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Mechanistic TK/TD-model simulating the effect of growth inhibitors on *Lemna* populations

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ABSTRACT

A mechanistic combined toxicokinetic–toxicodynamic (TK/TD) and growth model for the aquatic macrophytes *Lemna* spp. has been developed. This model simulates the development of *Lemna* biomass under laboratory and environmental conditions. Growth of the *Lemna* population is simulated on basis of photosynthesis and respiration rates which are functions of environmental conditions, *i.e.*, temperature, global radiation, N- and P-concentrations. The toxicodynamic sub-model describes the effects of growth-inhibiting substances by a respective reduction in the photosynthesis rate based on the *Lemna* spp. internal concentrations. Internal concentrations are calculated using a simple, one-compartment toxicokinetic model that considers the uptake of substances through the plant surface.

The growth model was parameterised based on literature data while toxicokinetic and toxicodynamic parameters were determined by calibrating the model using substance specific effect data. Both the growth model and the toxicokinetic model were independently tested by comparing model predictions to observed data.

In an exemplary case study, the model was applied to a risk assessment for the sulfonyl urea herbicide metsulfuron-methyl. This assessment was carried out for two standard scenarios used in European regulatory risk assessments for pesticides. Thereby, it was shown that the effect of transient concentration peaks of metsulfuron-methyl on *Lemna* populations is much lower than estimated in a low tier assessment considering the maximum surface water concentration and the EC50 obtained from the standard *Lemna* growth inhibition test. The model also predicts moderate effects for longer lasting exposures resulting from calculated drainage entries into the water body if the majority of the entry occurs during the cold season with no or slow growth of the plants.

1. Introduction

The assessment of ecotoxicological effects of complex exposure patterns of pesticides becomes increasingly necessary since it is becoming common practice in Europe to base environmental risk assessments for aquatic compartments on realistically simulated concentrations (European Commission, 2001) rather than on estimated maximum concentrations and simple dissipation. At the same time, the scope of risk assessments continues to shift to more realistic specific protection goals which are usually defined at the population level or even higher levels of biological organisation (European Food and Safety Agency, 2010). Ecotoxicological laboratory studies are usually limited to deal with sensitive individuals of representative species and consider only well-defined and more or less constant exposure. Higher tier studies may be able to investigate populations under more realistic conditions but for practical reasons, cannot consider complex temporally and spatially varying exposures. Therefore, further refinement options for realistic risk assessments based on experimental effect data alone are limited.

In contrast, toxicokinetic/toxicodynamic (TK/TD) simulation models in combination with population models have the potential to extrapolate from laboratory to more realistic conditions (Hommen et al., 2010). TK/TD models simulate the temporal development of effects based on internal concentrations in the organism and allow extrapolation to different temporal exposure patterns. Several applications of this approach in aquatic ecotoxicology have been described previously (Bedaux and Kooijman, 1994; Jager et al., 2006; Ashauer et al., 2007; Ashauer and Brown, 2008; Baas et al., 2010) but are restricted to invertebrates and were predominantly used for interpreting study results. Population models of different levels of complexity are also extensively described in the literature (Galic et al., 2010) and their potential use in aquatic risk assessment

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has been discussed (Hommen et al., 2010). Approaches combining TK/TD with a population model for aquatic biota have recently been published (Ashauer, 2010; Ashauer et al., 2011a). However, most published models deal with lethal effects where as the extrapolation of sub-lethal effects to the population level is rarely considered (Ashauer et al., 2011b).

Many modern herbicides have a reversible growth inhibiting effect rather than a lethal effect to aquatic plants. For such substances, a simulation approach as described above is particularly desired as it would allow an assessment of their effect at the population level under realistic conditions. Literature on mechanistic models dealing with aquatic plants is, however, rare. A simple model describing development of *Lemna* spp. biomass was described by Driever et al. (2005) as was a biokinetic approach describing uptake and elimination of lipophilic compounds in *Myriophyllum* (Gobas et al., 1991). The combination of the simulation of sub-lethal effects based on internal concentrations (TK/TD) with that of population growth of an aquatic plant, however, has not been published before, to our knowledge. We have developed such a combined TK/TD- and growth model for *Lemna* spp. which is described here together with an exemplary application in a risk assessment for the sulfonyl urea herbicide metsulfuron-methyl.

2. Model purpose

The primary objective of the model is the extrapolation of effects determined using standardised exposure patterns in laboratory studies to realistic, temporally varying exposures as they occur in small water bodies at the edge of fields treated with plant protection products. A key component of the model is thus a toxicokinetic sub-model translating external concentrations into internal concentrations. The model should additionally allow the prediction of effects on *Lemna* populations under realistic, temporally varying environmental conditions, *i.e.*, temperature, light and nutrition, based on observations derived under standard laboratory conditions.

For use of the model in risk assessments, pure extrapolation of exposure patterns and additional consideration of realistic environmental conditions are considered as two separate steps. The primary endpoint to be derived from the simulation results is the reduction of biomass compared to an unaffected control. As a secondary endpoint, the duration of such effect can also be determined.

3. Description of the model

3.1. Model concept

The model concept is visualised in Fig. 1. It comprises the combination of a one compartment TK model and a differential equation model describing the dynamic development of dry biomass based on photosynthesis and respiration rates. The TK model translates the external exposure to a toxic substance into its internal concentration. Based on the internal concentration, the photosynthesis rate is reduced, thus reflecting the growth inhibiting effect of the toxicant. It should be noted that here, the term photosynthesis rate is used for the biosynthesis rate for total biomass. Consequently, the TD model is applicable to all compounds that act on any step in the whole bio-synthesis pathway.

Apart from the influence of the toxicant, photosynthesis and respiration rates are also modulated by other external factors such as temperature, radiation, nutrition, and biomass density. This allows an extrapolation of the biomass growth dynamics to realistic environmental conditions.

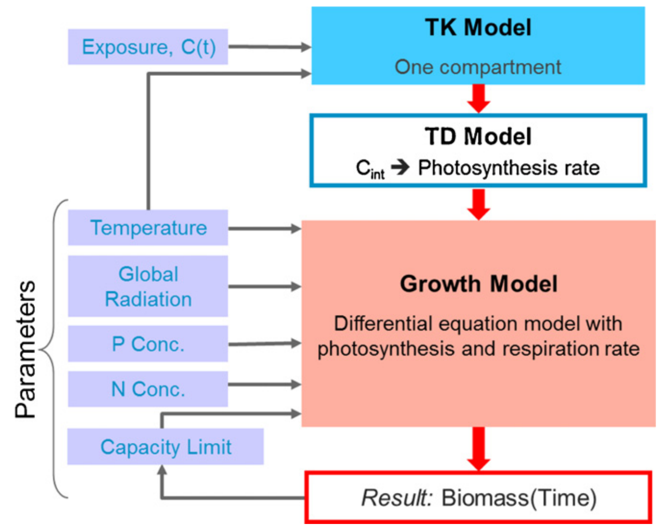

Fig. 1. Concept toxicokinetic/toxicodynamic and growth model for *Lemna* spp.

3.2. Growth model

The family of Lemnaceae is probably the best investigated group of aquatic macrophytes (Hillman, 1961; Landolt and Kandeler, 1987). Particularly, the growth of different *Lemna* spp. has been intensively investigated because these species are of interest for different potential applications due to their high growth rate, *e.g.*, water body remediation (Ansari and Khan, 2008; Benjawan, 2008; Cheng, 2002) and feed supply for animal breeding. It is generally agreed that the development of *Lemna* biomass can be described well with a growth rate that depends on environmental factors such as temperature, irradiation, and nutrient supply (Landolt and Kandeler, 1987). Thus, growth of a *Lemna* population in terms of dry biomass can be simulated using a very simple model given by the following differential equation (Eq. (1)) (Driever et al., 2005).

$$\frac{dBM}{dt} = f_{photo}(\theta)k_{photo}^{\max}BM - f_{resp}(\theta)k_{resp}^{ref}BM \qquad (1)$$

In this equation, BM = dry biomass, $k_{photo}^{\max}$ = maximum photosynthesis rate, k_{resp}^{ref} = respiration rate at reference temperature, f_{photo} = factor by which the maximum photosynthesis rate is reduced due to suboptimal conditions, f_{resp} = factor by which the maximum respiration rate is reduced, and $\theta = \{T, I, \mathrm{P}, \mathrm{N}, D\}$ is the set of environmental parameters potentially influencing the rates k_{photo} and k_{resp}. f_{photo} and f_{resp} are scaling factors that depend on environmental parameters, which for the present model are temperature (T), irradiation (I), phosphate concentration (P), and nitrate concentration (N). In addition, f_{photo} is considered to depend on population density (D) (=biomass/area) resulting in a carrying capacity. Overall, $f_x(\theta)$ is the product of functions depending on single parameters which are described below.

The toxic effect was included as an additional reduction factor. For growth inhibiting substances, the synthesis rate is reduced in relation to the internal concentration of the toxicant. For other modes of action, it might be desirable to increase the respiration rate in order to simulate increased mortality.

In the following, the single dependencies between influencing parameters and the rate constants are described in detail.

3.2.1. Temperature dependence

Experimentally, usually only the net growth rate of *Lemna* is determined which shows an asymmetric bell shaped temperature dependence (van der Heide et al., 2006; Lasfar et al., 2007). The net