

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

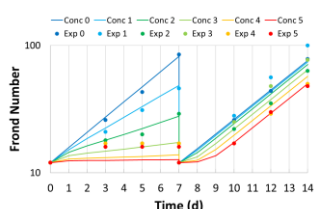


Figure 1: Calibration using a test with 7 days of exposure followed by 7 days of recovery in fresh medium without test item. Dots = data, lines = predictions. Model efficiency = 0.89

Step 2: Verification

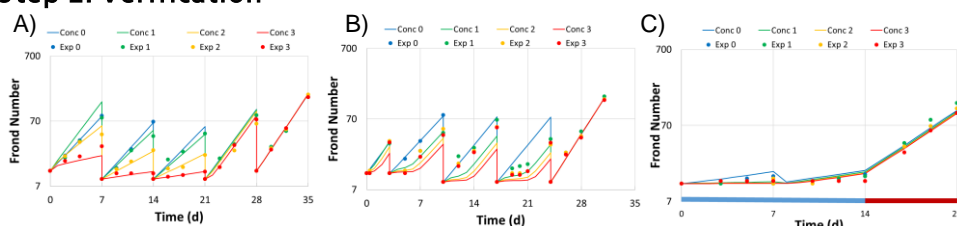


Figure 2: Verification using 3 refined exposure tests. A) a test with 21 days of exposure followed by 14 d in clean medium (weekly reset); B) four pulses (0.5 – 3d) in a test over 31 d (weekly reset after 1st pulse) and C) a test with exposure at 11 °C, followed by recovery at 11 °C (blue line) and later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

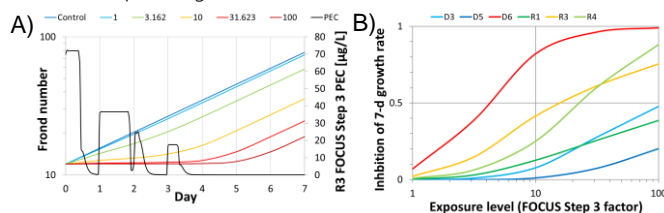


Figure 3: Simulation of 7 d growth inhibition tests. A: Simulation of a single exposure profile; B: Exposure response relation for different scenarios

- 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.

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.

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

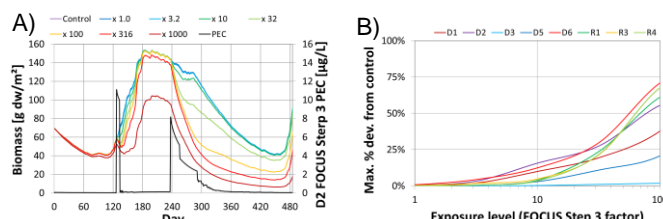


Figure 4: Simulation of the full exposure profile. A: Simulation of a single exposure profile; B: Exposure response relation for different scenarios

- 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).

References

- Schmitt W *et al.* 2013. Mechanistic TK-TD-model simulating the effect of growth inhibitors on *Lemna* populations. *Ecol Model* 255:1–10.
- Grimm V *et al.* 2014. Towards better modelling and decision support: documenting model development, testing, and analysis using TRACE. *Ecological Modelling* 280:129–139.
- EFSA PPR Panel 2013. Guidance on tiered risk assessment for plant protection products for aquatic organisms in edge-of-field surface waters. *EFSA Journal* 2013;11(7):3290, 268 pp.