Including Ecotoxic Effects on Warm-blooded Predators in Life Cycle Impact Assessment

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Goal of this lecture

Learn about the determinants of ecotoxicological impacts of organic chemicals on warm-blooded species

i.e. fate, exposure, bioaccumulation, effect

Contents

INTRODUCTION

Ecotoxicity

The potential for biological, chemical, or physical stressors to affect ecosystems

For instance: agricultural practice

Compare intensive and extensive farming

- What is the impact of pesticides?
- What is the impact of land use?

Life Cycle Impact Assessment (LCIA) is used to find environmentally best option

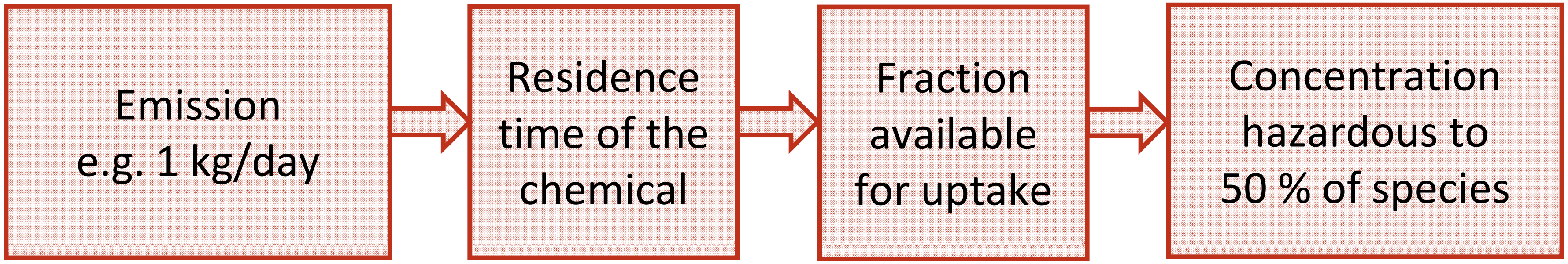
Ecotoxicity in LCIA: cause effect pathway

Emission

Concentration in the Environment

Effects on Aquatic Species

Ecotoxicity in LCIA: common modeling approach



Fate (FF) * Exposure (XF) * Effect (EF)

= Characterization Factor (CF)

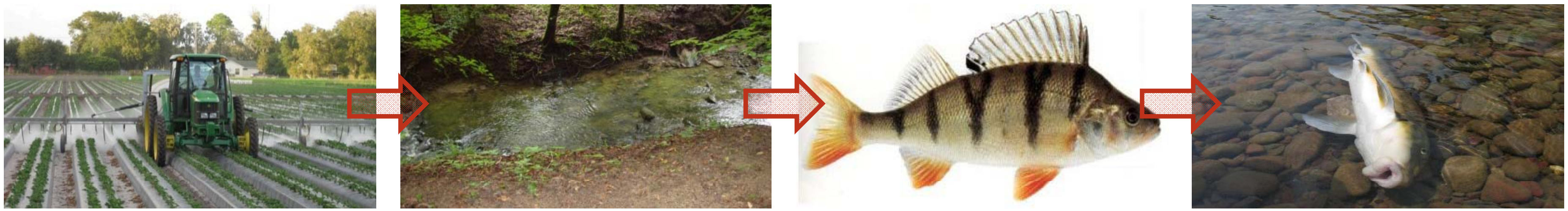
Ecotoxicity in LCIA: problems with the common approach

- Exposure from 1 uptake route is included, whereas for some species multiple uptake routes may be relevant
- Exposure within 1 compartment is included, whereas exposure may result from multiple compartments

- Focus is on cold-blooded species, but chemicals may have different effects in warm-blooded species

Approach for warm-blooded species: insert a bioaccumulation factor

Bioaccumulation Factor: Increase in chemical concentration from food & ambient medium to animal



$$CF_{x,i} = \sum_{j} \left(FF_{x,i,j} \cdot XF_{x,j} \cdot BF_{x,j} \right) \cdot EF_{x}$$

x = chemical

i = emission compartment

j = receiveing compartment

FATE FACTOR

Fate Factor

$FF = V \cdot dC_{tot}/dM$

V = Volume (m^3) - weighting factor

dC_{tot} = Total concentration change (kg/m^3)

dM = Emission change (kg/day)

<u>Application</u>

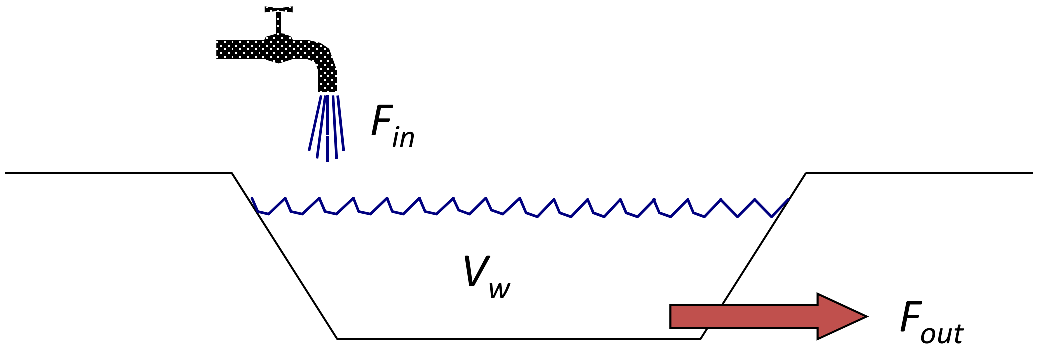
- Multi-media fate models
- Unit in Days

Steady-state concentration

Multi-media fate models

- Mass balance models
- Compartment models
- Box models

Mass balance



Balance:

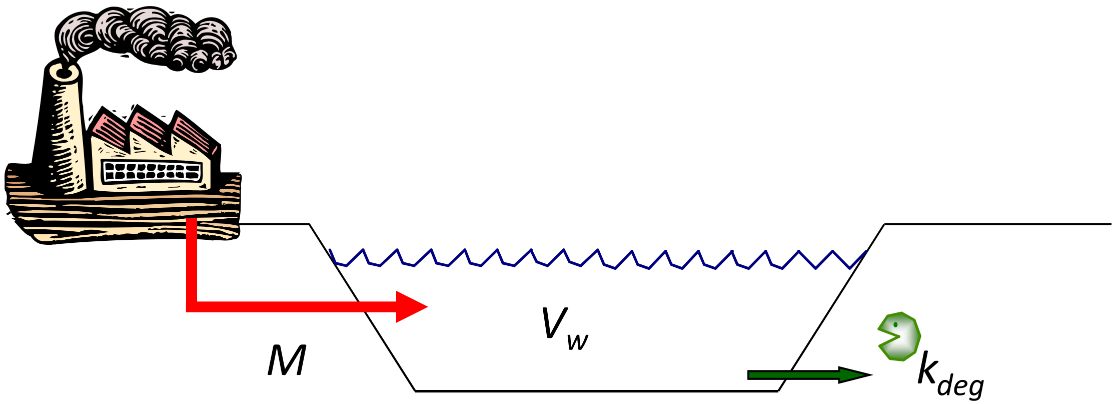
$$\text{Build-up} = \text{In} - \text{Out}$$

$$\frac{dV_w}{dt} = F_{in} - F_{out}$$

Steady state:

$$\frac{dV_w}{dt} = 0 = F_{in} - F_{out}; F_{in} = F_{out}$$

Chemical mass balance model



V_w = water volume (m^3)
M = emission (mol/s)
K_{deg} = degradation rate (s^{-1})
C = concentration (mol/m^3)

Balance:

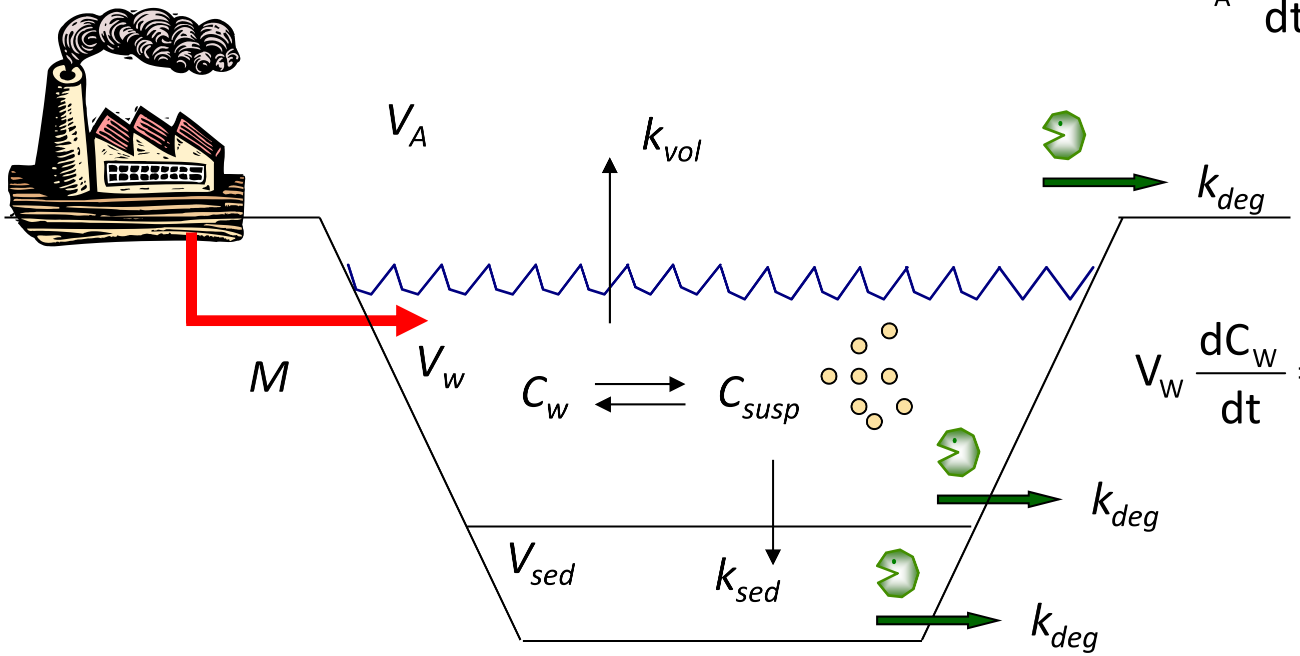
$$\text{Build–up} = \text{In} - \text{Out}$$

$$V_W \frac{dC_W}{dt} = M - k_{deg} V_W C_W$$

Steady state:

$$C(\infty) = \frac{M}{k \cdot V}$$

Multicompartment mass balance model



$$V_A \frac{dC_A}{dt} = -k_{deg} V_A C_A + k_{vol} V_W C_W$$

$$V_W \frac{dC_W}{dt} = M - (k_{deg} + k_{sed} + k_{vol}) V_W C_W$$

$$V_{sed} \frac{dC_{sed}}{dt} = -k_{deg} V_{sed} C_{sed} + k_{sed} V_W C_W$$

Important chemical properties

- Degradation
- Partitioning between compartments

Chemical properties: degradation

- Air
  - Oxidation by OH-radicals
  - Fast: $t_{1/2}$ order of hours-days

    rate constant: $k=\ln(2)/t_{1/2}$

- Water
  - Hydrolysis: pH-dependent
  - Aerobic degradation by bacteria
  - Slower: $t_{1/2}$ days-weeks

- Soil/sediment
  - Aerobic and anaerobic degradation by bacteria
  - Slow: $t_{1/2}$ order of weeks-years

Chemical properties: air-water partitioning

$K_{AW} = C_{air} / C_{water}$

- $K_{AW} = H / RT$
- $H = V_p \cdot Mw / Sol$

$V_{p\,=}$ Vapor pressure

Sol = Solubility

Mw = Molecular weight

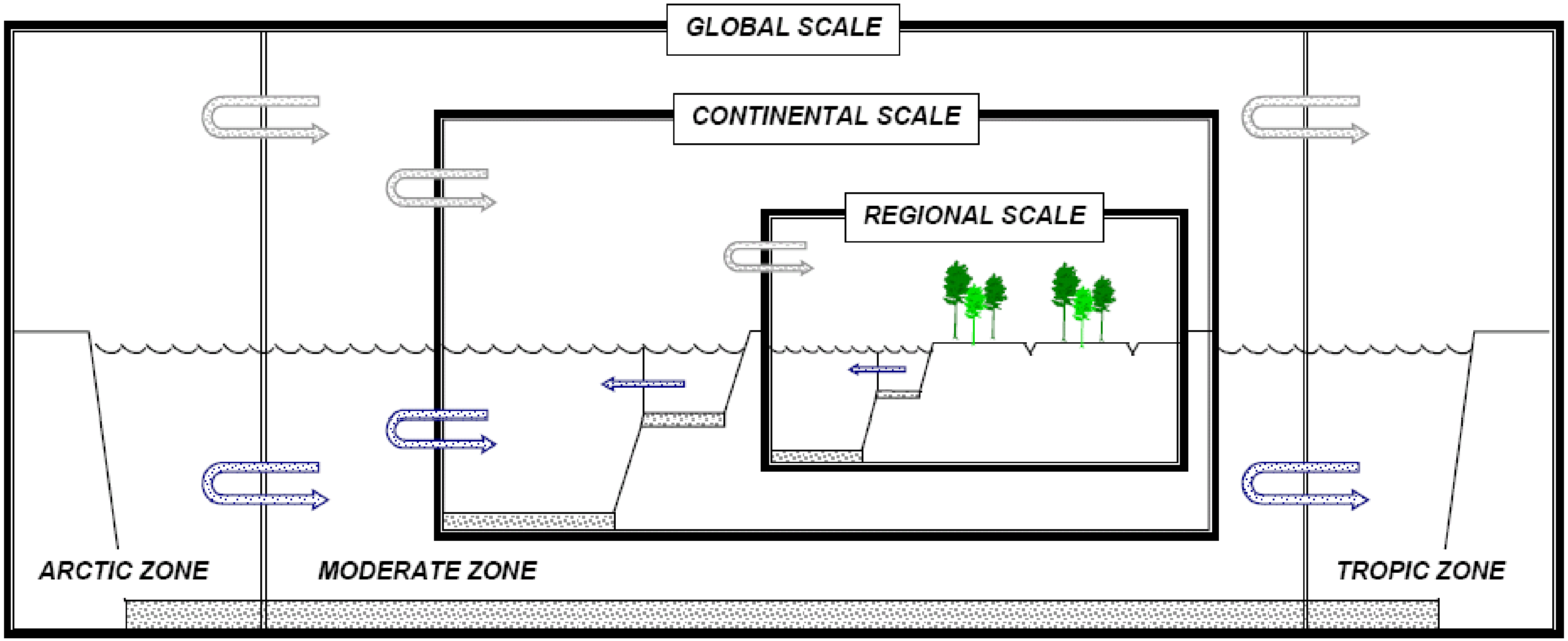
Chemical properties: solids-water partitioning

$K_{SW} = C_{solids} / C_{water}$

- $K_{SW} = f_{OC}\ K_{OC}$
- $K_{SW} = f_{OC}\ .\ b\ K_{OW}^{a}$
  - f_{OC} = fraction of organic carbon
  - K_{oc} = organic carbon partition coefficient
  - K_{ow} = octanol-water partition coefficient

  - Dependent on sedimentation, run-off, leaching…

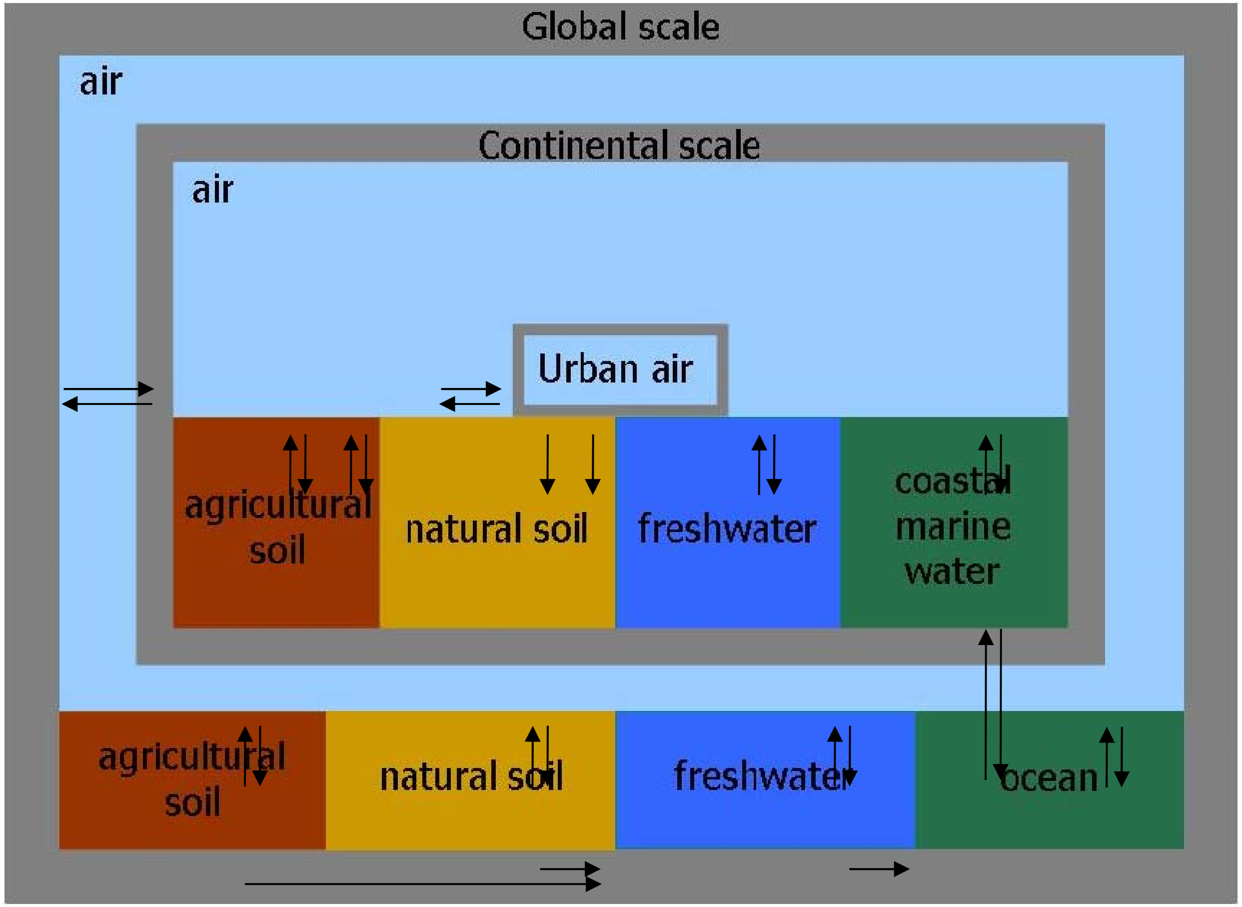
Multimedia fate and exposure model SimpleBox



Den Hollander HA, Van Eijkeren JCH, Van de Meent D (2004): **SimpleBox 3.0**: multimedia mass balance model for evaluating the fate of chemicals in the environment. RIVM, Bilthoven, The Netherlands

Van Zelm R, Huijbregts MAJ, Van de Meent D (2009): **USES-LCA 2.0**: a global nested multi-media fate, exposure and effects model. Int J LCA 14, 282-284

Consensus model USEtox



Rosenbaum RK, et al. (2008): **USEtox**—The UNEP-SETAC toxicity model: recommended characterisation factors for human toxicity and freshwater ecotoxicity in Life Cycle Impact Assessment. Int J LCA 13, 532-54

EXPOSURE FACTOR

Exposure factor

- Depends on binding to suspended solids and dissolved organic carbon:

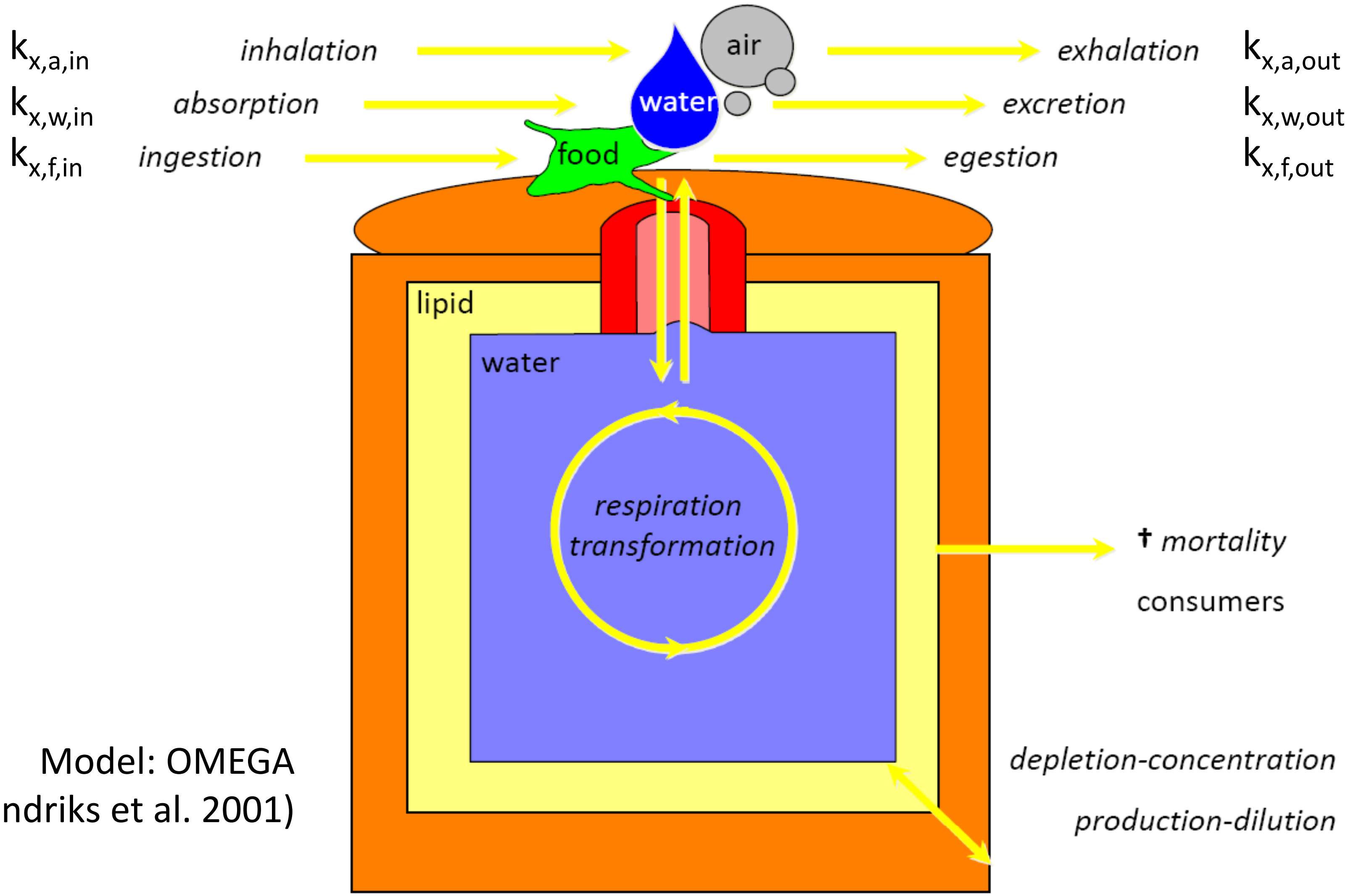
- Exposure of chemical concentration to the ecosystem

$$XF = dC_{dis}/dC_{tot} = F_{dis}$$

dC_{dis} = Dissolved Concentration change
dC_{tot} = Total Concentration change
F_{dis} = Fraction Dissolved (dimensionless)

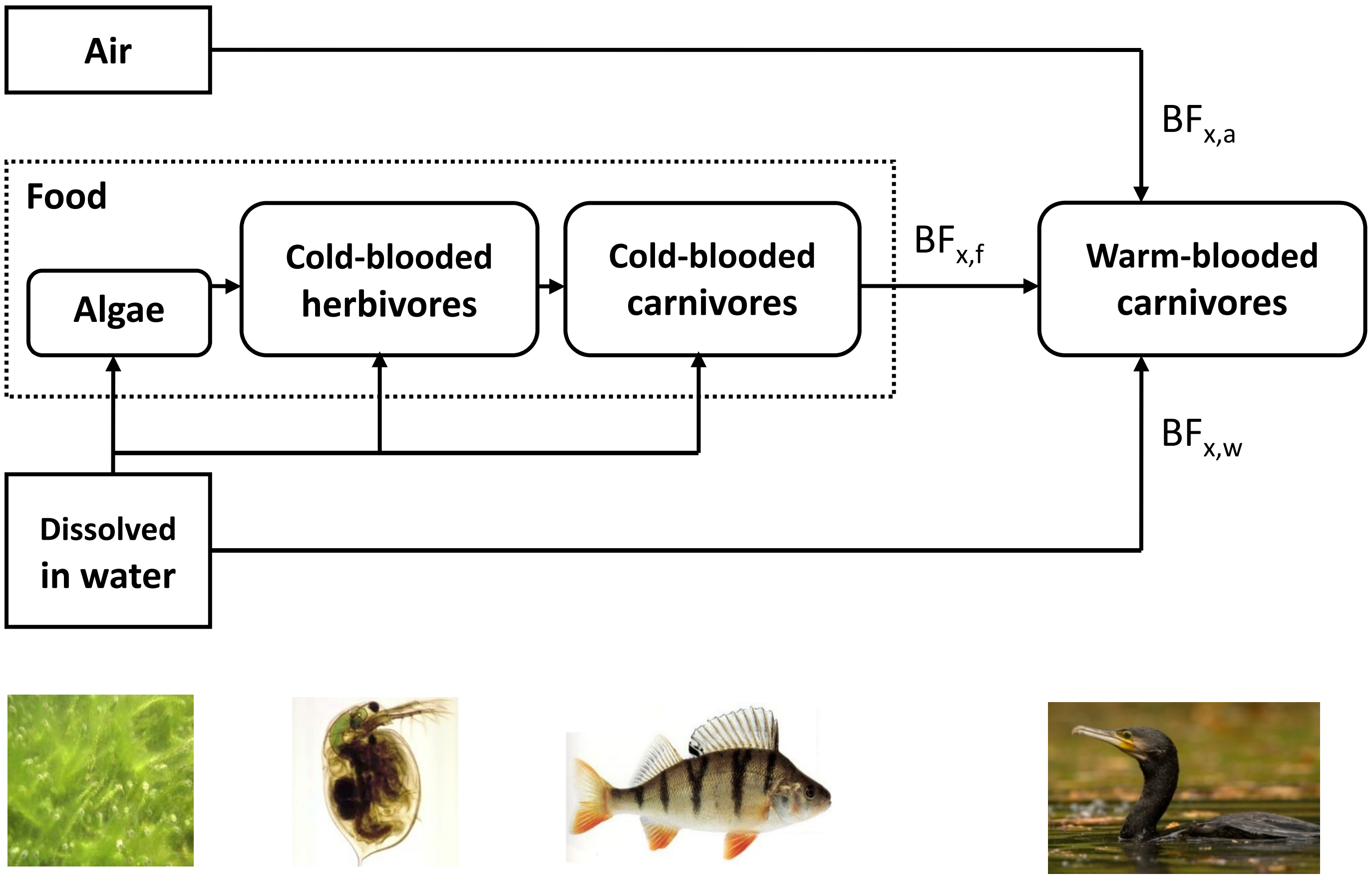
BIOACCUMULATION FACTOR

Bioaccumulation



Model: OMEGA
(Hendriks et al. 2001)

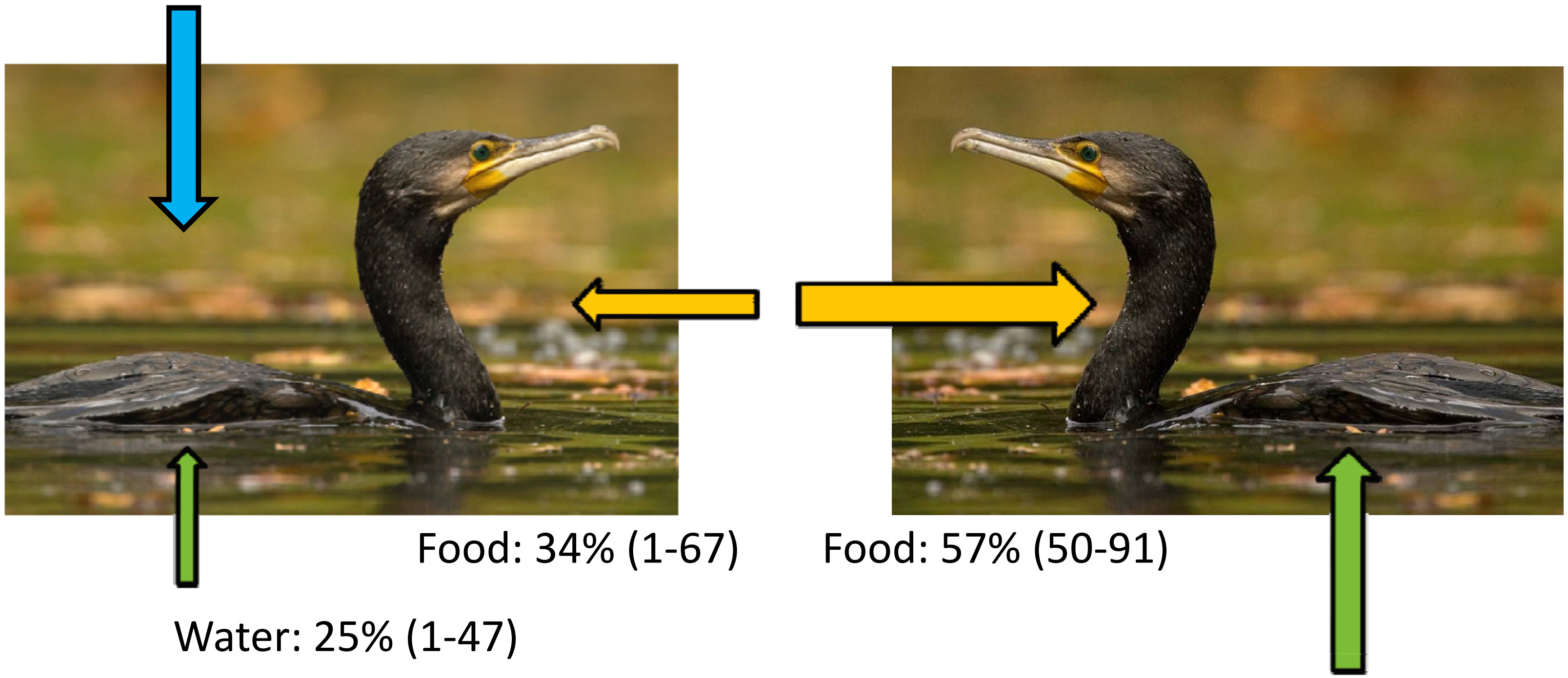
Schematic overview of the food chain



Importance of uptake routes depends on emission compartment

Emission to air

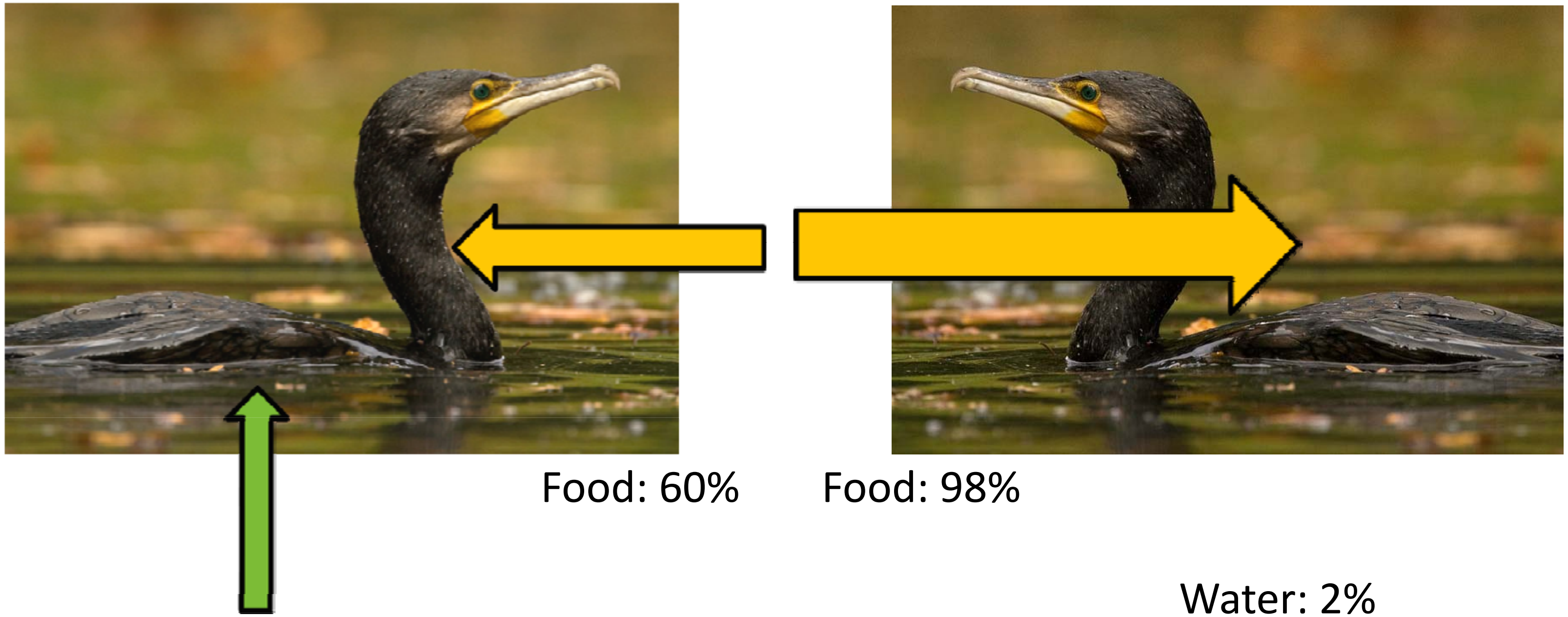
Emission to water



Importance of uptake routes depends on chemical

Lindane (K_{ow} $5.0 \cdot 10^3$)

DDT (K_{ow} $1.55 \cdot 10^6$)



Food: 60%

Food: 98%

Water: 2%

Water: 40%

Summarizing

- Uptake from air is mainly relevant for emissions to air
- Relative uptake from food increased with increasing K_{ow} at the expense of uptake from water
- For chemicals with a high K_{ow}, uptake from food is by far the most important uptake route

3 bioaccumulation factors for warm-blooded predators

- Bioaccumulation factor for uptake from water

$$BF_{x,w} = \frac{dC_{x,predator}}{dC_{x,w,diss}} = \frac{k_{x,w,in}}{\sum k_{x,out}}$$

- Bioaccumulation factor for uptake from food
  (depends on bioaccumulation in previous trophic levels 1-3)

$$BF_{x,f} = \frac{dC_{x,predator}}{dC_{x,w,diss}} = \frac{k_{x,f,in} \cdot BF_{x,3}}{\sum k_{x,out}}$$

- Bioaccumulation factor for uptake from air

$$BF_{x,a} = \frac{dC_{x,predator}}{dC_{x,a}} = \frac{k_{x,a,in}}{\sum k_{x,out}}$$

EFFECT FACTORS

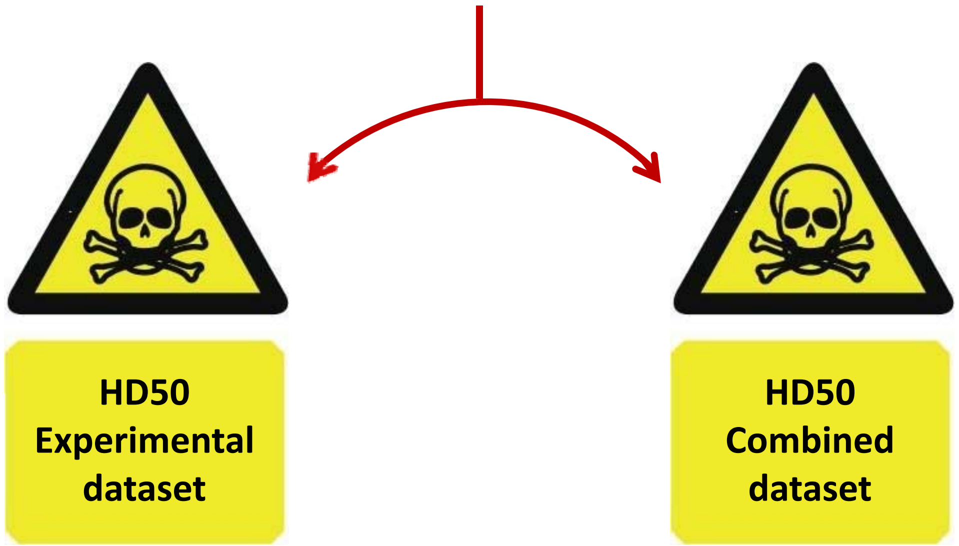
Chemical toxicity to wildlife species

The hazardous dose of a chemical (HD50): upcoming and important in the toxicity assessment of chemicals for wildlife species

- Small experimental sample size → Statistical uncertainty
- Unrepresentative sample of species → Systematic uncertainty
- Several ways to enlarge the sample size, a.o. interspecies correlation estimation (ICE) models, but these are uncertain

Effect factor can be based on experimental and / or estimated data

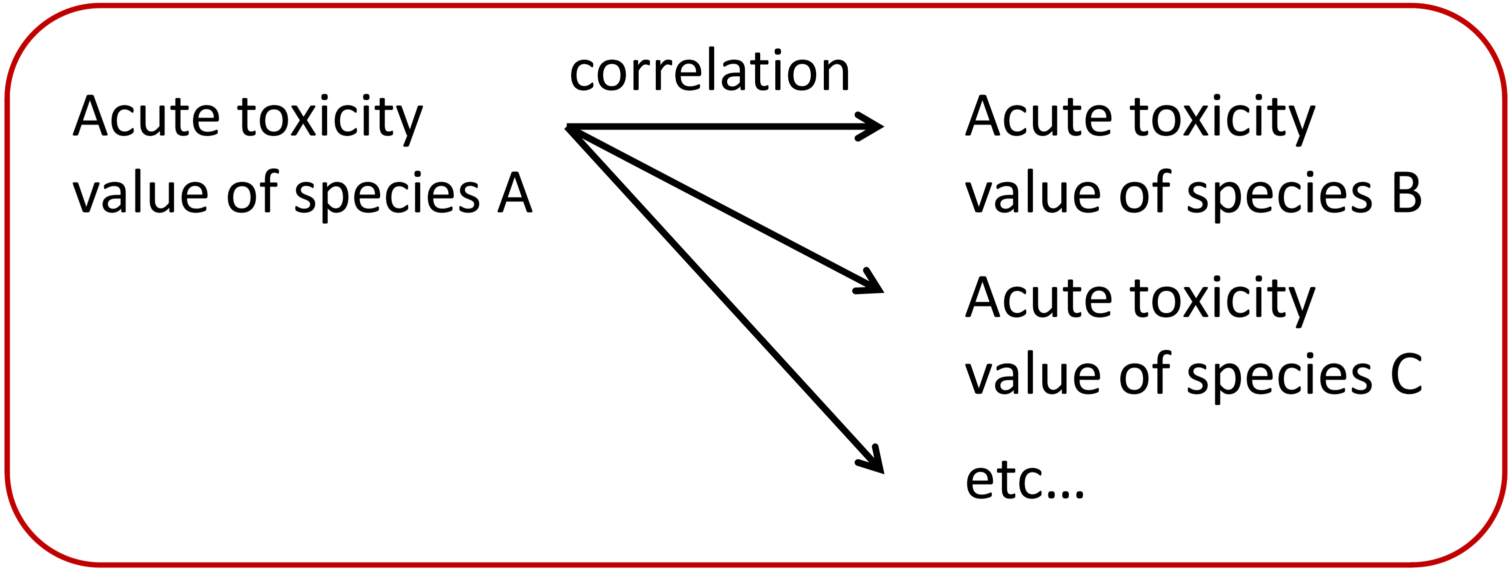
What is the difference for the effect factor?



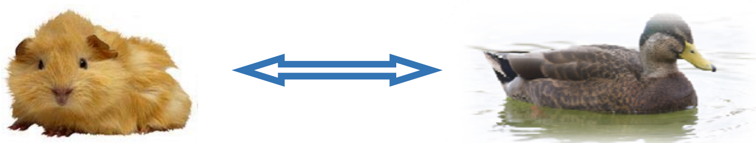
Experimental +
estimated data

Principle of Interspecies Correlation Estimation

- Raimondo et al. (2010) provide ICE-models to estimate the toxicity of 49 wildlife species.

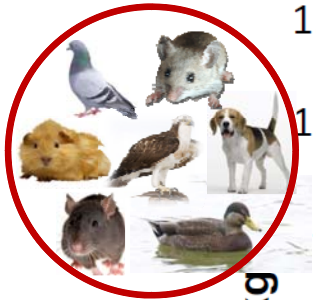


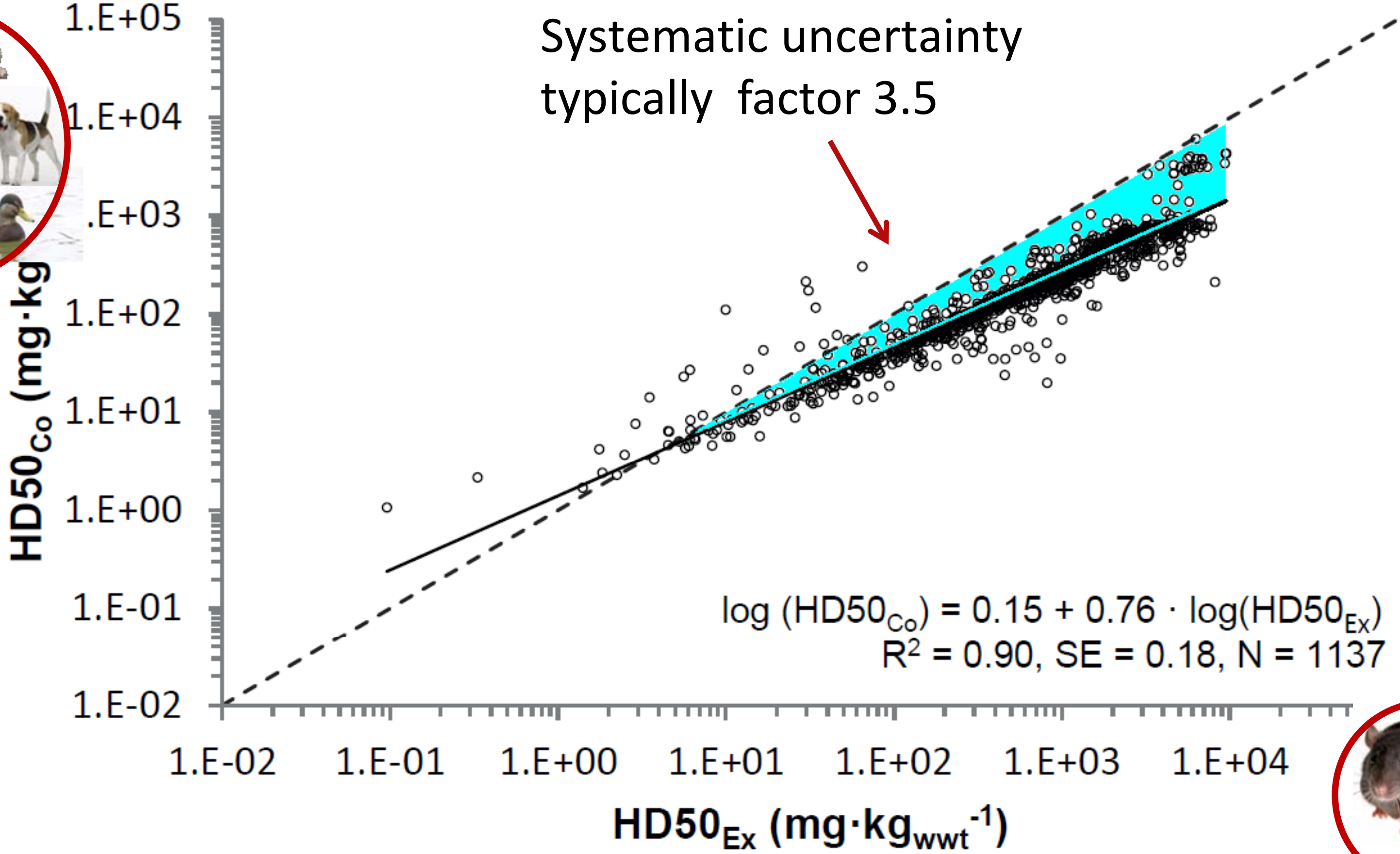
- *Log (tox. B) = a + b • Log (tox. A)* [mg/kg_{wwt}]



Extrapolate toxicity

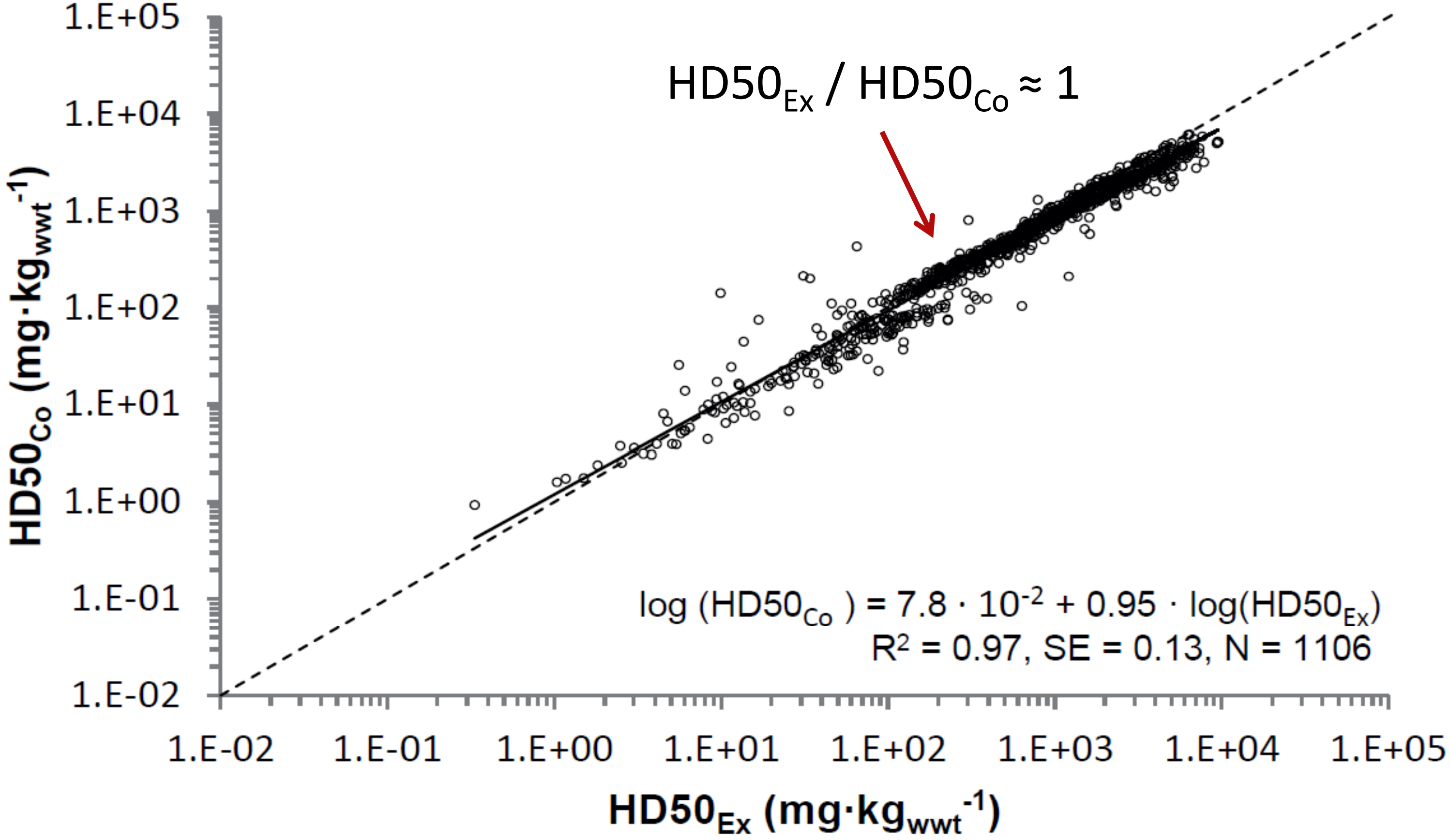
Hazardous dose (HD50): comparing the experimental and combined datasets





Hazardous dose (HD50) for *mammals* only

Birds are more sensitive!



Calculating the Effect Factor

Limited availability of experimental toxicity data, mainly for *mammals* → systematic underestimation of wildlife toxicity

Use HD50-values to calculate hazardous body burden:

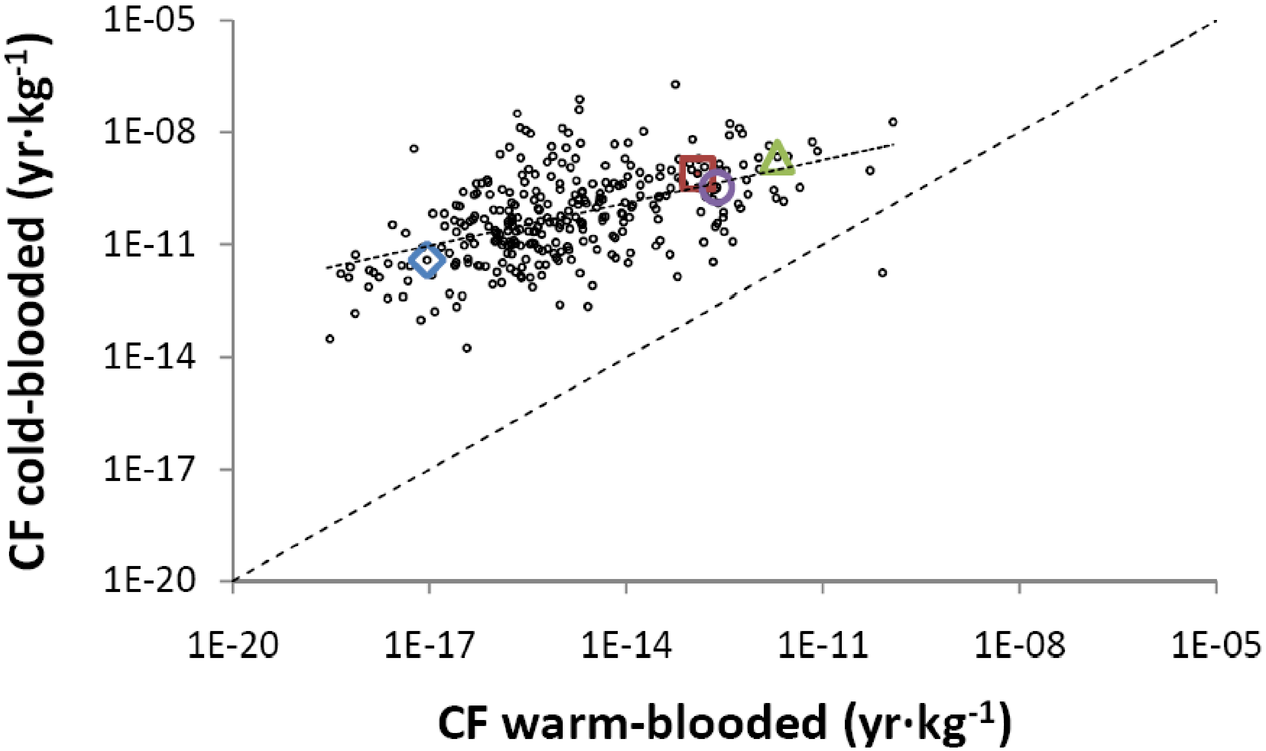
$HD50 \cdot p_{assimilated}$

EF = 0.5 / Hazardous body burden

LC-IMPACT

CHARACTERIZATION FACTORS

Comparison $CF_{warm\text{-}blooded}$ vs. $CF_{cold\text{-}blooded}$



R^2=0.26

Acephate (◇), Aldicarb (□),Lindane (Δ), and DDT (O)

Comparison $CF_{warm\text{-}blooded}$ vs. $CF_{cold\text{-}blooded}$

- $CF_{cold\text{-}blooded\ species}$ >> $CF_{warm\text{-}blooded\ species}$
- Different ranking of chemicals for warm-blooded compared to cold-blooded species

Best estimate for freshwater impact assessment

- Apply a (weighted) total CF for warm-blooded and cold-blooded species to study freshwater impacts
  - species density
  - the importance society attributes to protection per trophic level

- Depending on the weighting method, impacts on warm-blooded predators could change the CFs and relative ranking of toxic chemicals in freshwater impact assessment

Highlights of this presentation

- To estimate the impacts on warm-blooded species resulting from different uptake routes: insert a bioaccumulation factor

$$CF_{x,i} = \sum_{j} (FF_{x,i,j} \cdot XF_{x,j} \cdot BF_{x,j}) \cdot EF_{x}$$

- The importance of the different uptake routes depends on: the emission compartment and the properties of the chemical

- Effect factors can be based on experimental and/or estimated data

  Limited availability of experimental toxicity data, mainly for *mammals* → systematic underestimation of wildlife toxicity

- $CF_{\text{cold-blooded species}}$ >> $CF_{\text{warm-blooded species}}$ and the chemical ranking differs

  Implications depend on the weighting method for the total CF of freshwater impacts

More information?

Golsteijn L, van Zelm R, Veltman K, Musters G, Hendriks AJ, Huijbregts MAJ. 2012. *Including ecotoxic impacts on warm-blooded predators in life cycle impact assessment.* Integr. Environ. Assess. Manag. 8(2):372–378.

Golsteijn L, Hendriks HWM, van Zelm R, Ragas AMJ, Huijbregts MAJ. 2012. *Do interspecies correlation estimations increase the reliability of the chemical effect assessment for wildlife?* Ecotoxicol. Environ. Saf. 80: 238–243.

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