Estimation of degradation rates in water of outdoor cosms with pesticide measurements in water and sediment

Guidance for inverse modelling using TOXSWA

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Background

In water bodies with low flow velocities or with multiple spray drift deposition events, exposure concentrations of pesticides are influenced by their degradation rate in water.
However, guidance for estimating this rate for realistic outdoor studies is still lacking.

Objective

- To develop a method to estimate degradation rates in water from available higher-tier effect cosm studies, in which concentrations have been measured in water and in sediment.

These degradation rates may be used in higher-tier exposure assessments for registration of pesticides on a national and zonal level.

Methods

- Outdoor cosms (e.g. Figure 1) with at least water depth, five concentrations in water and three concentrations in sediment measured;
- Five compounds with K_{oc} values ranging from 10 to 300000 L/kg;
- Inverse modelling for at least three sets of sediment covering a range of bulk density, organic matter content and porosity;
- PEST 13.0 running FOCUS_TOXSWA_4.4.2 many times to minimize simulated-measured concentrations in water and in sediment simultaneously and
- Criteria for goodness of fit similar to FOCUS Degradation Kinetics (2006), but (i) one overall X^2 error with equal weight for water layer and sediment and (ii) X^2 errors up to 25% acceptable.

Results

Figure 1. Outdoor effect cosms used for higher-tier aquatic risk assessments (Leistra *et al.*, 2003).

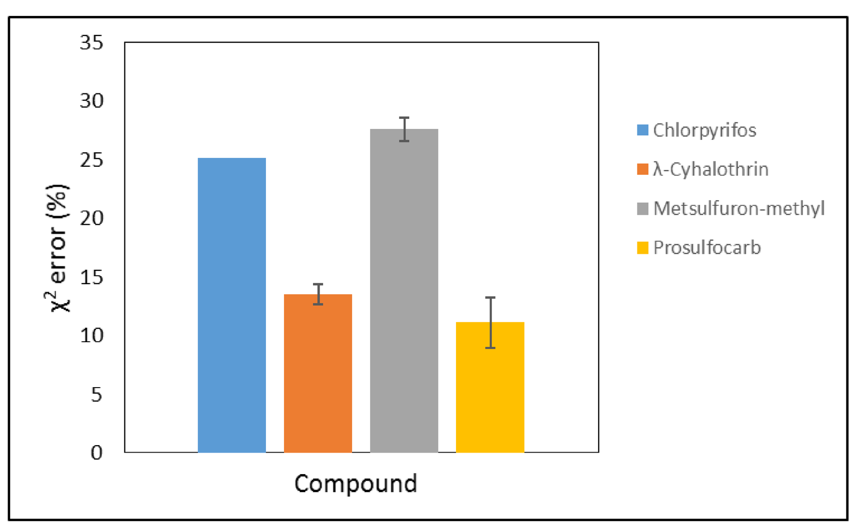

Figure 2. Error level of χ^2 test (average, lower and upper limit) for the four successful compound/cosm optimisations.

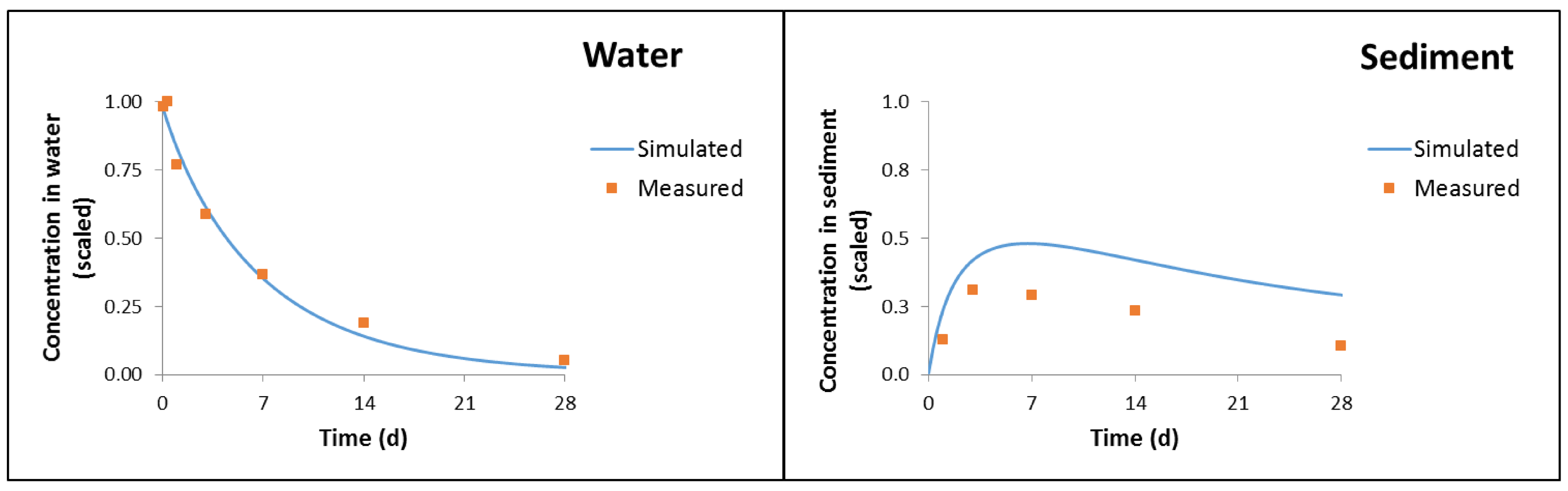

Figure 3. Measured and simulated concentration prosulfocarb in water and sediment of an outdoor ditch as a function of time; optimisation using a weight factor of 22 for the correspondence between measured and simulated in the water layer versus the correspondence in the sediment (data from Arts *et al.*, 2006).

- Two out of five compounds needed more than ten initial parameterisations and expert judgement adjustments to obtain successful optimisations;
- X^2 errors ranged from 8 to 28% (Figure 2);
- For four compounds fits were visually acceptable (e.g. Figure 3), as well as trends in residuals (not shown);

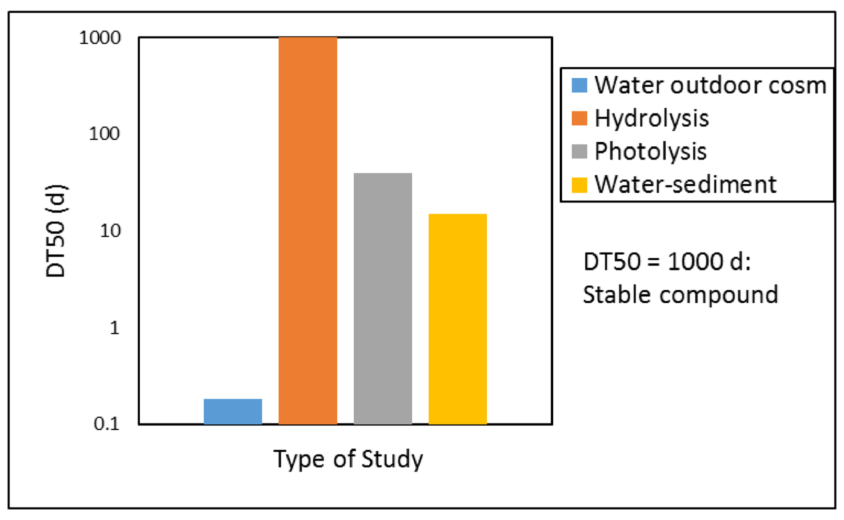

Figure 4. Geomean $DegT_{50,water}$ value for lambda-cyhalothrin for the outdoor cosm of Leistra *et al.* (2003) and DT_{50} values for hydrolysis (pH 9, 25°C), photolysis and water-sediment studies.

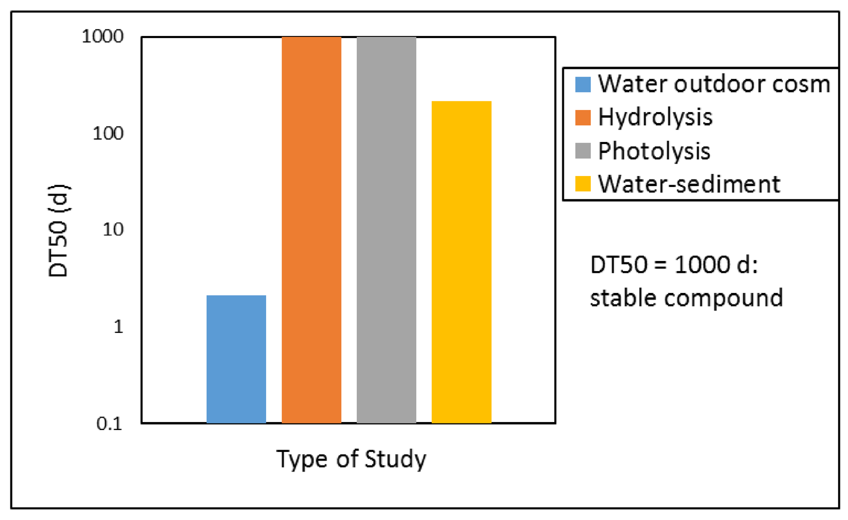

Figure 5. Geomean $DegT_{50,water}$ value for prosulfocarb for the outdoor cosm of Arts *et al.* (2006) and DT_{50} values for hydrolysis (pH 7, 20°C), photolysis and water-sediment studies.

- $DegT_{50,water}$ 95th confidence intervals were wide: typically within 30-170% of the fitted value (not shown) and
- For the four compounds with acceptable fits, the estimated $DegT_{50,water}$ values appeared to be shorter than the DT_{50} values derived from hydrolysis, photolysis and water-sediment studies (Figures 4 and 5). This difference was typically an order of magnitude and at least a factor of two.

Conclusions

- The estimation procedure resulted in sufficiently accurate $DegT_{50,water}$ values for four of the five compounds. So, the procedure seems suitable for use in registration.

- The $DegT_{50,water}$ values for outdoor cosms were considerably shorter than values for hydrolysis, photolysis and water-sediment studies. So, they have added value in the tiered aquatic exposure assessment.

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