Session: Effect Modelling for Regulatory Risk Assessment: Current Applications and Future Directions (I)
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Measure or extrapolate? Extended parameterisation of TKTD models for population modeling under outdoor conditions

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1. Introduction

Recently, the toxicokinetic-toxicodynamic (TKTD) model framework GUTS [1] is recommended to be used in regulatory risk assessment by EFSA [2]. TKTD models are species- and compound-specific and can be used to predict lethal effects of pesticides under untested and time-variable exposure conditions [2].

In the last few years, individual-based population models (IBMs) are being increasingly applied in risk assessment that take into account physiological temperature dependencies as well as the size structure of populations. These models are often coupled to TKTD effect models [e.g. 3], and can be used for extrapolating variable exposure scenarios to population effects under outdoor conditions. However, TKTD models usually take neither temperature nor size dependencies into consideration, although temperature and animal size can have a strong influence on the parameters of TKTD models [4,5].

TKTD models normally coupled to individual-based population models describe only the sensitivity which has been measured for one specific organism size at only one constant temperature. For practical reasons, it is not always possible to test the smallest and most sensitive stages of organisms in the laboratory. In addition, for a realistic effect modeling with dynamic population models, it is necessary to know the sensitivity of all relevant body sizes.

Measuring sufficient combinations of size and temperature is expensive and time consuming. An alternative could be the extrapolation of the required TKTD parameters from laboratory standard tests. The next step would be to examine which concepts are suitable for extrapolation from the size analyzed to other life stages or size classes and between different temperatures, and to what extent they are applicable to different organisms.

2. Materials and methods

Temperature and size dependencies of lethal effects on neonate and adult *Daphnia magna* exposed to the pesticide chlorpyrifos were measured in the laboratory in the range of 4-25 °C. These data are used to parameterize the effect model GUTS.

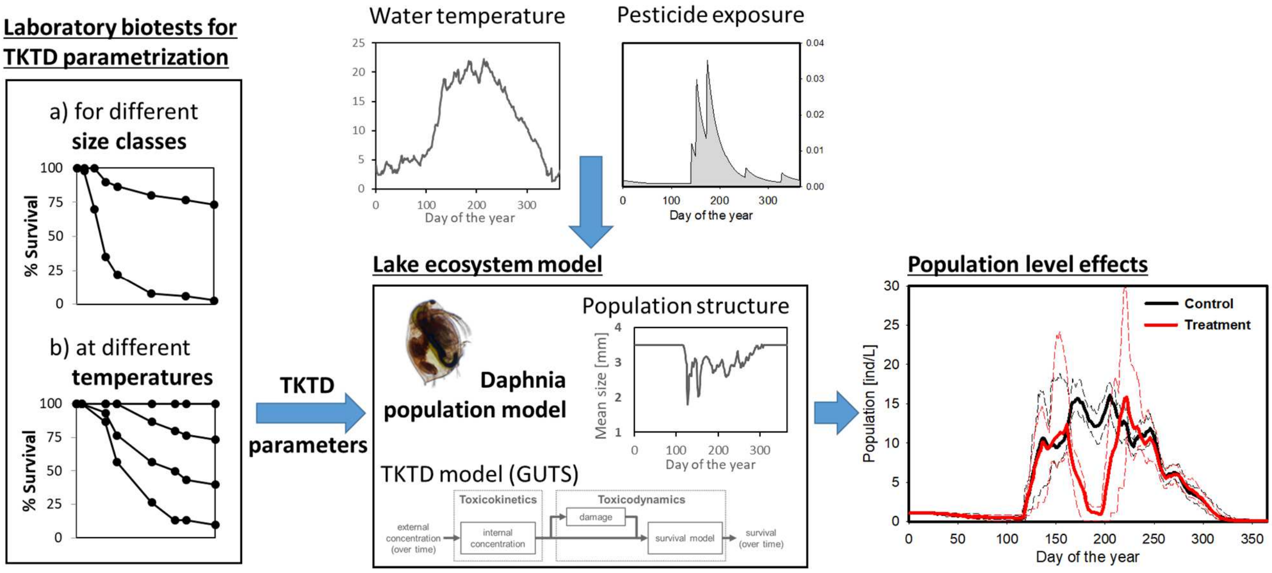

Figure 1: Simplified scheme of the modeling approach.

This presentation exemplarily examines the influence of seasonality on population-level toxicity under realistic field conditions. For this purpose, an individual-based population model for *Daphnia magna* is used [6], which has been coupled to a lake ecosystem model, which has been intensively tested using data from outdoor aquatic mesocosm studies [7]. The fluctuating water temperatures are simulated using the hydrodynamic lake model HyLaM [7], and are based on measured meteorological weather data with a high temporal resolution of at least 1 hour. This model framework includes the TKTD model GUTS [1], which now has been extended by temperature and body size dependencies.

This model approach was used to analyse different scenarios with i) measured, ii) extrapolated, and iii) ignored temperature and size dependencies of the TKTD parameters. Therefore, ecological as well as exposure scenarios for summer and winter conditions were selected. Additional population size and recovery time were considered as model endpoints to assess toxic effects on the population level.

3. Results and discussion

The implemented temperature and size dependencies of both biological and toxicological processes enables the analysis of the effect size of a pesticide as a function of exposure concentration and exposure time in the course of the year using size structured population models.

When extrapolating laboratory data to summer conditions with high water temperatures and the occurrence of the most sensitive small sized stages during the reproductive period, increased toxic effects on organisms generally are to be expected compared to simulations without temperature- and size dependent TKTD parameters. In case of winter scenarios with larger overwintering stages at low water temperatures, toxic effects are reduced, but are influenced by a slowed degradation of the substance and a lack of compensation for effects by reproduction on the population level.

We analyzed promising initial concepts for size [5] and temperature dependencies of TKTD parameters that can be used for TKTD parameter extrapolation from standard laboratory tests, but whose general application and validity for different species still needs further testing.

4. Conclusions

It is important to consider the dynamic and variable timing of toxic exposure, size composition in a population, and environmental stressors over the year.

While there are many factors that determine the effect size in the field which have to be addressed at the population and ecosystem level, temperature and body size already have an additionally strong influence directly on TKTD parameters.

Using temperature and body size dependencies for modelling the relevant biological and toxicological processes, this approach allows a more realistic risk assessment of pesticides for populations in the field, which can help to reduce the uncertainty in ecological risk assessment.

5. References

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