Fraunhofer IME

TK-TD MODELLING AS ADDITIONAL LINE OF EVIDENCE IN THE RISK ASSESSMENT FOR AQUATIC MACROPHYTES: CHLOROTOLURON AS A CASE STUDY

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Introduction

- Effects of pesticides including chlorotoluron on macrophytes are assessed by different standard tests.
- Exposure of chlorotoluron to aquatic organisms in edge-of-field waters can be highly dynamic.
- Refined exposure tests cannot cover every conceivable exposure scenario.
- Toxikokinetic-toxicodynamic (TK-TD) models offer a mechanistic way to predict the effects.
- Parameterisation, testing and application of a TK-TD model for *Lemna spec*. is presented.
- The model is based on Schmitt *et al*. (2013), and was re-implemented and described in detail in a TRACE documentation (after Grimm *et al*. 2014).

Step 1: Calibration

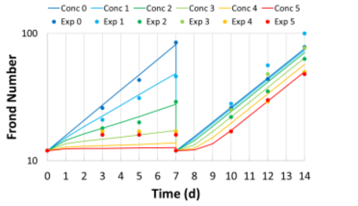

Figure 1: Calibration using a test with 7 days of exposure followed by 7 days of recovery in fresh medium without test item. Dots = data, lines = predictions. Model efficiency = 0.89

Step 2: Verification

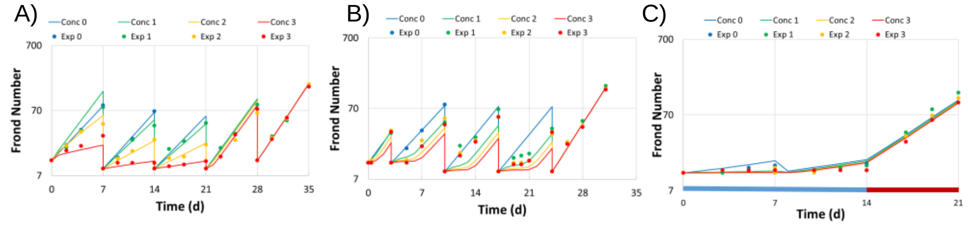

Figure 2: Verification using 3 refined exposure tests. A) a test with 21 days of exposure followed by 14 d in clean medium (weekly reset); B) four pulses (0.5 – 3d) in a test over 31 d (weekly reset after 1st pulse) and C) a test with exposure at 11 °C, followed by recovery at 11 °C (blue line) and later 24 °C (red line). Dots = data, lines = predictions. Model efficiencies = 0.90, 0.91 and 0.95

Step 3: Application

3.1 Simulation of standard tests with refined exposure according to the 7 d worst case time windows of the FOCUS step 3 profiles (example in Figure 3A)

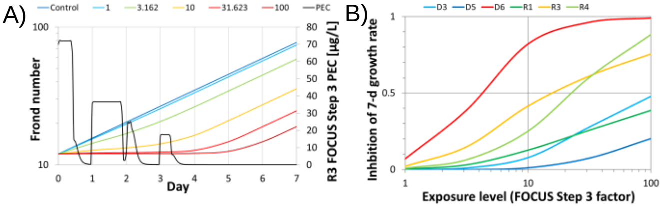

Figure 3: Simulation of 7 d growth inhibition tests. A: Simulation of a single exposure profile; B: Exposure response relation for different scenarios

- The margin of safety for a 50 % inhibition of the 7 d growth rate (Tier 1 assessment endpoint) is higher than the default assessment factor of 10 (Figure 3B).
- For scenarios with more prolonged exposure (D6 here), the margin of safety is lower.

3.2 Modelling the effect of the full FOCUS profiles on the growth of *Lemna* under field conditions (example in Figure 4A)

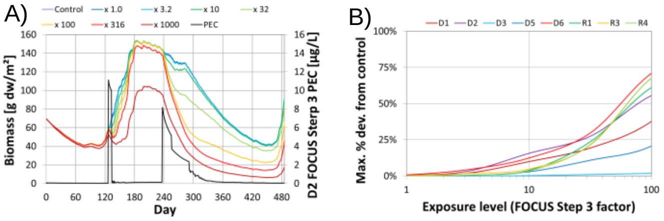

Figure 4: Simulation of the full exposure profile. A: Simulation of a single exposure profile; B: Exposure response relation for different scenarios

- The Ecological Threshold Option allows only 'negligible' effects on abundance or biomass (EFSA 2013).
- A deviation to control ≤ 25 % could be considered acceptable in the field.
- Margins of safety are then 20 or higher for all analyzed exposure scenarios (Figure 4B).

Conclusions

- The *Lemna* TK-TD model was successfully calibrated and verified.
- Simulation of refined exposure tests indicates acceptable risks for most of the FOCUS step 3 exposure scenarios.
- Modelling *Lemna* populations in the field introduces additional uncertainty but margins of safety were at least 20 for all scenarios.

➡ A combination of refined exposure tests and modelling can support the risk assessment for time variable exposure.

References

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TK-TD modelling as additional line of evidence in the risk assessment for aquatic macrophytes: chlorotoluron as a case study

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To assess effects of the use of plant protection products based on chlorotoluron as active substance, various designs of laboratory tests with Lemna sp. and other species and also mesocosm studies including different macrophyte species are available. Since it is not possible to experimentally study every possible exposure scenario, TK-TD modelling was used as an additional approach to address the potential effects of short-term exposure as predicted for some FOCUS surface water scenarios. The Lemna TK-TD model developed by Schmitt et al. (2013) was used to simulate laboratory tests assuming exponential growth as observed in the experimental controls. Growth under field conditions was modelled as dependent on time variable temperature and light conditions as well as density dependence. The substance-specific TK-TD parameters were calibrated using the results of a growth inhibition test with 7 days of exposure followed by 7 days of recovery in fresh medium without test item. The so calibrated model was verified by comparing its predictions with results of three other tests with different exposure patterns, some of which were designed with this purpose in mind. Modelling efficiencies were close to or above 0.9 for all four tests and, thus, the model was considered suitable for simulating effects of different exposure patterns on the growth of Lemna. We simulated laboratory refined exposure tests with PEC profiles of the 7 days worst-case time window of the FOCUS step 3 scenarios as well as field populations using the full FOCUS profiles as inputs. For the exposure profiles characterized by short-term pulses, margins of safety were above 10 to reach a 50 % inhibition of the growth rate over 7 days, the endpoint used in Tier 1. For the simulated field tests, maximum deviation of biomass under control and exposure conditions was used as assessment endpoint. If up to 25 % deviation of biomass of an exposed population from a control population is considered a negligible effect, the Margins of Safety was above 20 all analysed scenarios. The experimental results and the additional line of evidence provided by the modelling indicate that the exposure profiles considered here will, with a high probability, not lead to unacceptable effects on macrophytes. This project demonstrates the usefulness of modelling as additional tool in risk assessment of plant protection products, particularly for extrapolation between scenarios which cannot all be tested experimentally.