IMPROVING AVAILABLE GUIDANCE FOR PERSISTENCE ASSESSMENT OF SUBSTANCES (CEFIC-LRI ECO52) – SENSITIVITY ANALYSIS TO IDENTIFY KEY MODELLING INPUT PARAMETERS FOR OVERALL PERSISTENCY

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Software MUST is freely available at software.ime.fraunhofer.de, contact: judith.klein@ime.fraunhofer.de

Introduction

- Chemical persistence plays a key role in risk assessment and regulation
- Existing frameworks have shown some limitations
- Many substances are problematic, or fall outside the applicability domain of existing frameworks due to their specific characteristics
- Evaluating degradation half-lives using a compartment-by-compartment approach is overly simplistic because it neglects dynamic multimedia exchanges and degradation processes that may have an important bearing on the overall persistence of a substance in the environment
- Overall persistence as joint persistence criterion can be used to integrate several compartments
- A sensitivity analysis is used to identify important model parameters with respect to overall persistence
- The software MUST is analyzed representatively for a regional/continental level III and level IV model

Materials & Method

1 Scenario definition

Emission

- 4 emission scenarios are considered
  1. 100% emission to air
  2. 100% emission to water
  3. 100% emission to soil
  4. Equal distribution to air, water and soil
- For level III constant emission is used, for level IV 10 years constant emission followed by a 2 years recovery period is applied

2 Scenario definition

Substance

- 5 example substance are investigated
  1. HBCDD,
  2. **D4 (details see Results & Discussion),**
  3. Bisphenol A,
  4. Dechlorane Plus and
  5. DecaBDE
- Sewage treatment plant (STP) is used to model a more realistic emission to water and soil

3 Selection of assessment endpoints

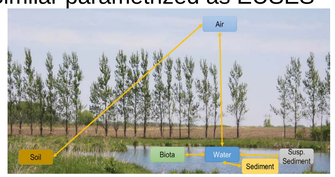
Endpoints

- Steady state distribution (%) in compartment,
- Regional/continental DT50,
- **Overall persistence,**
- Residence time (a) in compartment,
- Area under the curve in compartment, and
- Reduction (%) (maximum value divided by end value)

4 Multimedia model MUST

MUST

- Regional/continental level III and level IV model
- Similar parametrized as EUSES



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Results & Discussions

Case Study: D4

Results of the deterministic default scenario (substance D4)

- Level III and level IV differ within substance and emission scenario
- Overall persistence yields higher values than regional DT50

100% air

Pov 14.6 d

100% soil

Pov 25.55 d

100% water (STP: 25% water, 75% soil)

Pov 51.1 d

Equal distribution (STP: 8% water, 58% soil)

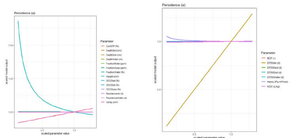
Pov 32.85 d

- Using STP influences the emission of 100% water scenario and equal distribution scenario, the resulting emission scenario differed within the substances
- The steady state distribution and hence persistence depend on the emission scenario

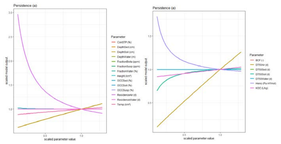
Air (%)	Water (%)	Soil (%)	Sediment (%)	Susp. Sediment (%)	Biota (%)

Result of sensitivity analysis

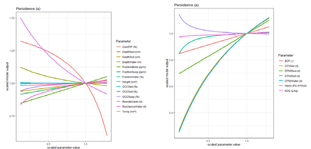
100% air



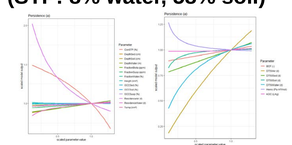
100% soil



100% water (STP: 25% water, 75% soil)



Equal distribution (STP: 8% water, 58% soil)



- The most sensitive parameter when simulating D4 is DT50 air (mean sensitivity coefficient 0.77 over all scenarios)
- For 100% air, DT50 air is even the only sensitive parameter
- Average connection percentage to STP is sensitive for 100% water and equal distribution scenario
- Soil depth (0.41) and residence time air (-0.39) are sensitive for 100% soil, DT50 water (0.48) for 100% water and residence time air (-0.42) for equal distribution

Conclusions

- A sensitivity analysis is essential before models are used in risk assessment
- It is important to agree on environmental parameters as they influence the result and thus, it is also important to agree on parameterization of environmental scenarios
- In case of sensitive substance specific parameters, it is important to have reasonable, reliable values
- Multimedia fate modelling has potential to improve the evaluation of chemical persistence in the environment

References

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