USEtox ecotoxicity effect modelling

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USEtox characterisation factor

Effect Factor
For aquatic ecotoxicity

$$CF = FF \cdot XF \cdot EF$$

USEtox effect factor for aquatic ecotoxicity

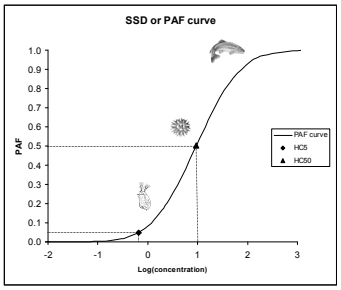
$$EF = \frac{0.5}{HC50} = \frac{0.5PAF}{HC50_{EC50}} \qquad (PAF*m^3/kg)$$

HC50 is the hazardous concentration (kg/m³) of a chemical at which 50% of the species (in an aquatic ecosystem) are exposed to a concentration above their EC50 (e.g. the concentration at which 50% of a population dies in a laboratory test). It is calculated by:

$$\log HC50 = \frac{1}{n_s} \cdot \sum_s \log EC50_s$$

where n is the number of species (or taxa or throphic levels) for which EC50 values are available

Species Sensitivity Distribution
Potentially Affected Fraction of species (PAF)



$$PAF = \frac{1}{1 + e^{-(\log C - \alpha)/\beta}}$$

Where:
C is the concentration
α is the location parameter = logHC50
USEtox: α = logHC50

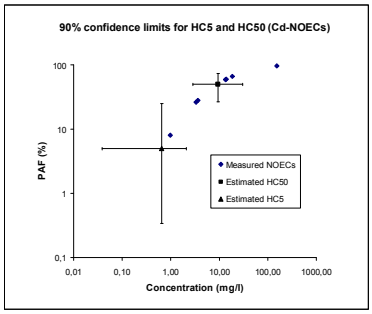
$$\log HC50 = \frac{1}{n_s} \sum_s \log EC50_s$$

β is the scale parameter:

$$\beta = \frac{\sqrt{3}}{\pi} \sigma$$

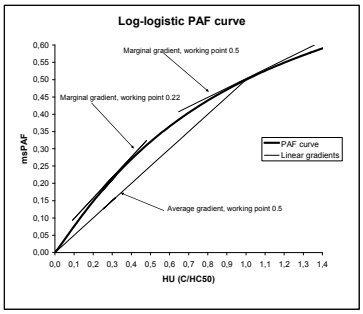
σ is the standard deviation

Different uncertainties for HC50 and HC5



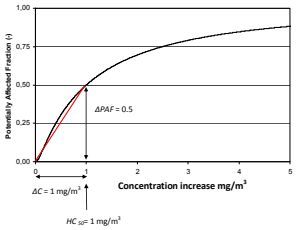
(Larsen and Hauschild 2007; Int J LCA 12 (1) 24-33)/Straalen & Denneman 1989)

Different linear gradients and working points



(Larsen and Hauschild 2007; Int J LCA 12 (1) 24-33)

Example visualisation of the extrapolation procedure for the ecotoxicological effect factor in USEtox



(USEtox™ manual v. 1.00, Januar 2010)

Calculation of HC50

$$HC50 = anti\log(\frac{1}{n_s} \cdot \sum_s \log EC50_s)$$

OR IN EXCEL

$$HC50 = GEOMEAM(EC50s)$$

Critical issues:

1. **Which EC50s to include as raw data**
2. **Which avg. EC50 to include**

EC50s recommended for USEtox

(based on recommendations from the UNEP-SETAC "ecotox effect investment team"; EVS, RIVM, EPFL, DTU)

- At least three different EC50 values (species) from at least three different trophic levels
  - Otherwise the estimated HC50 value is designated "interim"
- Chronic (long-term) EC50s are preferred with population relevant endpoints, e.g.:
  - Reproduction
  - Growth
  - Mortality
- If a sufficient number of $EC50_{chronic}$ is available (≥ 3) an $HC50_{chronic}$ is calculated and used directly in the EF (0.5/HC50)
- If the number of $EC50_{chronic}$ values are insufficient (< 3) but sufficient $EC50_{acute}$ values (≥ 3) are available an $HC50_{acute}$ is calculated. On this basis a $HC50_{chronic}$ is calculated by use of an assessment factor of 2: $HC50_{chronic} = HC50_{acute}/2$
- In the majority of cases only enough acute data are available
- No consensus on averaging principle but level of single species chosen for pragmatically reasons

Choosing among acute EC50s

- In order to treat chemicals as equally as possible and avoid bias is the LCA comparison (try to) choose results from standard tests with standard organism:
  - Primary producers (algae):
    - Time duration: 72 - 120 hours
    - End point: Inhibition of growth
    - Species: *Raphidocelis subcapitata*, *Scenedesmus subspicatus*, *Scenedesmus quadricauda*, *Chlorella vulgaris*, *Anabaena flos-aqua*, *Microcystis aeruginosa*, *Navicula seminulum* and *Navicula pelliculosa*.
  - Primary consumers (crustacean):
    - Time duration: 24 - 96 hours (48 hours preferred)
    - End point: Mortality or immobility (*Daphnia*)
    - Species: *Daphnia magna*, *Daphnia pulex*, *Daphnia sp.*, *Ceriodaphnia dubia*, *Neomysis mercedis* and *Brachionus calyciflorus*
  - Secondary/tertiary consumers (fish):
    - Time duration: 96 - 336 hours (96 hours preferred)
    - End point: Mortality
    - Species: *Ambassis macleayi, Carassius auratus auratus, Cyprinus carpio carpio, Danio rerio (Brachydanio rerio), Ictalurus punctatus, Lepomis cyanellus, Lepomis macrochirus, Leuciscus idus, Melanotaenia splendida inornata, Onchorhynchus kisutch, Onchorhynchus mykiss (Salmo gairdneri), Oryzias latipes, Pimephales promelas, Poecilia reticulate* and *Salvelnius fontinalis*

(Larsen and Hauschild 2007; Int J LCA 12 (2) 79-91)

Data sources for EC50s

- ECOTOX: ECOTOXicology Database system. US EPA: http://cfpub.epa.gov/ecotox/
- ESIS: Including IUCLID: http://ecb.jrc.ec.europa.eu/esis/
- RIVM (1999): Appendix A in: Environmental Risk Limits in The Netherlands. Part III Data. Könemann H (ed.). Report No. 601640 001. RIVM, Bilthoven, The Netherlands

Geometric means (GMs) - for the calculation of HC50 - and lowest EC50 for tetrachlorophenol

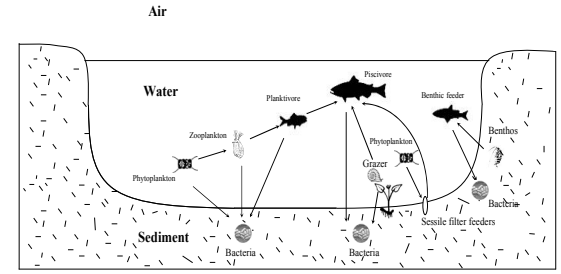
Taxa/trophic level	Species	EC50acute (mg/l)	GMspecies	GMgenus	GMtropic level
Algea	Chlorella vulgaris	10,10	10,10	10,10	3,62
(primary producers)	Selenastrum capricornutum	1,30	1,30	1,30	
Crustacean (primary consumers)	Daphnia galeata mendotae	0,58	0,58	0,31	0,31
	Daphnia magna	0,29	0,17		
	Daphnia magna	0,18			
	Daphnia magna	0,09			
Fish (secondary consumers)	Lepomis macrochirus	0,14	0,14	0,14	0,47
	Oncorhynchus mykiss	0,33	0,33	0,33	
	Poecilia reticulata	1,09	0,81	0,81	
	Poecilia reticulata	0,60			
	Oryzias latipes	0,62	0,62	0,62	
	Pimephales promelas	1,03	1,03	1,03	
	Geometric mean	0,55	0,68	0,75	0,81
	LoEC50	0,09	0,14	0,14	0,31

Exercise:

Calculating the HC50-value for 4-methyl-2-pentanone

Species	EC50acute (mg/L)
Selenastrum capricornutum	400
Daphnia magna	170
Pimephales promelas	780
Pimephales promelas	540
Pimephales promelas	537
Pimephales promelas	509
Pimephales promelas	505
Oncorhynchus mykiss	600

What is it we want to protect?



(Larsen and Hauschild 2007; Int J LCA 12 (2) 79-91)

Two main approaches for estimating the ecotoxicity effect factor, EF

- Species Sensitivity Distribution (SSD) or PAF based approaches; *Effect based*, average approach (e.g. Impact 2002+, EDIP200X, **USEtox**)

$$EF = \frac{PAF = 0.5}{HC_{50}} = \frac{0.5}{HC_{50}}$$

- Assessment Factor based approaches (PNEC); *No effect based (e.g. EDIP97, CML):*

$$EF = \frac{1}{PNEC}$$

Examples of existing approaches for ecotoxicity effect factors

Criteria	PNEC-based approaches				PAF-based approaches		
	AF-based PNEC (only acute data)	AF-based PNEC (only chronic data)	AF- based PNEC (chronic (preferred) and acute data)	SSD-based PNEC ($HC5_{SCEC}$)	'Marginal PAF increase' (fixed β value)	Average PAF increase, HC5 (fixed β value)	Average PAF increase, HC50
Compatibility	+	++	+(+)	++	++	++	+++
Environmental relevance	+	+++	++(+)	+++	+++	+++	+++
Reproducibility	++	+(+)	+(+)	++(+)	+++	++(+)	+++
Transparency	++++	+++(+)	+++(+)	++	+(+)	+(+)	+(+)
Low data demand	++++	+++	+++(+)	++	+	++	++
High data availability	++++	++	++++	+(+)	+	+(+)	+(+)
Spatial differentiation possible	+	+(+)	+	++	+++	++ [b]	+(+)
Quantification of uncertainty included	+	+	+	++ [c]	++ [b]	++ [c]	++++ [b]

++++: Very high degree of fulfilment
+++: High degree of fulfilment
++: Moderate degree of fulfilment
+: Low degree of fulfilment

a: Payet fixed
b: Implemented in AMI (Payet 2004, 2005)
c: Not implemented but possible

(Larsen and Hauschild 2007; Int J LCA 12 (1) 24-33)

Pros and cons for the 0.5/HC50 approach

(as opposed to the PNEC approach)

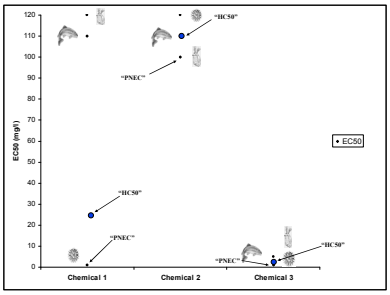
PROS

- The risk of bias from the laboratory test set-up is low compared to a no-effect based indicator (PNEC), where the highest tested concentration, which is not statistically different in toxicity from the control concentration, is typically reported.
- The use of a value which is estimated and placed in the centre of the concentration response curve (i.e. HC50) gives the lowest uncertainty.
- The quantification of damage in terms of potential loss of species is possible (at least in theory).

CONS

- The focus is shifted away from protection of the function and structure of ecosystems.
- The importance of very sensitive species may be neglected.

PNEC (low. EC50) as opposed to HC50 (geo. mean)



Definitions and abbreviations

- HC50 : **The hazardous concentration of a chemical at which 50% of the species (in an aquatic ecosystem) are exposed to a concentration above their EC50**
- EC50 : **The concentration at which 50% of a population (e.g. fish) is affected (e.g. dies) in a laboratory test**
- PAF : **Potentially affected fraction of species**
- PNEC : **Predicted no effect concentration**
- NOEC : **No observed effect concentration**

References/Further information

- Larsen HF, Hauschild M (2007). GM-troph: A low data demand ecotoxicity effect indicator for use in LCIA. *Int J LCA 12(2) 79-91.*
- Larsen HF, Hauschild M (2007). Evaluation of Ecotoxicity Effect Indicators for Use in LCIA. *Int J LCA 12(1) 24-33 (Erratum for p. 32 in: Int J LCA 12(2) 92).*
- *Payet J (2004): Assessing Toxic Impacts on Aquatic Ecosystems in Life Cycle Assessment (LCA). PhD thesis No. 3112 (2004). EPFL, Lausanne, Switzerland*