USEtox ecotoxicity effect modelling

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USEtox characterisation factor

\[ CF = FF \cdot XF \cdot EF \]

For aquatic ecotoxicity

USEtox effect factor for aquatic ecotoxicity

\[ EF = \frac{0.5}{HC50} = \frac{0.5PAF}{HC50EC50} \] (PAF m/\(\text{kg}\))

HC50 is the hazardous concentration (kg/m\(^3\)) 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:

\[ \log HC50 = \frac{1}{n} \sum \log EC50_i \]

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

Species Sensitivity Distribution

Potentially Affected Fraction of species (PAF)

Where:

- \(C\) is the concentration
- \(n\) is the number of species
- \(\alpha\) is the location parameter = \(\log HC50\)
- \(\beta\) is the scale parameter
- \(\sigma\) is the standard deviation

Different uncertainties for HC50 and HC5

90% confidence limits for HC5 and HC50 (CE/NOECs)

Different linear gradients and working points

Log-logistic PAF curve

Marginal gradient, working point 0.5
Marginal gradient, working point 0.22
Marginal gradient, working point 0.5
Marginal gradient, working point 0.22
Example visualisation of the extrapolation procedure for the ecotoxicological effect factor in USEtox

Calculation of HC50

\[ HC_{50} = \text{anti } \log \left( \frac{1}{n} \sum \log EC_{50_i} \right) \]

OR IN EXCEL

\[ HC_{50} = \text{GEOMEAN} (EC_{50s}) \]

Critical issues:
1. Which EC50s to include as raw data
2. Which avg. EC50 to include

Choosing among acute EC50s

• In order to treat chemicals as equally as possible and avoid bias in the LCA comparison (try to) choose results from standard tests with standard organisms:
  - 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 pelliculosa and Navicula perminuta
  - 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 Salvelinius fontinalis (Larsen and Hauschild 2007; Int J LCA 12 (2) 79-91)

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

Data sources for EC50s

• ECOTOX: ECOTOXicology Database system.
  US EPA: [http://cfpub.epa.gov/ecotox](http://cfpub.epa.gov/ecotox)


### Exercise:

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

<table>
<thead>
<tr>
<th>Chemical</th>
<th>PNEC (low EC50)</th>
<th>HC50 (geo. mean)</th>
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</thead>
<tbody>
<tr>
<td>Chemical 1</td>
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<td>Chemical 2</td>
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<td>Chemical 3</td>
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</table>

### What is it we want to protect?

**Air**

**Water**

**Grazer**

**Phytoplankton**

**Zooplankton**

**Benthos**

**Phytoplankton**

**Sessile filter feeders**

**Bacteria**

**Bacteria**

**Bacteria**

### 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)

\[ EF = \frac{PAF}{0.5} \frac{HC50}{HC50} \]

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

\[ EF = \frac{1}{PNEC} \]

### Examples of existing approaches for ecotoxicity effect factors

<table>
<thead>
<tr>
<th>Criteria</th>
<th>AF-based PNEC (only acute data)</th>
<th>AF-based PNEC (only chronic data)</th>
<th>AF-based PNEC (chronic and acute data)</th>
<th>SSD-based PNEC (HC50 NOEC)</th>
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<tbody>
<tr>
<td>Compatibility</td>
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<td>Environmental relevance</td>
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<td>Low data demand</td>
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<td>High data availability</td>
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<td>Spatial differentiation</td>
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<td>Quantification of uncertainty included</td>
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### 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.
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