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Theoretically exploring direct and indirect chemical effects across ecological and exposure scenarios using mechanistic fate and effects modelling

F. De Laender [a,*], M. Morselli [b], H. Baveco [c], P.J. Van den Brink [c,d,1], A. Di Guardo [b]

[a] Namur University, Research Unit in Environmental and Evolutionary Ecology, Rue de Bruxelles 61, 5000 Namur, Belgium
[b] Department of Science and High Technology, University of Insubria, Via Valleggio 11, 22100 Como, Italy
[c] Alterra, Wageningen University and Research Centre, P.O. Box 47, 6700 AA Wageningen, The Netherlands
[d] Department of Aquatic Ecology and Water Quality Management, Wageningen University, Wageningen University and Research Centre, P.O. Box 47, 6700 AA Wageningen, The Netherlands

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ABSTRACT

Predicting ecosystem response to chemicals is a complex problem in ecotoxicology and a challenge for risk assessors. The variables potentially influencing chemical fate and exposure define the exposure scenario while the variables determining effects at the ecosystem level define the ecological scenario. In absence of any empirical data, the objective of this paper is to present simulations by a fugacity-based fate model and a differential equation-based ecosystem model to theoretically explore how direct and indirect effects on invertebrate shallow pond communities vary with changing ecological and exposure scenarios. These simulations suggest that direct and indirect effects are larger in mesotrophic systems than in oligotrophic systems. In both trophic states, interaction strength (quantified using grazing rates) was suggested a more important driver for the size and recovery from direct and indirect effects than immigration rate. In general, weak interactions led to smaller direct and indirect effects. For chemicals targeting mesozooplankton only, indirect effects were common in (simple) food-chains but rare in (complex) food-webs. For chemicals directly affecting microzooplankton, the dominant zooplankton group in the modelled community, indirect effects occurred both in food-chains and food-webs. We conclude that the choice of the ecological and exposure scenarios in ecotoxicological modelling efforts needs to be justified because of its influence on the prevalence and magnitude of the predicted effects. Overall, more work needs to be done to empirically test the theoretical expectations formulated here.

1. Introduction

Ecosystems are inherently complex and understanding how chemicals impact on their structure and functioning is at an incipient phase (Naito et al., 2003; De Laender et al., 2008b; Park et al., 2008; De Laender and Janssen, 2013). The number of variables potentially influencing how ecosystems respond to chemicals represents one dimension of this complexity. Although widely used, the concept of the 'ecological scenario' is, to the best of our knowledge, rarely defined. One approach to characterizing an ecological scenario consists of allocating one value to each variable potentially influencing population- and ecosystem-level responses to an environmental perturbation. Note that this approach does not constrain the number of variables needed to describe a given scenario, as this will depend on the ecosystem considered and the research questions asked.

* Corresponding author. Tel.: +32 81 724 405.
E-mail addresses: frederik.delaender@unamur.be (F. De Laender), melissa.morselli@uninsubria.it (M. Morselli), paul.vandenbrink@wur.nl (P.J. Van den Brink), antonio.diguardo@uninsubria.it (A. Di Guardo).
[1] Tel.: +31 317 481615; fax: +31 419000.

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Examples of variables making up an ecological scenario include trophic state, the degree of isolation of the exposed system, the interaction strength between species in a food-web and the complexity of this food-web. Trophic state may determine the response of individuals, populations, and ecosystems to chemicals through modifying resource availability (Noel et al., 2006; Pieters et al., 2006; Alexander et al., 2013; De Hoop et al., 2013; Gabsi et al., 2014). The degree of isolation will determine if immigration from areas with lower exposure levels can compensate for chemical effects and/or facilitate recovery and recolonization (Liess and Schulz, 1999; Caquet et al., 2007). Based on the ecological literature on disturbances in ecosystems, also interaction strength and food-web complexity can be hypothesised as key variables making up the ecological scenario. For example, the influence of these two variables on various stability measures has been a major topic in community and ecosystem ecology (May, 1972; Neutel et al., 2002; Allesina and Tang, 2012), although existing efforts have focused on random (non-specific) perturbations. To our knowledge, the influence of these two ecosystem descriptors on the response of ecosystems to chemicals has not been tested yet. We expect this response to be different for chemicals than for random perturbations because chemicals often affect specific taxa only. The way in which such direct impacts of chemicals travel through an ecological network such as a food-web will most likely depend on the identity of the impacted taxa.

Next to the ecological scenario, the exposure scenario is another dimension to the complexity surrounding ecological effect assessments at higher levels of biological organisation. Again, an approach to defining an exposure scenario consists of attributing values to variables determining chemical exposure. Such exposure is often related to chemical emissions in the environment (application and/or discharge). The timing of application is one potentially important variable making up the exposure scenario, although the influence of the application season is unclear at present (Willis et al., 2004; Van Wijngaarden et al., 2006). Other variables that characterize exposure include those determining chemical fate (e.g. partitioning coefficients) as well as chemical movement across compartments and degradation. In such view, the role of the ecological complexity in defining the exposure is often neglected or overlooked (Di Guardo and Hermens, 2013).

The influence of the exposure scenario on a chemical's effects on ecosystems needs to be examined in concert with that of the ecological scenario, as both scenarios may share common variables. More precisely, certain variables making up the ecological scenario will also define the exposure scenario, and vice versa. For example, trophic state, essentially a characteristic of the challenged ecosystem determining resource availability, will also influence chemical bioavailability in water, and therefore the actual exposure pelagic biota are facing. The timing of application, often considered as a part of the exposure scenario, will likewise determine the ecological scenario in case of strong seasonal fluctuations in community composition.

At present, no information is available on how ecosystem response to chemicals varies across different ecological and exposure scenarios. This may be partly due to the practical difficulty to experimentally test chemical effects on population- and ecosystem-level endpoints for a range of ecological and exposure scenarios and the resources that are required to do so. As opposed to experimental approaches, the use of mechanistic models does not suffer such constraints. Indeed, modelling can play a key role in theoretically exploring how ecological scenarios co-determine the ecological effects triggered by an array of exposure scenarios.

In the field of exposure and fate modelling, efforts are on-going to refine the incorporation of bioavailability into the exposure assessment of organic pollutants (Di Guardo et al., 2006; Infantino et al., 2013). Future efforts will include the evaluation and expression of the spatial and temporal variability of chemical fate in order to define more realistic exposure scenario (Di Guardo and Hermens, 2013). In recent years, advancements have been made in the field of mechanistic effect modelling as well, mostly at the population level (Grimm et al., 2009; Martin et al., 2013), and these efforts have led to strategies to enhance the realism of ecological effect assessments (Forbes et al., 2009). Currently, efforts are on-going to continue the upscaling of effects towards higher levels of biological organisation (De Laender et al., 2011; De Laender and Janssen, 2013).

The objective of the presented paper is to formulate theoretical expectations for ecological effects and recovery across a range of exposure and ecological scenarios, using a combined chemical fate and ecosystem model. The chemical fate model is based on the fugacity approach. The choice for a fugacity approach was based on the availability of a dynamic fugacity-based aquatic model (Di Guardo et al., 2006; Infantino et al., 2013), which could be easily modified to simulate exposure for this exercise. The ecosystem model is defined as a set of coupled ordinary differential equations, at present the only approach available to model ecosystem dynamics in ecotoxicology. We summarize effects on the biomasses of the included functional groups in two ways: (1) using the maximum difference in time between the exposed and control biomass, and (2) using the time-integrated biomass difference between the exposed and control dynamics. We consider both direct and indirect effects (Fleeger et al., 2003) across sixteen ecological scenarios, differing in trophic state (oligo- vs. mesotrophic), the interaction strength between producers and consumers (high vs. low), the immigration rate (fast vs. slow), and the complexity of the ecological system (food-web vs. food-chain). The four chemicals considered represent all combinations of two sorption characteristics (hydrophobic vs. hydrophilic), and two toxicological profiles (targeting micro- vs. mesozooplankton). By also varying the season of emission between spring and late summer, a total of eight exposure scenarios were considered. The fate model was used to predict the dynamics of the water dissolved chemical concentrations, taking into account trophic state by using phytoplankton and detritus mass for bioavailability calculations. We stress that our exercise should be interpreted as a model-aided quantification of the theoretical expectations on how ecological effects of chemicals vary across ecological and exposure scenarios. In our discussion, we qualitatively confront our predictions with results from micro- and mesocosm studies but this comparison does not waive the need for a more formal confrontation with data in the future, when these become available.

2. Material and methods

2.1. Chemical fate model

Chemical fate was calculated using a modified version of the DynA (Di Guardo et al., 2006) and EcoDynA (Infantino et al., 2013) models. These models are fugacity-based (Mackay, 2001) and were developed to investigate the fate of organic chemicals in a dynamic aquatic system. Model dynamics depend on chemical emission (which can be varied on an hourly basis) and on environmental parameters. More specifically, model input includes hourly values of water temperature, water inflow and outflow rates and suspended solid concentration in water. Suspended solids are modelled as a water sub-compartment; equilibrium with water is therefore assumed. The presence of particulate organic carbon (POC) is simulated by defining the organic fraction of the suspended solids. In the implementation of the model used in the present work, also a dissolved organic matter (DOM) sub-compartment was included. More details concerning model formulation and the application in this paper can be found in Text S1.

For all simulations, the model was parameterized to represent a typical shallow pond, characterized by an area of 450 m^2 and a depth of 1 m. A water residence time of six months, sufficiently high to prevent the chemical outflow with POC and DOC to become the dominant fate process, was simulated, as the result of constant input and output water fluxes of 0.1 $m^3\ h^{-1}$. A seasonal profile of water temperature similar to those measured in a set of UK temperate ponds, with values ranging from 3 to 15 °C in winter and summer, respectively, was adopted (Martin, 1972; Young, 1975) (Fig. S1, Supporting information). The sediment compartment, in terms of the fraction of solids and fraction of organic carbon in solids, was parameterized elsewhere (Armitage et al., 2008).

2.2. Food-web model

A food-web model was implemented in R (R Development Core Team, 2010) as a set of ordinary differential equations. Each equation represented the dynamics of one functional group (mg C/m^2), based on gain and loss processes quantified as surface-specific carbon exchange rates (mg $C/m^2/d$), including functional group-specific immigration (Table 1 lists all parameters). The model included 6 functional groups: phytoplankton, omnivores, microzooplankton, mesozooplankton, detritivores, and invertebrate predators (consuming all heterotrophs) (Fig. 1). Phytoplankton growth was described as:

$$\frac{dPhy}{dt} = Phy \cdot \left[\left[1 - a \cdot \cos\left(\frac{2 \cdot \pi \cdot t}{365}\right)\right] \cdot Gpp \cdot (1 - Resp - Excr) \cdot \left(1 - \frac{Phy}{K}\right) - Mort\right] - Predation + I$$