Uncertainty in fugacity-based multimedia modeling: probabilistic and non-probabilistic methods

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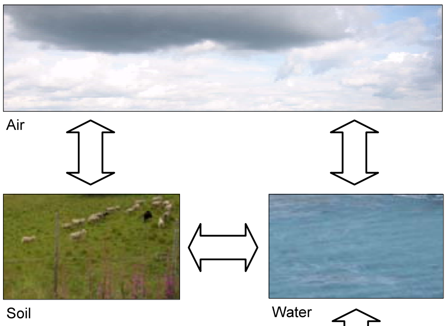
Level I model – a conservative equilibrium



$Z_{air} = 1/R \cdot T$

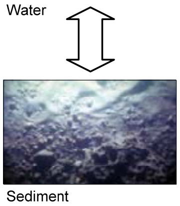
$Z_{water} = Z_{air} / K_{aw}$

$Z_{soil} = Z_{water} \cdot \rho_{soil} \cdot \Phi_{oc} \cdot K_{oc}$

$Z_{sed} = Z_{water} \cdot \rho_{sed} \cdot \Phi_{sed} \cdot K_{oc}$

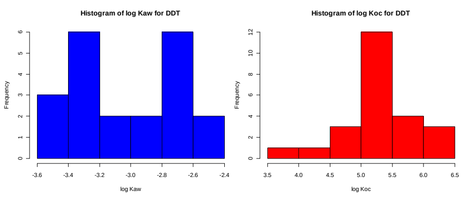
$Z_{susp} = Z_{water} \cdot \rho_{susp} \cdot \Phi_{susp} \cdot K_{oc}$

$f = \frac{M}{\sum V_i \cdot Z_i}, m_i = V_i \cdot Z_i \cdot f.$



K_{aw} and K_{oc} determine the partitioning

The partition constant between air and water (K_{aw}) and the soil-sediment sorption constant normalized to organic carbon (K_{oc}) are the two compound specific properties in these calculations. The empirical data are uncertain, here exemplified by DDT.



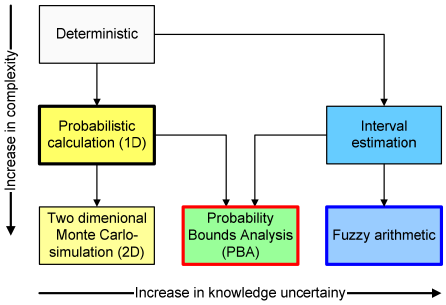
Randomness and systematic errors

Measurement or estimation uncertainty can be separated into random and systematic (incompleteness) components. Randomness does arise from the natural variability of observations (heterogeneity) while a systematic estimation and measurement errors are examples of imprecision or epistemic (knowledge) uncertainty.

K_{aw}: Systematic errors (imprecision)
K_{oc} : Systematic errors and variability

Different methods are needed

Random variability can be described by probability distributions, but knowledge uncertainty can not. We simply do not know which distribution to choose.

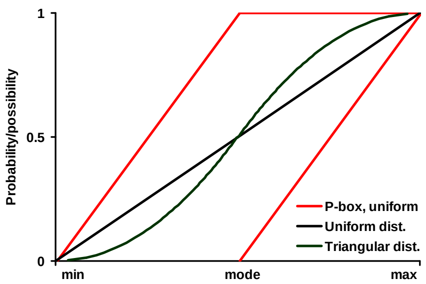


Probabilistic or possibilistic?

Probability boxes are bound by pairs of cumulative probability distributions (CDF):

$$\underline{F}(x) \leq F(x) \leq \overline{F}(x) \ \forall x \in \Re$$

A triangular fuzzy number (possibility distribution) can be expressed as a probability box. This p-box covers all distributions with the same **min**, **max** and **mode**.



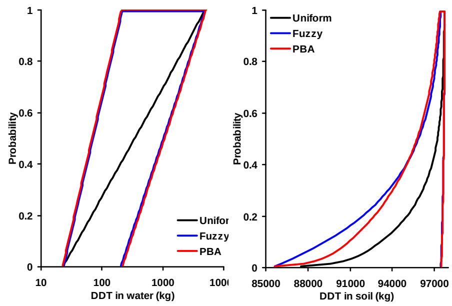
Distribution between compartments

We have modeled partitioning and uncertainty after the release of 100000 kg of DDT into a standard evaluative environment. Best estimates and interpercentile ranges (5-95) for each compartment are given below.

	Fuzzy arithmetic		Probabilistic (p-box)		Probabilistic (uniform)	
	Best	**Range**	**Best**	**Range**	**Best**	**Range**
Air	94.1	4.51-6290	98.4	5.73-4320	178	10.0-2820
Water	211	25.3-4300	212	24.8-4300	336	28.2-3860
Soil	97500	87600-97700	97500	89400-97700	97200	91200-97700
Sediment	2170	1950-2170	2170	1990-2170	2160	2030-2170
Susp. sed.	67.7	60.9-67.9	67.7	62.1-67.9	67.5	63.3-67.9

Precise distributions may underestimate uncertainty

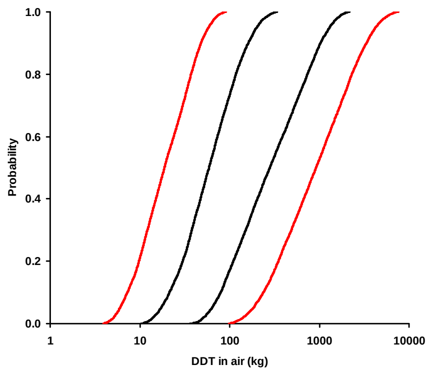
The differences in estimates are modest in this example, but precise distributions may underestimate uncertainty. In higher level models, when degradation rates are added, the differences will increase.



Uncertainty propagation, discrete or Monte Carlo

Uncertainty propagation by discrete calculations is flexible and computationally effective, but if repeated parameters are not algebraically eliminated the uncertainty estimates will be inflated.

To avoid this problem, probability bounds analysis can also be run as a Monte Carlo-simulation. Below a p-box is generated for DDT in air, bound by the leftmost and rightmost CDF.



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