

USEtox® 2.0 – Characterization factors for human toxicity and freshwater ecotoxicity for new and updated substances, exposure pathways, and regions

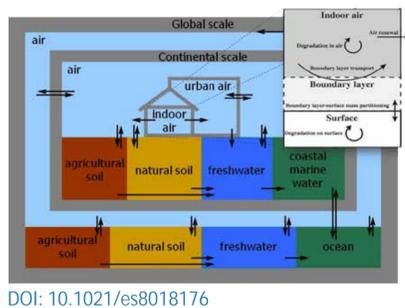
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USEtox is the UNEP/SETAC scientific consensus model for assessing human toxicological and ecotoxicological impacts of chemical emissions. Based on scientific progress in assessing fate, exposure and effects of toxic chemical emissions on humans and ecosystems, ongoing scientific consensus building and harmonization, and a survey of USEtox user requirements, effort was put into updating the first USEtox release version. The next official release version is **USEtox® 2.0 released in 2015**. All updates implemented in USEtox® 2.0 are outlined below. Further details can be found at <http://usetox.org>. All USEtox users are invited to submit data, substances and other proposals to further improve USEtox!

Indoor environments

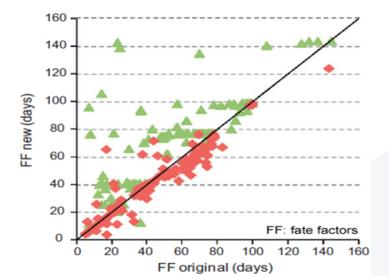
- Household and industrial indoor air compartments for 9 exposure settings
- Ventilation and adsorption considered
- Integration with rate constant matrix (fate)



DOI: 10.1021/es8018176

Ionizing organic chemicals

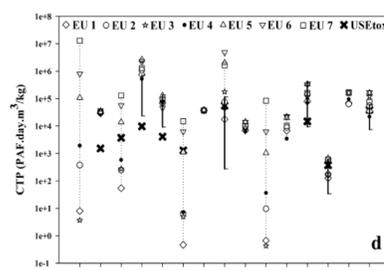
- Degree of ionization based on compartment/phase pH and pKa
- Speciation-specific partitioning in soil based on QSAR equations
- Integrated in modelling of environmental fate processes as input for rate constant matrix



DOI: 10.1016/j.chemosphere.2012.07.014

Freshwater ecotoxicity for metals

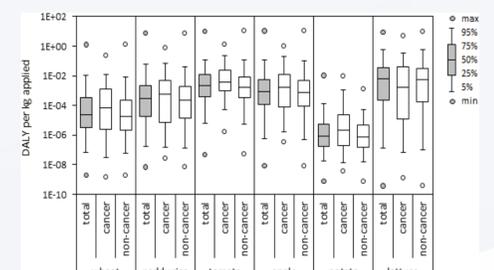
- Generic freshwater ecotoxicity characterization for cationic metals
- Partitioning adjusted for truly dissolved fraction
- Based on parameterized freshwater archetypes



DOI: 10.1016/j.chemosphere.2014.03.046

Exposure to pesticide residues

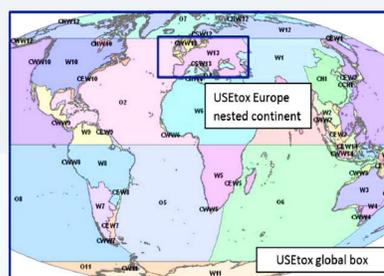
- Human health impacts via exposure to pesticide residues in food crops
- 6 major crop archetypes with crop-specific data
- Integration with human Intake fraction matrix



DOI: 10.1021/es201989d

Sub-continent landscape data

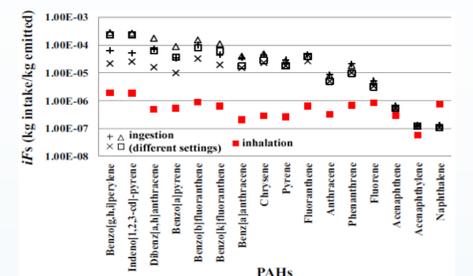
- Landscape datasets for 8 continental and 17 sub-continental regions
- Wind speed, rain, human population, human intake
- Applied as sensitivity study to default dataset



DOI: 10.1016/j.envint.2014.04.004

New chemicals and updated data

- Data and factors for new chemicals (pharmaceuticals, PAHs, triazoles, metals, ...)
- Updated soil half-lives for pesticides
- Small corrective updates of chemical and fate data



DOI: 10.1007/s11367-014-0810-6

User-friendly model interface and full documentation

SINGLE SUBSTANCE or FIRST ROW		FINAL ROW		FIND A SUBSTANCE Row/ir	
Row/ir	Substance	Row/ir	Substance	Search term	Row/ir
1163	Benzyl chloride	1167	benzylbelyde	Benzyl	1163
103-44-7		103-52-7			103-44-7

Loss processes - [day ⁻¹]		Emission compartment	
removal	degradation	home air	occ air
0.00E+00	0.00E+00	4.76E-03	1.88E-01

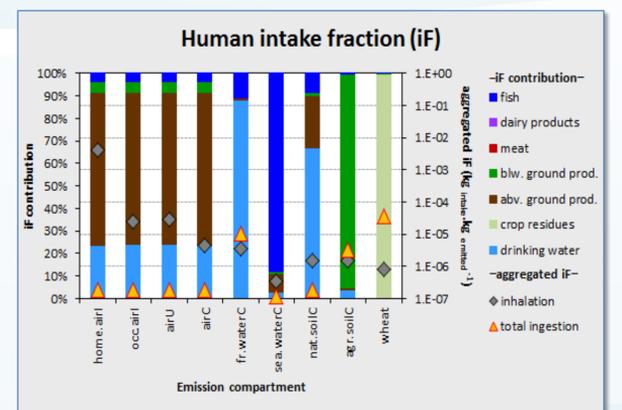
Mass balance rate constants - k [day ⁻¹]		Emission compartment	
home air	occ air	airU	airC
-1.95E+01	0	0	0

Improved scenario definition interface

Data name	Unit	Value	Default value
kdegA - Degradation rate in air	day ⁻¹	8.00E-06	
kdegW - Degradation rate in water	day ⁻¹		
kdegS - Degradation rate in sediment	day ⁻¹		
kdegSI - Degradation rate in soil	day ⁻¹		
kdisP - Disposition rates in above-ground plant tissues	day ⁻¹		
kdisWheat - Disposition rates in wheat	day ⁻¹		
kdisRice - Disposition rates in rice	day ⁻¹		
kdisTomato - Disposition rates in tomato	day ⁻¹		
kdisApple - Disposition rates in apple	day ⁻¹		
kdisLettuce - Disposition rates in lettuce	day ⁻¹		
kdisPotato - Disposition rates in potato	day ⁻¹		

Data name	Unit	Value	Default value
avglogCS0 - Average of the log-values of the species-specific ecotoxicity data	mg L ⁻¹		
ED50h,noncanc - Human equivalent lifetime dose per person that causes a non-cancer disease probability of 50% after inhalation	kg Lifetime ⁻¹		
ED50h,noncanc - Human equivalent lifetime dose per person that causes a non-cancer disease probability of 50% after ingestion	kg Lifetime ⁻¹		
ED50h,canc - Human equivalent lifetime dose per person that causes a cancer probability of 50% after inhalation	kg Lifetime ⁻¹		
ED50h,canc - Human equivalent lifetime dose per person that causes a cancer probability of 50% after ingestion	kg Lifetime ⁻¹		

New interactive user input interface



Additional dynamic output graphs