Fate and effects of chemicals including their transformation products

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November 19th 2009

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Life Cycle Impact Assessment modeling

- Provide *input* to quantify impacts of stressors

  - ✓ Putting a score to the effects of a chemical on the environment or humans caused by its emission

  - ✓ Including fate and effects

Characterization factors

Goal

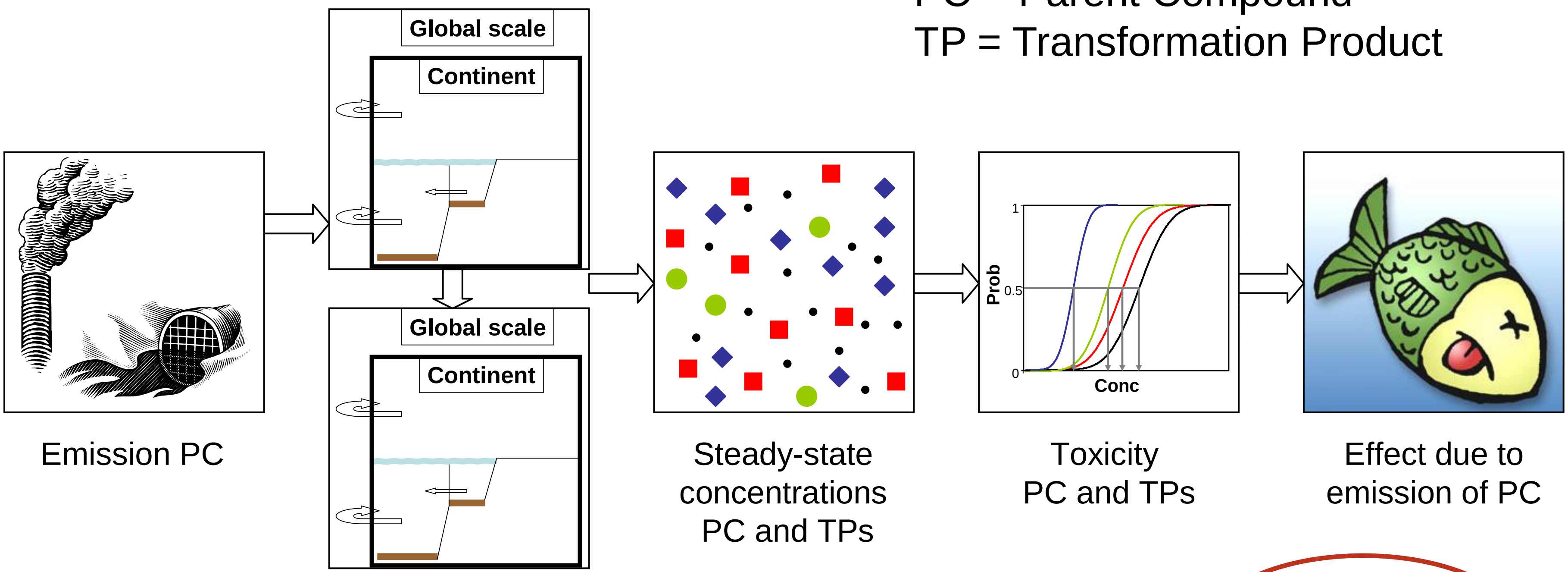
Provide characterization factors for 16 chemicals including their transformation products

- Persistence, mobility *and* toxicity
- Including uncertainty analysis
- Case study atrazine application on corn

Ecotoxic effects

Fate and transformation PC

PC = Parent Compound
TP = Transformation Product



Emission PC

Steady-state concentrations PC and TPs

Toxicity PC and TPs

Effect due to emission of PC

Fate and transformation TPs

Potentially Affected Fraction of species

Fate Factor

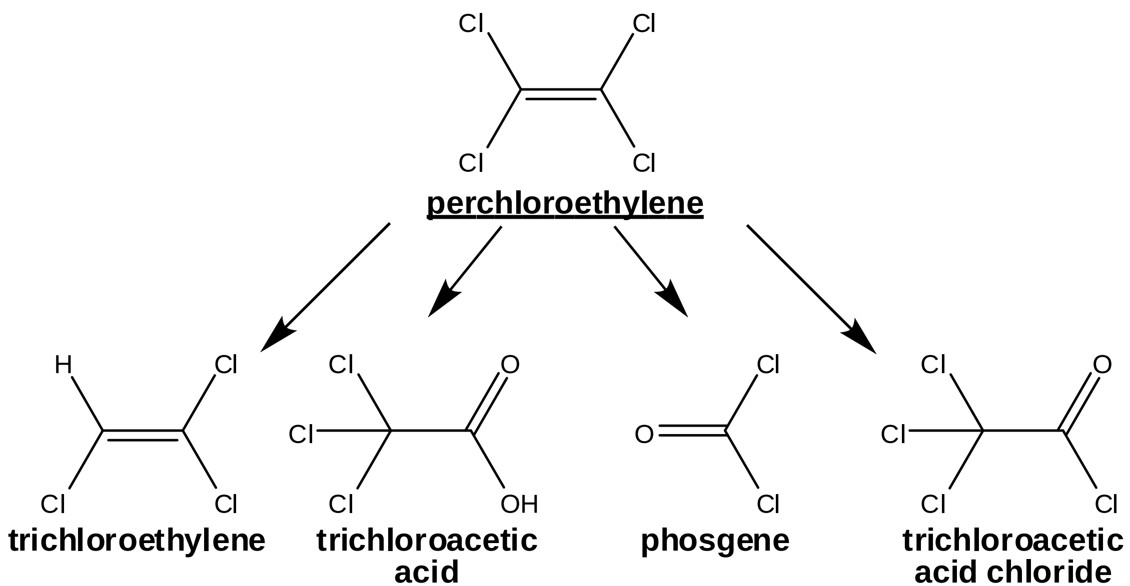
Effect Factor

Ecotoxic effects

Characterization Factor of chemical *x*: $CF_{x,p} = FF_{x,p} \cdot EF_{x,p}$

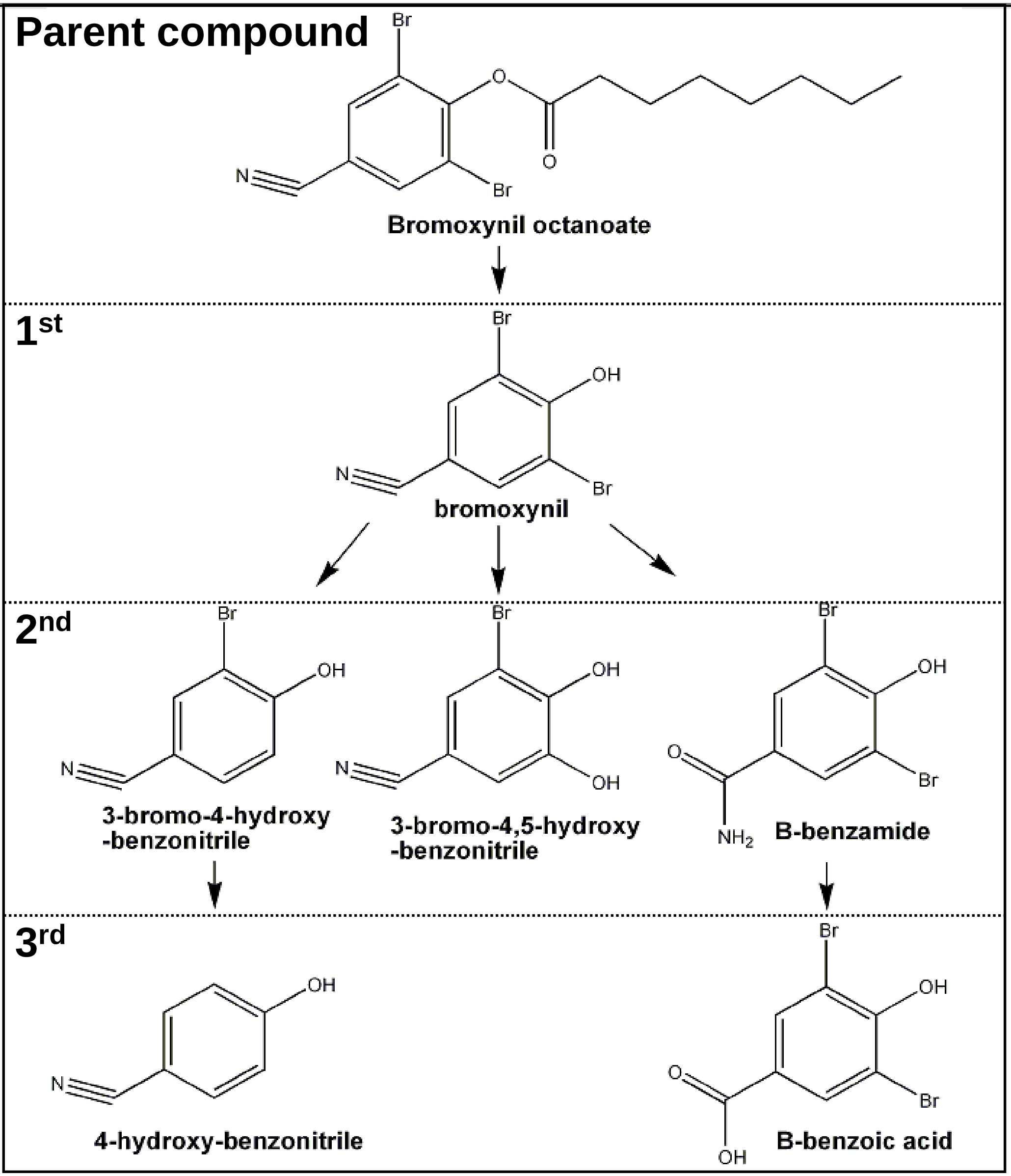
Including *n* transformation products *t*:

$$CF_x = FF_{x,p} \cdot EF_{x,p} + \sum_{a=1}^{n} \left(FF_{t_a} \cdot EF_{t_a} \right)$$



Fate

- Multimedia fate model SimpleBox3.0
- Up to 4 generations of transformation products
- Degradation rates
- Formation yields



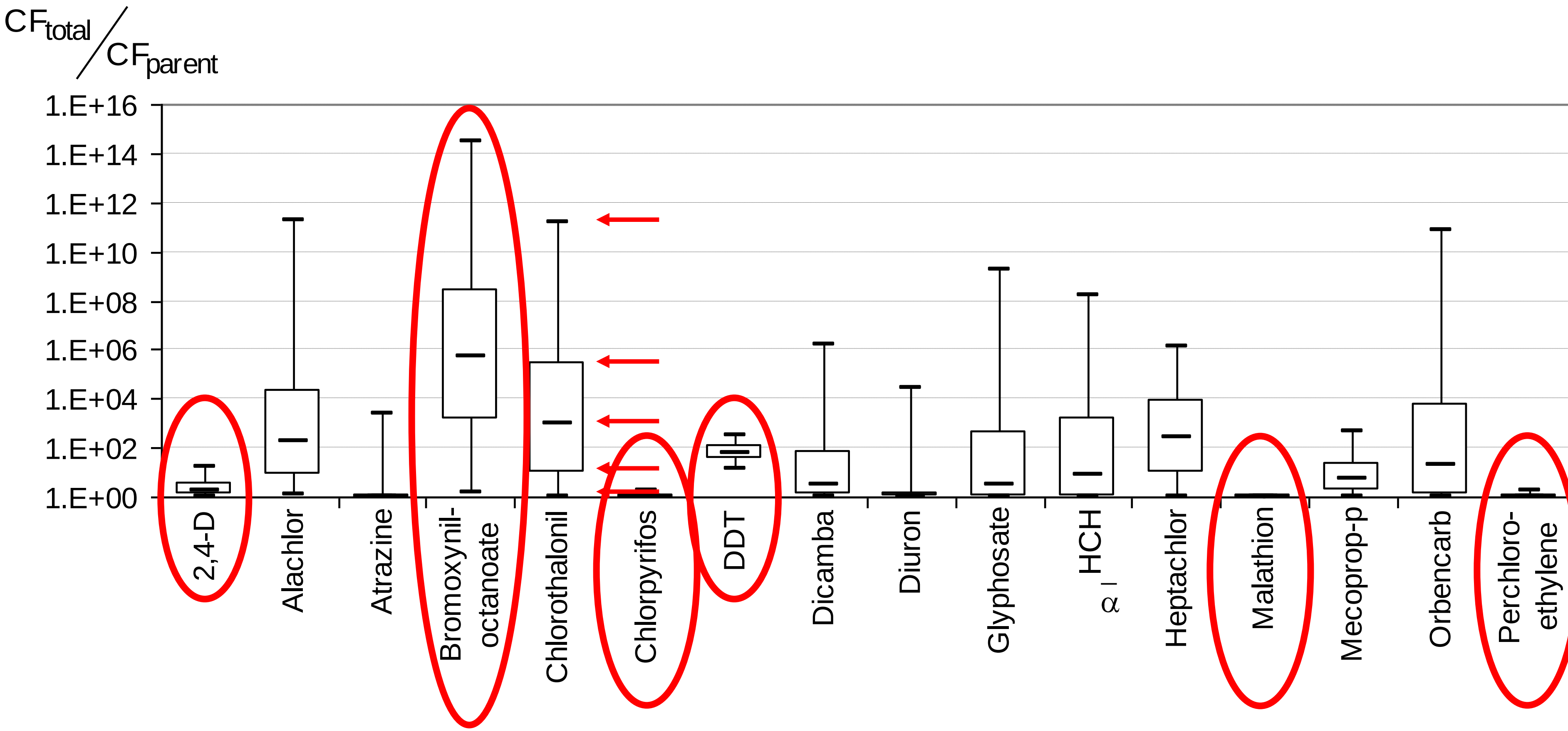
Effect

- Per parent compound/ transformation product
- $\frac{dE}{dC} = S \cdot \frac{1}{HC50}$
- Acute freshwater toxicity of a chemical
- Experimental (e.g. e-toxBase) or estimated with ECOSAR
- Toxic mode of action e.g. e-toxBase or ASTER

Characterization factors

- Emission compartments air, freshwater, agricultural soil
- Concentrations in freshwater ecosystem
- A number of chemicals:
  - ✓ Perchloroethylene
  - ✓ 15 pesticides, i.e. atrazine, DDT, and heptachlor
- Uncertainty assessment
  - ✓ Chemical-specific input parameters
  - ✓ Monte Carlo: 10,000 iterations

Increase in characterization factors



Emissions to agricultural soil

Including transformation products

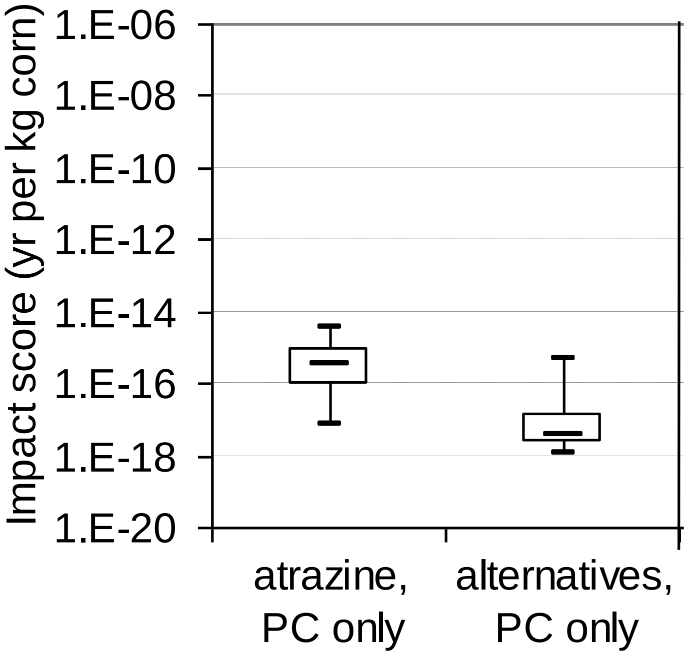
- Median increase of up to 5 orders of magnitude
- Fate *and* toxicity of importance
- Reliable data, uncertainty range does not need to increase
- Uncertainty in effect factor largest
  - ✓ unknown EC50 data
  - ✓ no TMoA-specific data

Case study – atrazine on corn

- Possible atrazine ban
- Replacing pesticides
  2,4-D, bromoxynil, dicamba, nicosulfuron
- Total Impact Score (IS) [PAF*yr per kg corn]
  - ✓ $$IS_{ecotox} = \sum_{x} \left[AR_x \cdot \left(M_{x,a} \cdot CF_{x,a} + M_{x,s} \cdot CF_{x,s} \right) \right]$$

AR_x = Application rate (kg/kg_{corn}) of pesticide x
M_a = Emission to air
M_s = Emission to agricultural soil
CF_a = Characterization factor for emissions to air
CF_s = Characterization factor for emissions to agricultural soil

Case study – atrazine on corn



- Not certain IS will increase
- Alternative pesticides might not be an improvement
- 2,4-D best alternative

Conclusions

- Transformation products should not always be disregarded
  - ✓ Bromoxynil-oct, chlorothalonil, DDT, heptachlor >50% chance that CF will increase more than factor of 10
  - ✓ Alachlor, bromoxynil-oct, chlorothalonil, heptachlor, orbencarb >25% chance CF will increase more than factor of 100
- Data input can be highly uncertain
  - ✓ Reliable data, CFs can be substantially larger, while uncertainty does not need to increase
- A ban on atrazine will not necessarily lead to a decrease in pesticide impacts