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Development of a dynamic model for estimating the food web transfer of chemicals in small aquatic ecosystems

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ABSTRACT

A dynamic combined fate and food web model was developed to estimate the food web transfer of chemicals in small aquatic ecosystems (i.e. ponds). A novel feature of the modeling approach is that aquatic macrophytes (submerged aquatic vegetation) were included in the fate model and were also a food item in the food web model. The paper aims to investigate whether macrophytes are effective at mitigating chemical exposure and to compare the modeling approach developed here with previous modeling approaches recommended in the European Union (EU) guideline for risk assessment of pesticides. The model was used to estimate bioaccumulation of three hypothetical chemicals of varying hydrophobicity in a pond food web comprising 11 species. Three different macrophyte biomass densities were simulated in the model experiments to determine the influence of macrophytes on fate and bioaccumulation. Macrophytes were shown to have a significant effect on the fate and food web transfer of highly hydrophobic compounds with log $K_{OW} >= 5$. Modeled peak concentrations in biota were highest for the scenarios with the lowest macrophyte biomass density. The distribution and food web transfer of the hypothetical compound with the lowest hydrophobicity (log $K_{OW} = 3$) was not affected by the inclusion of aquatic macrophytes in the pond environment. For the three different hypothetical chemicals and at all macrophyte biomass densities, the maximum predicted concentrations in the top predator in the food web model were at least one order of magnitude lower than the values estimated using methods suggested in EU guidelines. The EU guideline thus provides a highly conservative estimate of risk. In our opinion, and subject to further model evaluation, a realistic assessment of dynamic food web transfer and risk can be obtained using the model presented here.

1. Introduction

Several models for assessing the uptake, fate and distribution of organic chemicals in food webs have been developed (e.g. Clark et al., 1990; Thomann et al., 1992; Gobas, 1993; Morrison et al., 1996; Nfon and Cousins, 2007). Common features in these models are (i) their general applicability to large ecosystems and (ii) the use of a steady-state assumption. These steady-state models however are not appropriate for predicting the fate and food web uptake of chemicals in small aquatic ecosystems where emissions are often periodic (e.g. in the case of pesticides; Crossland, 1982; Rand and Clark, 2000), and chemical levels therefore fluctuate substantially over time.

Carbonell et al. (2000) addressed some of these concerns when they developed a simple, generic and dynamic (time dependent or unsteady-state) food web model. They demonstrated that bioaccumulation becomes important for hydrophobic chemicals even if the chemical is only moderately persistent. The approach of Carbonell et al. (2000) has gained acceptance at the European level for registration of pesticides by being incorporated into the Aquatic Guidance Document on Aquatic Ecotoxicology as a higher tier study in the context of the Directive 91/414/EEC (EU 2002).

There is interest among regulators, the agrochemical industry and researchers in the ability of aquatic vegetation (macrophytes) to mitigate against chemical exposure (e.g. Maund et al., 2002; Bouldin et al., 2004). Apart from playing a vital role in aquatic ecosystems as primary producers at the base of aquatic food webs, macrophytes may reduce the dispersion and assist the removal of chemical from aquatic environments by sorbing residues or trapping particulate containing chemicals (Hinman and Klaine, 1992; Karen et al., 1998) and thus limiting the ability of the chemical for aquatic transport or uptake from the water-phase (reducing the exposure of aquatic animals). Aquatic plants have also been shown to enhance the overall degradation of chemical residues facilitating the irreversible removal of toxic compounds from contaminated water bodies (Muir et al., 1985; Hand et al., 2001). Armitage et al. (2008) developed and applied a fugacity-based model to describe the fate of chemicals in small ponds and specifically their mass transfer to macrophytes. They concluded that uptake by macrophytes is particularly strong for hydrophobic chemicals (log K_{OW} >5.5), where the mass transfer is dominated by particle deposition.

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This study describes a dynamic food web model for studying the food web transfer of chemicals in small-scale ecosystems such as ponds, streams, ditches or mesocosms. It represents a logical extension of the work of Carbonell et al. (2000) because (i) uptake/elimination parameters are derived from chemical properties using similar approaches used in large-scale steady state food web models (ii) the transfer of chemical residues between environmental compartments and biota is explicitly calculated using the fugacity concept (iii) aquatic macrophytes are included as component of the aquatic ecosystem and as a food item for food web species and (iv) a realistic pond food web is modeled. The paper aims to investigate whether macrophytes are effective at mitigating chemical exposure and to compare the modeling approach developed here with the previous modeling approaches recommended in the aforementioned EU guidance document, including the approach of Carbonell et al. (2000).

2. Methods

The general structure of the model consists of a chemical fate module linked to a food web bioaccumulation model representative of a generic pond ecosystem.

2.1. Pond fate model

The pond fate model is represented by three compartments (water, sediment and submerged vegetation) and has been previously described in Armitage et al. (2008). The water compartment is modeled as three phases (water, suspended solids and dissolved organic matter); the sediment compartment comprises two phases (pore water and sediment solids) and the submerged vegetation is modeled as a single phase. The model uses the fugacity concept (Mackay, 2001). The different methods used to calculate fugacity capacities (Z-values) ($\text{mol m}^{-3}\,\text{Pa}^{-1}$) and transport D-values ($\text{mol Pa}^{-1}\,\text{h}^{-1}$) are explained in full in Armitage et al. (2008).

Three differential equations representing the mass distribution (or fugacity) of the chemical in the pond were generated in fugacity format as:

$$V_W Z_W df_W/dt = f_S D_{SW} + f_M D_{MW} - f_W D_{TW} \quad (1)$$

$$V_S Z_S df_S/dt = f_W D_{WS} + f_M D_{MS} - f_S D_{TS} \quad (2)$$

$$V_M Z_M df_M/dt = f_W D_{WM} + f_S D_{SM} f_M D_{TM} \quad (3)$$

where V, Z, f and D are the volumes (m^3), fugacity capacities ($\text{mol m}^{-3}\,\text{Pa}^{-1}$), fugacities (Pa), and the fugacity transport coefficients or D-values ($\text{mol Pa}^{-1}\,\text{h}^{-1}$), respectively, the subscripts W, S and M refer to the water, sediment and macrophyte compartments and the subscripts on the D-values refer to different D-values for intermedia transport (W, S and M again refer to water, sediment and macrophytes, thus D_{SW} refers to intermedia transport from sediment to water and so on) and total loss (i.e. D_{TW} refers to the total loss D value for the water compartment which comprises several processes; degradation, volatilisation, diffusive and particulate deposition to sediments and macrophytes).

A solution of the system of equations is generated by numerical integration (with initial conditions $f_S = f_M = 0$ and $f_W = C_{WO}/Z_W$) and the output is the change in fugacity with time for each compartment in the modeled system. C_{WO} is the concentration in the system following an initial pulse release of chemical. With modification, the model can be used to model other emission scenarios such as continuous steady inputs or time-varied inputs. Full details of the pond fate model are given in Armitage et al. (2008).

2.2. Pond food web model

The pond food web model comprises five trophic levels of 11 guilds (see Fig. 1). Defining guilds rather than specific organisms was preferred because it allows a more generic representation of the pond ecosystem. The food web is representative of a typical pond food web, but the selection of number/type of species and guilds is arbitrary. The food web modeling approach is based on the model developed by Campfens and Mackay (1997) using the fugacity approach of Mackay (2001) with the main difference that the model is dynamic (concentrations can be calculated as a function of time) rather than steady-state. Eleven equations of the form of Eq. (4) describing the fugacity of each species in the food web were generated

$$V_i Z_i df_i/dt = \sum \left(D_{Aji} f_j\right) + D_{Vi}(f_W . X_{Wi} + f_S . X_{Si}) - D_{Ti} f_i \quad (4)$$

where i can be any one of eleven species; V is volume, f is fugacity and Z is fugacity capacity, D_{Aji} is the food uptake D-value to species i

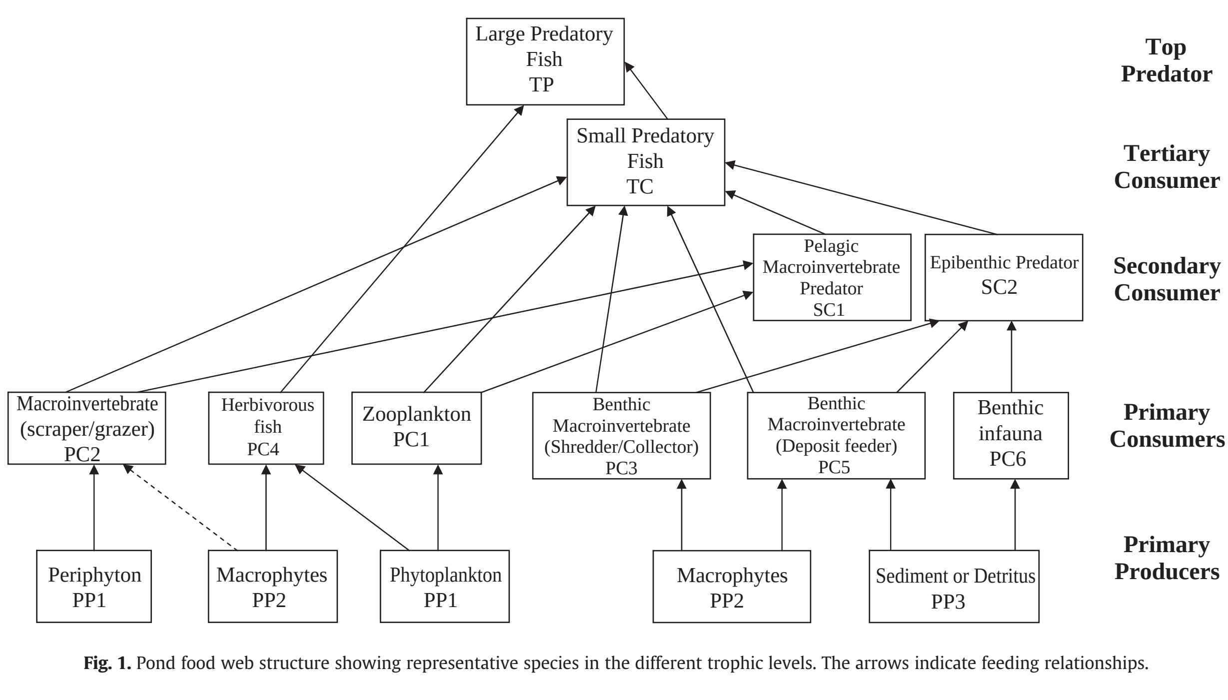

Fig. 1. Pond food web structure showing representative species in the different trophic levels. The arrows indicate feeding relationships.