

DEGKINMANAGER - EVALUATION OF WATER SEDIMENT STUDIES INCLUDING VOLATILISATION

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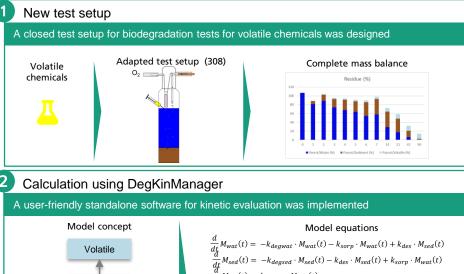
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Software DegKinManager is freely available at software.ime.fraunhofer.de Contact: judith.klein@ime.fraunhofer.de

Introduction

- Biodegradation kinetic data is key parameter in environmental risk assessment of chemicals
- Guidelines are not suitable for testing highly volatile chemicals (e.g. OECD 308)

Materials & Method

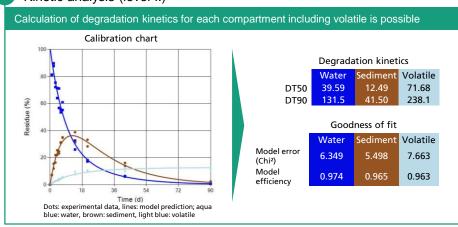


Sediment

$\frac{d}{dt}M_{vol}(t) = k_{degvol} \cdot M_{wat}(t)$

Initial conditions $M_{wat}(0) = M_{wat_0} \in \mathbb{R}_+, \, M_{sed}(0) = M_{sed_0} \in \mathbb{R}_+, \\ M_{vol}(0) = M_{vol_0} \in \mathbb{R}_+$

Kinetic analysis (level II)



Results & Discussions

- DegKinManager is suitable to describe experimental residue data
- Parent in water is best described, parent in volatile is worst described
- In general, there is a good correspondence between model prediction and data

Conclusions

- Test setup is suitable for obtaining the complete mass balance for a range of volatile chemicals
- Optimization in the test setup is necessary to improve test conditions
- The software is able to evaluate water sediment studies at level II
- Rate constants and DT50 or DegT50 values according to the recommendations of **FOCUS Degradation** Kinetics (FOCUS 2014) are calculated
- DegKinManager is able to handle volatilising substances