/person/lifetime using a default lifetime of 70 years and a default body weight of 70 kg per person. 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 2 (see next section) provides an overview of interspecies conversion factors applied in constructing the USEtox inorganic 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). Inorganic substances with all negative carcinogenic effect data were also included as true zero carcinogenic effect factors and distinguished from inorganic substances with missing data.

Note that for the following inorganic substances the carcinogenic ED_{50} are not directly reported, but derived from closely related substances via molar mass correction:

- The carcinogenic ED_{50} of Cd(II) for ingestion were derived from information available for cadmium chloride.
- The carcinogenic ED_{50} of Hg(II) for ingestion was derived from information available for mercuric chloride.
- The carcinogenic ED_{50} of Pb(II) for ingestion was derived from information available for lead acetate.

3.2 Human toxicity – non-cancer

In the case of effects other than cancer, for most of the inorganic substances insufficient data were available to recalculate an ED₅₀ with dose–response models. In those cases the ED₅₀ has been estimated from no-observed effect level (NOEL) by a NOEL-to-ED₅₀ conversion factor of 9 (Huijbregts et al. 2005). In case only a LOEL was available, a LOEL-to-ED₅₀ 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 m³/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 ED₅₀ for ingestion (see Table 2). 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 ED₅₀ between inhalation and ingestion route.

Note that for the following inorganic substances the non-carcinogenic ED₅₀ values were not directly reported, but derived from closely related substances via molar mass correction:

- The non-carcinogenic ED₅₀ of Tl(I) for ingestion was derived from information available for thallium(I) chloride.
- The non-carcinogenic ED₅₀ of V(V) for ingestion was derived from information available for vanadium pentoxide (V₂O₅).

Table 2. 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 ED₅₀ for inorganic substances are identified:

1. Gather experimental (i) carcinogenic oral (ingestion exposure) ED₅₀ data, (ii) carcinogenic inhalation exposure ED₅₀ data, (iii) non-carcinogenic oral (ingestion exposure) ED₅₀ data, and (iv) non-carcinogenic inhalation exposure ED₅₀ data;
2. Specify for every ED₅₀ value whether it is chronic, subchronic or subacute exposure;
3. In case of subchronic or subacute ED₅₀ data, derive the chronic-equivalent ED₅₀ 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 ED₅₀ data, derive the human-equivalent ED₅₀ by dividing by an extrapolation factor for interspecies differences (see Table 2);
5. In case only carcinogenic, low-dose, slope factors are available, derive the carcinogenic ED₅₀ via multiplication of 1/q* with the extrapolation factor for 1/q* to ED₅₀, which is a factor of 0.8;
6. In case only NOAEL-data or NOAEC-data are available, derive the non-carcinogenic ED₅₀ via multiplication with the extrapolation factor for NOAEL to ED₅₀, which is a factor of 9;
7. In case only LOAEL-data or LOAEC-data are available, derive the non-carcinogenic ED₅₀ 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 ED₅₀, which is a factor of 9;
8. Implement the human-equivalent ED₅₀ values (maximum 4 values) in columns AE:AH of the sheet «Substance data» of USEtox model file or of the USEtox inorganic substances database file.
9. Always be careful with the units!

3.3 Freshwater ecosystem toxicity

The EC₅₀ data for inorganic substances are taken from three studies (Dong et al. 2014, Gandhi et al. 2011, Gandhi et al. 2010), all of which are based on chronic and acute EC₅₀ values from the ECOTOX database (<http://cfpub.epa.gov/ecotox/>). First priority is given to chronic data. If chronic data is not available, acute data is used, applying an acute-to-chronic ratio (ACR) of 10 for crustaceans, 20 for fishes (Dong et al. 2014) and 15 (average of crustaceans and fishes) for all other trophic levels. In cases where ecotoxicity data were not provided in Dong et al. (2014), acute toxicity data 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/>) are used, applying an acute-to-chronic ratio (ACR) of 10 for crustaceans, 20 for fishes (Dong et al. 2014) and 15 (average of crustaceans and fishes) for all other trophic levels.

The following calculation steps of the HC₅₀ for inorganic substances are identified:

1. Gather experimental or estimated EC₅₀ data for the chemical of interest;
2. Specify for every EC₅₀-value whether it is based on chronic or acute exposure;
3. For acute EC₅₀-data, derive the chronic-equivalent EC₅₀ per species by dividing by a chronic-to-acute ratio (ACR). For cationic metals as specific inorganic substances group, ACR depends on the trophic level, that is 10 for crustacean and 20 for fish (Dong et al. 2014). For all other trophic levels, we recommend to apply an ACR of 15 as average between crustaceans and fishes;
4. Calculate the geometric mean of EC₅₀ (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 EC₅₀ per species and calculate the average of the log-values. This average equals the logHC₅₀ (log mg/L);
6. Implement this value in column AD of the sheet «Substance data» of USEtox model file or of the USEtox inorganic substances database file.
7. Always be careful with the units!

4. SUBSTANCES DATABASE IMPORT

The inorganic 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

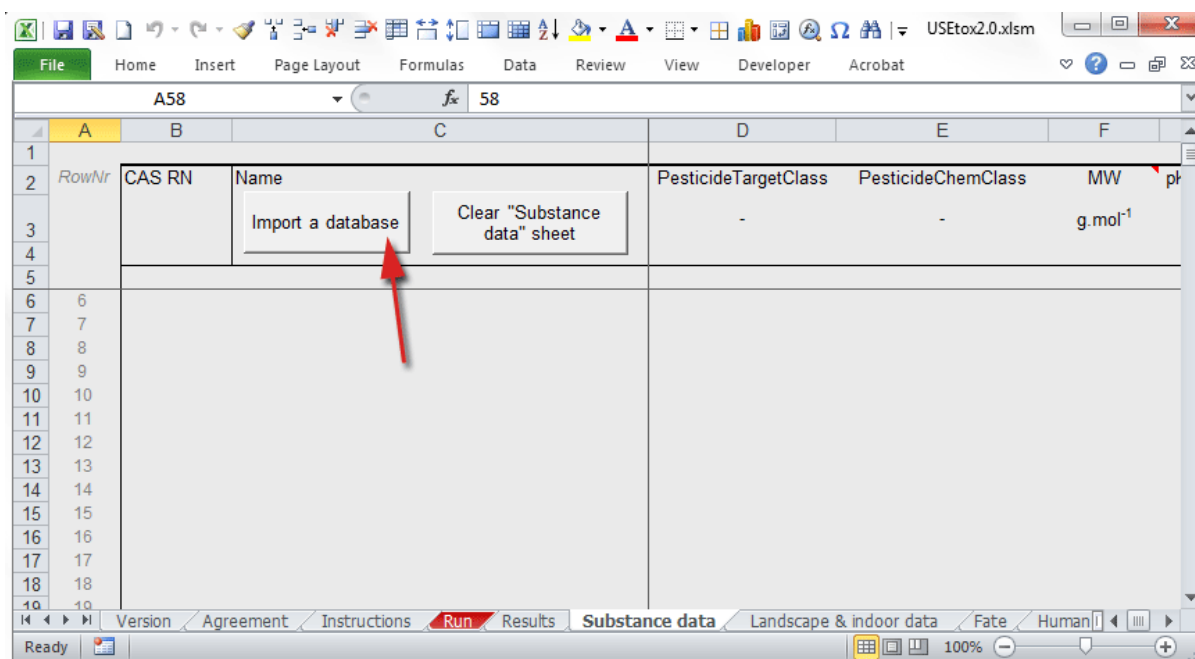


Figure 1. Importing substances database into the USEtox model file.

You have now successfully imported the substances database into your USEtox model file which is ready to calculate (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>.

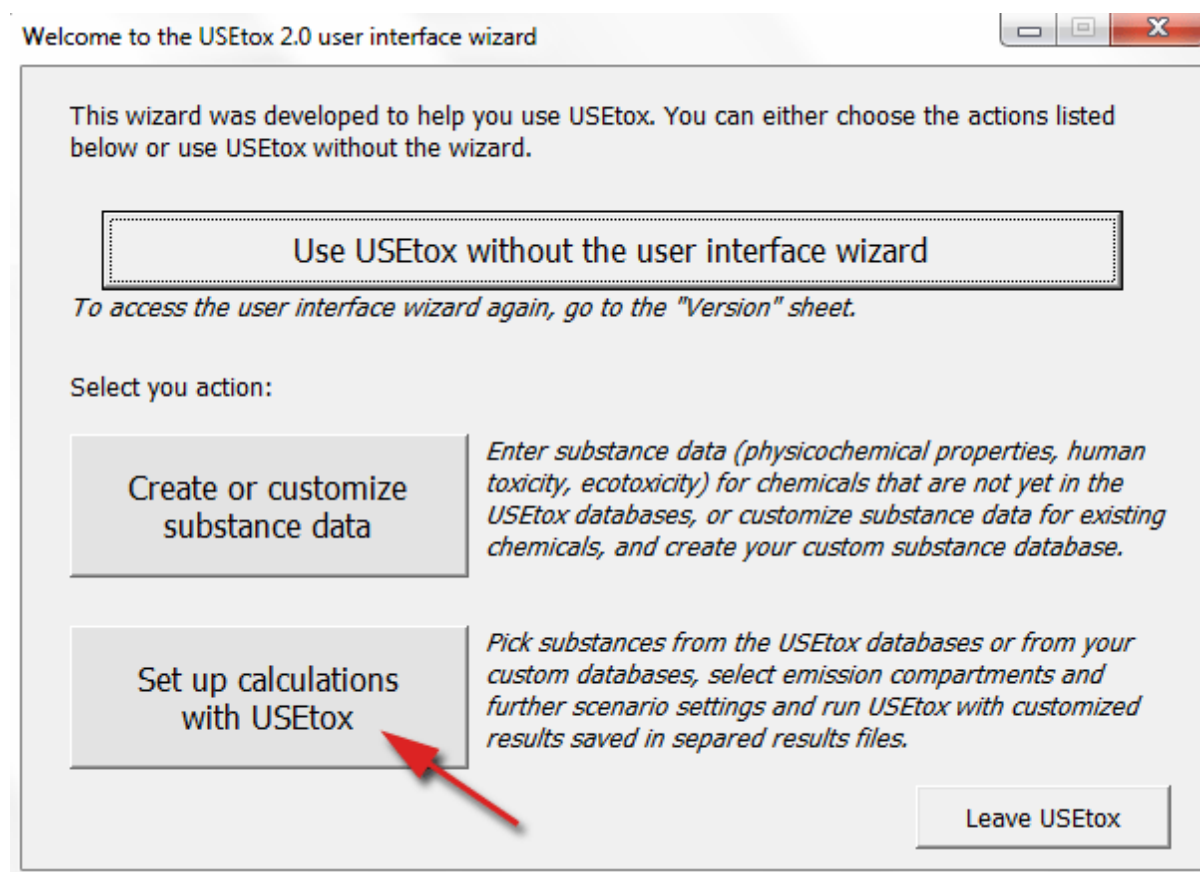


Figure 2. USEtox user interface wizard start screen.

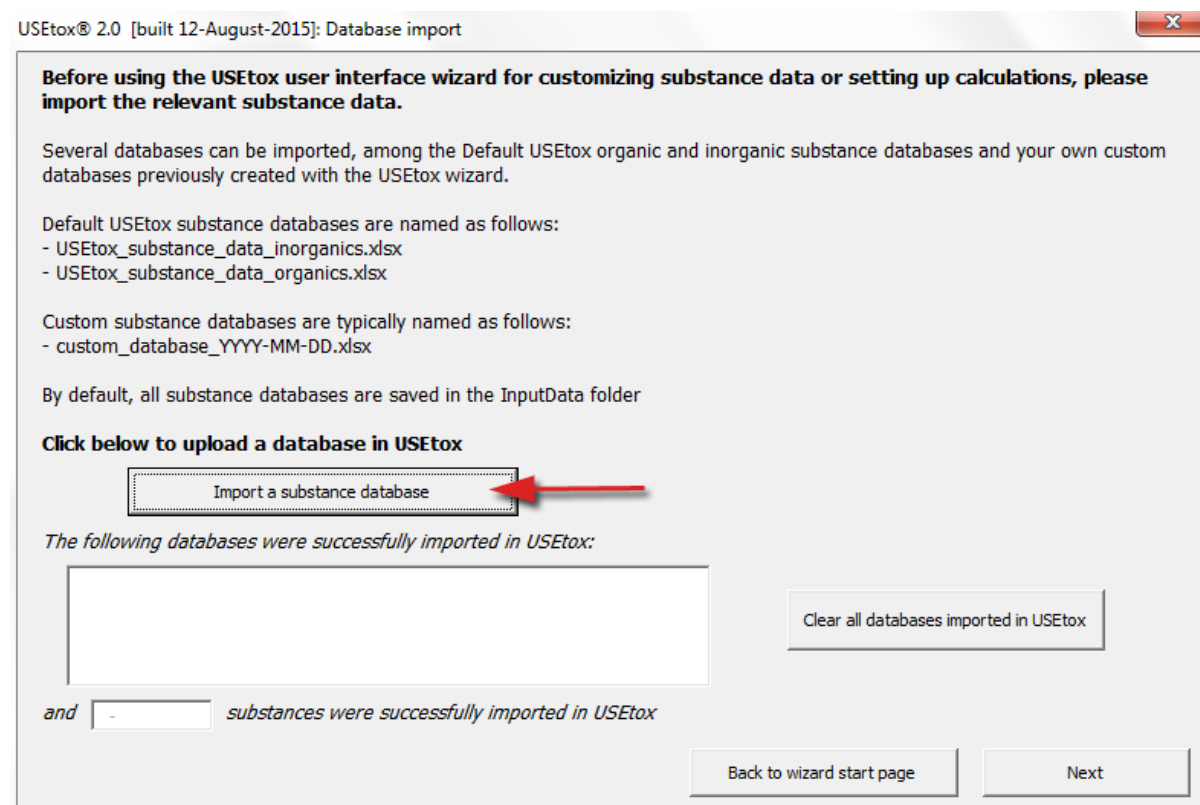


Figure 3. USEtox user interface wizard database import page.

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