

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

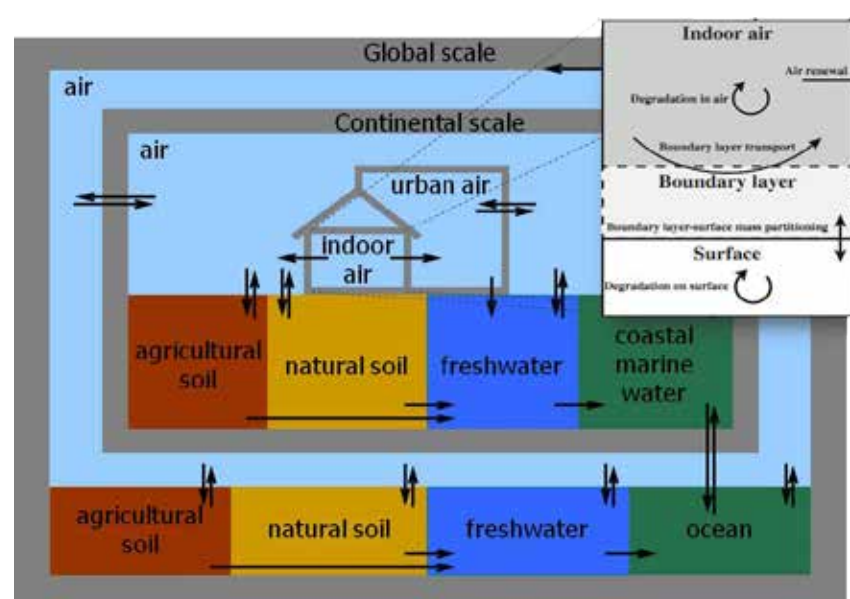
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USEtox is the UNEP/SETAC **scientific consensus model** for assessing **human toxicological and ecotoxicological impacts** of chemical emissions. Based on scientific progress in assessing fate, exposure and effects of toxic chemical emissions on humans 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

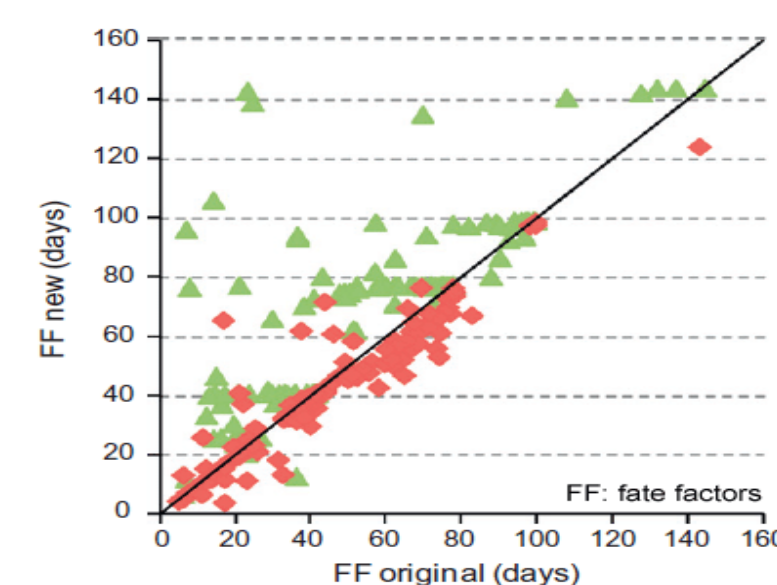
- Household and industrial indoor air compartments for 9 exposure settings
- Ventilation and adsorption considered
- Integration with rate constant matrix (fate)



DOI: 10.1021/es8018176

Ionizing organic chemicals

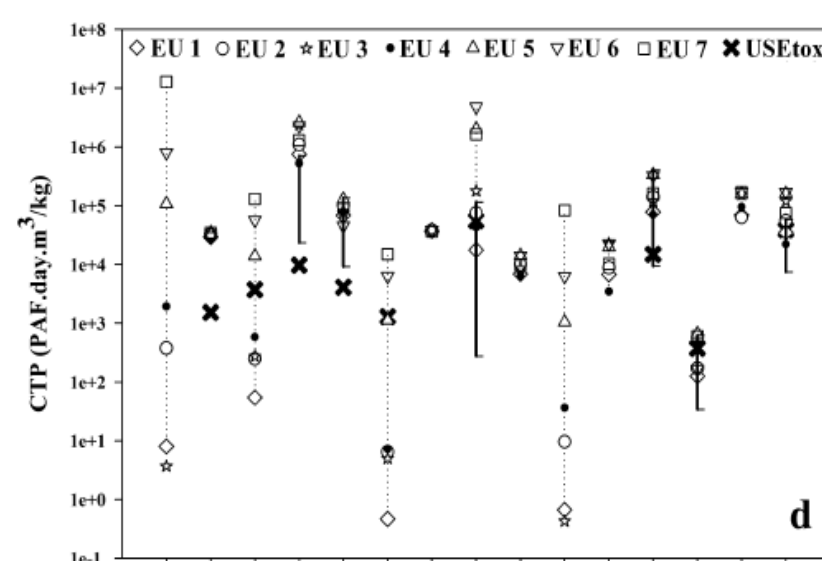
- Degree of ionization based on compartment/phase pH and pKa
- Speciation-specific partitioning in soil based on QSAR equations
- Integrated in modelling of environmental fate processes as input for rate constant matrix



DOI: 10.1016/j.chemosphere.2012.07.014

Freshwater ecotoxicity for metals

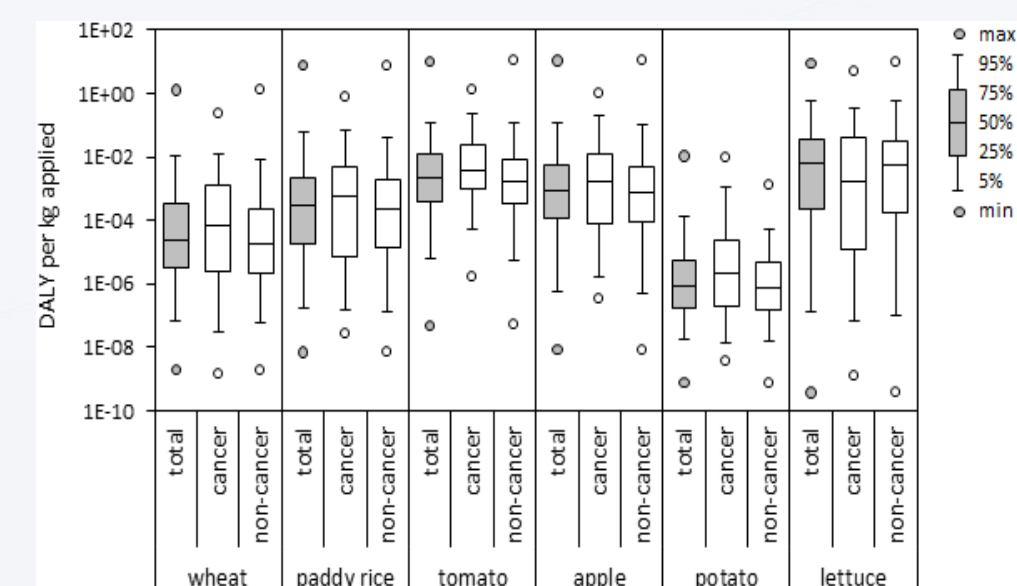
- Generic freshwater ecotoxicity characterization for cationic metals
- Partitioning adjusted for truly dissolved fraction
- Based on parameterized freshwater archetypes



DOI: 10.1016/j.chemosphere.2014.03.046

Exposure to pesticide residues

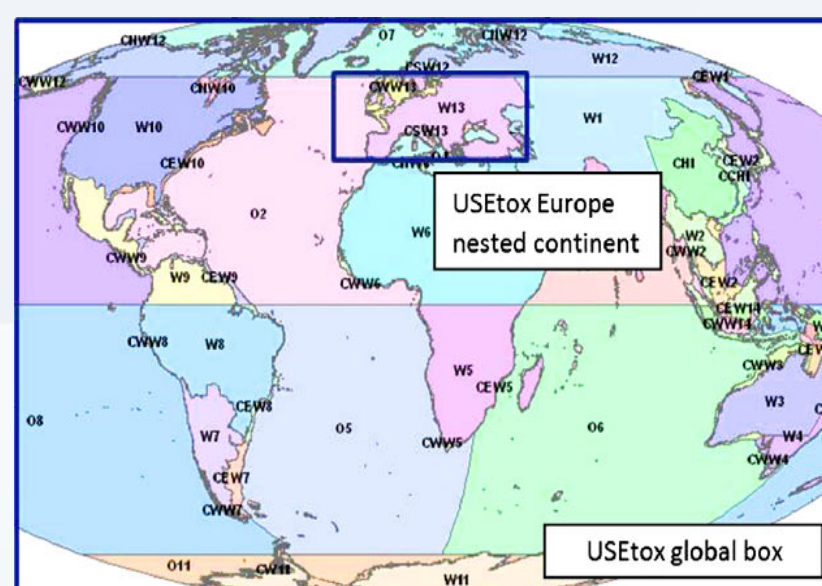
- Human health impacts via exposure to pesticide residues in food crops
- 6 major crop archetypes with crop-specific data
- Integration with human Intake fraction matrix



DOI: 10.1021/es201989d

Sub-continent landscape data

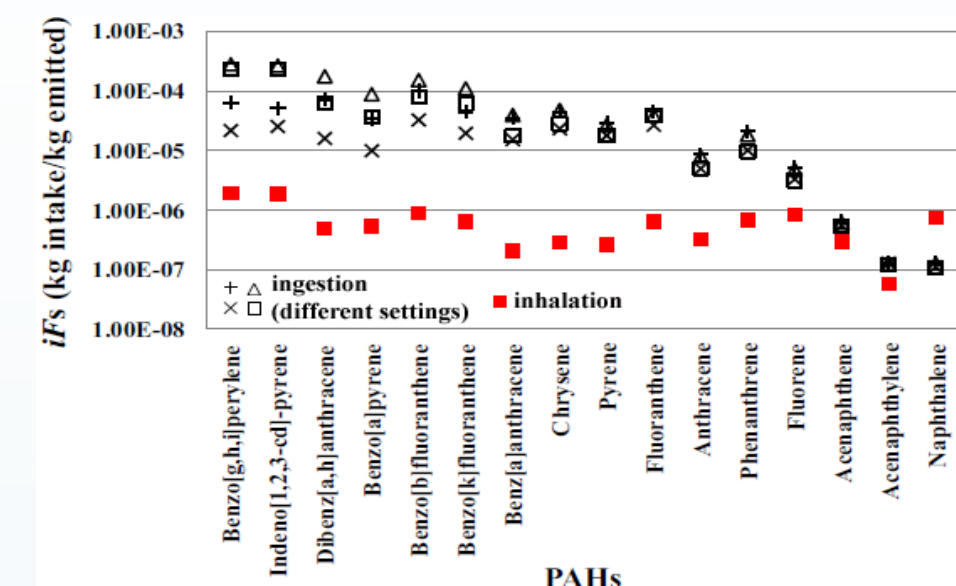
- Landscape datasets for 8 continental and 17 sub-continental regions
- Wind speed, rain, human population, human intake
- Applied as sensitivity study to default dataset



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

CALCULATION OF CHARACTERIZATION FACTORS										
Enter a single substance to see set of matrices below or enter range of rows to create series of results in 'Results multiple substances'										
SINGLE SUBSTANCE or FIRST ROW			FINAL ROW		FIND A SUBSTANCE RowNr					
RowNr	Substance	1163 Benzyl chloride	RowNr	Substance	1167 benzylchloride	Search terms	Benzyl	RowNr	Substance	1163 Benzyl chloride
CAS		100-44-7	CAS		100-52-7	Run series	Search	Apply	CAS RN	100-44-7
Substance running			REGION		INDOOR EXPOSURE			CROP RESIDUES		
RowNr 1163			RegionRowNr 7		HomeName OECD countries average			CropName wheat		
Model USEtox 2.0 [built 11-Mar-2015]			RegionName Default USEtox		OccupationName Industry, OECD					
Date of run 28-Apr-2015										
Loss processes - [day ⁻¹]										
Emission compartment										
	home air	occ air	airU	airC	fr waterC	sea waterC	nat soilC	agr soilC		
removal	0.00E+00	0.00E+00	4.78E-03	3.17E-05	4.69E-04	1.07E-05	4.06E-04	4.06E-04		
degradation	0.00E+00	0.00E+00	1.88E-01	1.98E-01	4.62E-02	4.62E-02	2.31E-02	2.31E-02		
Mass balance rate constants - k [day ⁻¹]										
Emission compartment										
Receiving compartment	home air	occ air	airU	airC	fr waterC	sea waterC	nat soilC	agr soilC		
	home air	-1.90E+01	0	0	0	0	0	0		
	occ air	-2.88E+02	0	0	0	0	0	0		
	airU	9.48E+00	2.30E+02	-1.88E+01	1.07E-04	0	0	0		
	airC	4.68E+00	5.78E-01	1.89E+01	-3.95E-01	1.64E-01	4.11E-03	1.14E-02		
	fr waterC	0	0	2.38E-03	1.30E-03	-2.18E-01	0	4.07E-04	4.07E-04	
	sea waterC	0	0	0	4.73E-03	6.97E-03	-5.31E-02	0	0	
	nat soilC	0	0	0	7.81E-04	0	0	-3.53E-02	0	
	agr soilC	0	0	0	7.81E-04	3.99E-04	0	0	-3.53E-02	
	airU	0	0	0	1.09E-01	0	0	0	0	
	fr waterC	0	0	0	0	0	0	0	0	
	oceanU	0	0	0	0	0	2.76E-03	0	0	
nat soilC	0	0	0	0	0	0	0	0		
agr soilC	0	0	0	0	0	0	0	0		
nat soilC	0	0	0	0	0	0	0	0		
agr soilC	0	0	0	0	0	0	0	0		