**Bridging across OECD 308 and 309 data in search of a robust transformation indicator**

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The OECD guidelines 308 and 309 define simulation tests aimed at simulating chemical transformation in stagnant, layered aerobic and anaerobic, versus stirred, purely aerobic water-sediment systems, respectively. The objectives of these tests are two-fold, they should serve both the direct estimation of persistence indicators for hazard assessment and the estimation of half-lives for use in exposure modelling.

While system- or compartment-specific dissipation half-lives of the parent compound are directly extractable from the experimental data, they are strongly system-specific and mix up phase-transfer with transformation. They therefore are not suitable to make generalised statements about persistence or compartment-specific half-lives. Due to the complexity of the 308 system, compartment-specific transformation rate constants are best extracted by inverse modelling (according to the FOCUS guideline). Models, however, suffer from structural and parameter identifiability problems and therefore the extracted transformation rates are highly uncertain and at least partly system- and model-specific (Honti & Fenner 2015). In contrast, 309 experiments with suspended sediments can be mostly treated as fully aerobic bioreactors. Therefore, assuming first-order kinetics and fast sorption equilibration, the estimation of biotransformation rate constants from 309 data should be better accessible and less uncertain. As such, there is scope for 309 tests with suspended sediment to serve as proxy for degradation in the aerobic phase of the more complicated 308 test. However, it remains unclear whether there is any correspondence between aerobic degradation in 308 and 309 systems.

The two aims of our study therefore were: (i) to find a way to extract transformation rates that are universally valid across different experimental systems and hence more representative of the compound’s behaviour in the environment, and (ii) to analyse the potential of simpler experiments (as 309) to predict the transformation rates of more complicated ones (308) by finding a common denominator between experimental systems.

We performed 4 different types of experiments for 4 compounds, covering a broad range of water:sediment ratios (from 309 to 308) and degradability (from aniline to voriconazole), for details see Junker et al. (submitted). We developed a unified model that was able to simulate all 4 experimental types by using a biomass-corrected, generalised biotransformation parameter (kbio) and specialised descriptions of the different physical conditions in the 308 and 309 family of systems. We used a Bayesian calibration and uncertainty assessment framework to calibrate the models for individual experimental types separately and across all 4 experimental setups at once. It was possible to attain a good fit to the data in both setups and kbio turned out to be quite robust across systems when certain additional assumptions were made. However, the uncertainty of kbio remained significant and therefore predictions from one experimental type to another remained very uncertain as well.

References

Junker, Hennecke, Shrestha, Fenner, Honti(submitted to ICCE2015) Improvement strategies for the assessment of chemical persistence at the water-sediment interface–experimental approach

Honti, Fenner (2015) Deriving persistence indicators from regulatory water-sediment studies: Opportunities and limitations in OECD 308 data. *ES&T* doi:10.1021/acs.est.5b00788