USEtox™

- Chemical database: inorganics -

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Colophon

Title: USEtox™ Chemical-specific database: inorganics

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1. Background

The USEtox™ model is an environmental model for characterisation of human and ecotoxicological impacts in Life Cycle Impact Assessment (LCIA) and Comparative Risk Assessment (CRA) of chemicals. It has been developed by a team of researchers from the Task Force on Toxic Impacts under the UNEP-SETAC Life Cycle Initiative. USEtox™ is designed to describe the fate, exposure and effects of chemicals. The UNEP-SETAC Initiative supports the development, evaluation, application, and dissemination of USEtox™ to improve understanding and management of chemicals in the global environment.

The USEtox™ model has been implemented in Microsoft Excel® and applied for 3000+ organic chemicals and 21 inorganic chemicals to calculate characterisation factors for human toxicity and freshwater aquatic ecotoxicity. The chemical-specific data selection for the calculations of the inorganic chemicals is described in this report. It should be stressed that the characterisation factors are useful for a first tier assessment only. In case an inorganic chemical 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 chemical and improve the data whenever possible.

A database of chemical properties was set up with data aiming to (a) have a consistent set of data (b) of a certain minimum quality (c) for as many inorganics as possible for which characterisation factors can be computed. This includes three types of datasets: (1) physico-chemical 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 metals for which partitioning coefficients and effect data for aquatic ecosystems or humans were found.

In USEtox™, characterisation factors for inorganics are all specified as 'interim', reflecting the relatively high uncertainty associated with estimates of fate, exposure and effects for this substance group. In contrast to organic compounds, for which the substance-to-substance variations in transport properties can be attributable to basic chemical 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 (E_H) and cation-exchange capacity. 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 metals, as is done for organic chemicals. In addition, inorganic species are not "removed" by chemical reactions in the same way that most organic chemicals are transformed by actions such as biodegradation, photolysis, and hydrolysis. The biodegradation of an organic chemical in soil, water, or sediment effectively removes it from the system, but species such as lead, cadmium, and arsenic can only be truly removed form water, soil, or sediment by advection and tend to persist for very long time periods. However, many inorganic species can be effectively removed 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 chemicals 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 species.

Additionally, we included an ‘extra’ interim factor in the following cases:

- aquatic ecotoxicological characterisation factors are specified as interim, if effect factors are based on species toxicity data covering less than three different trophic levels. This is to ensure a minimum variability of biological responses.
- human health characterisation factors based on route-to-route extrapolation were considered interim when the primary target site is specifically related to the route of entry.
- human health characterisation factors based on extrapolation from the ingestion to inhalation route of entry were considered interim if the expected fraction absorbed via inhalation is much higher than the fraction absorbed via ingestion, e.g. a factor of 1,000. Fraction absorbed for metals 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 interim characterisation factor can underestimate the potential impact by inhalation. This is the case for Hg(II).

2. Fate and exposure data

Physico-chemical properties and bioaccumulation factors of inorganics were derived in the following way:

1. Molecular weights (MW in g/mol) were taken from the periodic table;
2. The Henry coefficient (K_H25C in $Pa.m^3/mol$) was set at 1.10^{-20} $Pa.m^3.mol^{-1}$, indicating negligible transfer of inorganic species from soil and water to air via volatilisation.
3. Partition coefficients for soil, sediment, suspended solids and dissolved organic carbon were taken from IAEA (2009) and US-EPA (2005), prioritising the IAEA-data. The average partioning coefficients for soil from IAEA (2009) were used and refer to 'all soils'. The average partioning coefficients for suspended solids from IAEA (2009) are preferably based on field data. The exception is for Ag(I) with an average partioning coefficient for suspended solids derived with adsorption experiments in the lab (IAEA, 2009). In case IAEA (2009) does not report partitioning coefficients, the average partitioning coefficients reported by US-EPA (2005) were applied. This is the case for for all metals in case of sediment and dissolved organic carbon partitioning, and for the majority of the metals in case of suspended solids partitioning.
4. Degradation rates in air, water, soil and sediment of inorganics were set at 1.10^{-20} s^{-1}, indicating no degradation of inorganic in the environment.
5. Bioconcentration factors (BCF) for fish were preferably taken from IAEA (2009). For Beryllium and Cadmium no BCF information was provided for fish by IAEA (2009). For these two metals, BCFs for fish were taken from US-EPA (2002).
6. Biotransfer factors for milk and meat were taken from IAEA (2009) and US-EPA (2002) with a preference for the IAEA-data. For Copper, however, these two data sources did not provide a biotransfer factor for milk and meat. In this case, the biotransfer factor to milk and meat for Copper was taken from Ng (1982).
7. Bioconcentration factors for root crops were derived from IAEA (2009) and US-EPA (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' were taken from IAEA (2009) and US-EPA (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.
8. Bioconcentration factors for leaf crops were derived from IAEA (2009) and US-EPA (2002) with a preference for the IAEA-data. For leaf crops, the bioconcentration factors specified for 'cereals - grain' were taken from IAEA (2009) and US-EPA (2002), as cereals dominantly contributes 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 bioconcentrations 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 effect data were found, i.e. no human health characterisation factors were caculated for this metal.

3. Toxicity

Ecotoxicity

Two databases with ecotoxicity effect data on average EC50 values (i.e. HC50s) were available, covering, respectively, 41 (Van Zelm et al. 2009) and 17 metal species (Payet 2004), the first one being based on acute EC50 values from the RIVM e-toxBase (www.e-toxbase.com) and the second one on chronic and acute EC50-data mainly from ECOTOX (http://www.epa.gov/ecotox) and IUCLID (2000). We prioritise chronic values from Payet (2004) as long as they represent measured EC50 values. Second priority is given to acute data from Payet (2004), applying a best estimate extrapolation factor as an acute-to-chronic ratio (ACR) of 2. In case Payet (2004) does not provide ecotoxicity information for an inorganic substance, acute toxicity data from the RIVM e-toxBase was used, applying an acute-to-chronic ratio (ACR) of 2.

Human carcinogenic toxicity

The following order of preference in toxicity data has been used in the USEtox^{TM} calculations of carcinogenic effect factors:

1. The carcinogenic effect factor takes as a point of departure the effect dose 50% (ED50) which is preferably estimated from the low-dose, slope factor (q*), based on human data. 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 ED50 is derived by 0.8/q* where 0.8 is a 1/q*-to-ED50 conversion factor (Huijbregts et al., 2005). After that, the unit was converted from mg/kg/day to kg/person/lifetime, using a lifetime of 70 years and a body weight of 70 kg. Low-dose, slope factors for inhalation are reported in units of $m^3/\mu g$. Again, the ED50 is derived by 0.8/q* where 0.8 is a 1/q*-to-ED50 conversion factor. After that, the unit was converted from $\mu g/m^3$ to kg/person/lifetime, using a lifetime of 70 years and an inhalation rate of 13 m^3/day.
2. In case no quantitative effect information on humans was available from the IRIS database, ED50s from the carcinogenic potency database were taken (CPDB; http://potency.berkeley.edu/). ED50s for ingestion and inhalation are reported in units of mg/kg/day and converted to kg/person/lifetime, using a lifetime of 70 years and a body weight of 70 kg. For cancer, the harmonic mean of all positive ED50s in the CPDB is retained for the most sensitive species of animal cancer tests after application of an allometric interspecies conversion factor proportional to bodyweight to the power of 0.25. Table 2 provides an overview of interspecies conversion factors applied in constructing the USEtox^{TM} chemical database (Huijbregts et al., 2005). Experimental data in the CPDB are available for rats, mice, hamsters, dogs, monkeys.
3. In case no quantitative effect information was available from the CPDB, the carcinogenic ED50 has been estimated from the low-dose, slope factor (q*) by a 1/q*-to-ED50 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 ED50 or slope factor between inhalation and ingestion route. Inorganics with all negative carcinogenic effect data were also included as true zero carcinogenic effect factors and distinguished from missing data.

Note that for the following inorganics the carcinogenic ED50s were not directly reported, but derived from closely related substances via molecular weight correction:

- the carcinogenic ED50s of Cd(II) for ingestion were derived from information available for cadmium chloride;
- the carcinogenic ED50 of Hg(II) for ingestion was derived from information available for mercuric chloride;

- the carcinogenic ED50 of Pb(II) for ingestion was derived from information available for lead acetate.

Non-cancer human toxicity

In the case of effects other than cancer, for most of the inorganics 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. In case only a LOEL was available, a LOEL-to-ED50 conversion factor of 2.25 has been applied. 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. 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 lifetime of 70 years and a body weight of 70 kg for ingestion and an inhalation rate of 13 m^3/day and a lifetime of 70 years for inhalation. An allometric interspecies conversion factor proportional to bodyweight to the power of 0.25 has been applied to the ED50 for ingestion (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 pharmaco-kinetic 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 inorganics the non-carcinogenic ED50s were not directly reported, but derived from closely related substances via molecular weight 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 pentaoxide (V2O5).

Table 2: Interspecies conversion factors to humans for various species

Type	***CF interspecies (-)***	***Average bodyweight (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

4. Database import into USEtox™

The inorganics database, which can be downloaded from www.usetox.org, will be independently updated from USEtox™ itself. To ensure a proper connection between database and USEtox™, we provide a step-by-step procedure to import the database for inorganic substances into the model below. The proposed procedure assures that the database for inorganic substances will be fully and correctly functional and readable by USEtox™:

1. Open both the USEtox™ model ("USEtox.xls") and the database file for the inorganics ("Database_inorganics.xls").
2. Select the worksheet named "Substance data" in the "USEtox.xls" file.
3. Click on the button 'Import Database Metals' located in cel C3.

You have now successfully imported the new metal database into your USEtox™ model which is ready to calculate new updated characterisation factors. See the User Manual for further information on the calculation procedure.

5. Literature

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