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Importance of environmental and biomass dynamics in predicting chemical exposure in ecological risk assessment

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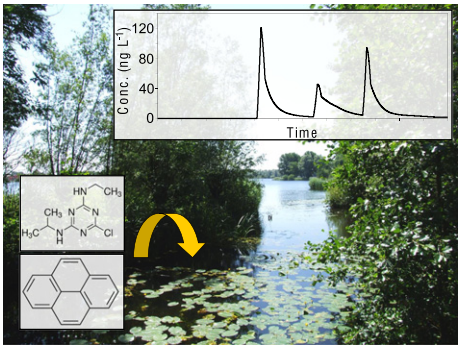
HIGHLIGHTS

- Exposure is generally modelled using static environmental and biomass conditions.
- The spatio-temporal heterogeneity of such conditions may cause exposure variations.
- A new dynamic spatially-explicit model for aquatic environments was developed.
- Spatial and temporal dynamics were predicted for four organic chemicals.
- Variations of bioavailable concentrations can be up to several orders of magnitude.

GRAPHICAL ABSTRACT



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ABSTRACT

In ecological risk assessment, exposure is generally modelled assuming static conditions, herewith neglecting the potential role of emission, environmental and biomass dynamics in affecting bioavailable concentrations. In order to investigate the influence of such dynamics on predicted bioavailable concentrations, the spatially-resolved dynamic model "ChimERA fate" was developed, incorporating macrophyte and particulate/dissolved organic carbon (POC/DOC) dynamics into a water-sediment system. An evaluation against three case studies revealed a satisfying model performance. Illustrative simulations then highlighted the potential spatio-temporal variability of bioavailable concentrations after a pulsed emission of four chemicals in a system composed of a pond connected to its inflow and outflow streams. Changes in macrophyte biomass and POC/DOC levels caused exposure variations which were up to a factor of 4.5 in time and even more significant (several orders of magnitude) in space, especially for highly hydrophobic chemicals. ChimERA fate thus revealed to be a useful tool to investigate such variations and to identify those environmental and ecological conditions in which risk is expected to be highest.

1. Introduction

Ecological risk assessment of chemicals (ERA) is a procedure which is commonly used to evaluate the impact of chemicals on ecosystems.

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This is generally done comparing the environmental exposure and the potential (ecological) effect threshold levels. The need for regulating a large number of chemicals and the complexity of the ecosystems to protect led to the development of simple and standardized tools (EPA, 1998; EC, 2003). However, most of these approaches do not properly address environmental realism in terms of, for example, the spatial and temporal variability of exposure and ecological scenarios (affecting both exposure and effects) (De Laender et al., 2014, 2015), the interactions among individuals and populations and the co-occurrence with other stress factors (such as chemical or physical ones). A recent joint scientific opinion document from the three scientific committees of the European Commission (EC, 2013; Vighi, 2013) tried to address the new challenges for risk assessment for human health and the environment. Among the points devised, a number were related to the improvement of environmental exposure assessment (EEA) in ERA. It was underlined that EEA deserves particular attention when predictions should cover a large variety of habitats at different spatial scales, as well for terrestrial as aquatic environments (Di Guardo, 2014). Moreover, in a recent publication specifically devoted to challenges for EEA (Di Guardo and Hermens, 2013), the need of accounting for the bioavailability of chemicals (here defined as the freely dissolved concentration of a chemical, in e.g., water) is remarked. This concentration, which is regarded as available for uptake by organisms, can exhibit spatio-temporal variations in surface water bodies in response to the presence of relevant amounts of organic carbon-rich materials like primary producers (e.g., algae and/or macrophytes) (Taylor et al., 1991; Berglund et al., 2001; Leistra et al., 2003), particulate/dissolved organic carbon (POC/DOC) (Schwarzenbach et al., 2003), or sorbing materials (e.g., organic matter or soot) in sediment (Gustafsson et al., 1997). Despite the fact that a number of exposure models exist accounting for the presence of primary producers (e.g., Armitage et al., 2008; Nfon et al., 2011) or incorporating variable degrees of environmental complexity (e.g., Adriaanse, 1997; FOCUS, 2001), there is a need to develop a model unit incorporating such processes to reflect realistic ecosystem heterogeneity and suitable for regulatory purposes. Indeed, most of the exposure models adopted for regulatory purposes (such as EUSES in the European Union; EC, 2004) rely on simplistic assumptions (such as steady-state) or they use fixed values for environmental parameters (temperature, organic carbon fractions, volumes of compartments and phases, etc.).

The aim of this study was to develop a new dynamic, spatially-explicit fate model for shallow-water environments ("ChimERA fate"), capable of accounting for spatio-temporal variability of emissions and compartment properties and considering the role of macrophytes, POC and DOC dynamics in affecting bioavailable concentrations. Although phytoplankton can be relevant in affecting exposure in shallow waters, its modelling will be included in a following paper. Comparisons between model predictions and experimental observations for three case studies allowed a preliminary assessment of model performance. The results of illustrative simulations run for chemicals with different hydrophobicity and persistence are then presented in order to show (I) the potential temporal and spatial variability of bioavailable concentrations after a pulsed emission in a stream–pond–stream system, (II) the role of macrophytes, POC and DOC and their dynamics in influencing bioavailability and (III) the added value of adopting time–variable profiles of macrophyte biomass and POC/DOC concentrations compared to the use of constant or averaged values.

2. Materials and methods

The ChimERA fate model is based on the fugacity approach (Mackay, 2001) and was developed starting from an existing dynamic water–sediment model (Di Guardo et al., 2006). New compartments and sub-compartments were added and different model units were connected to obtain a spatial discretization. In this first version of ChimERA fate, the model incorporates the macrophyte compartment, while the inclusion of the phytoplankton compartment will be the object of future work. In Fig. 1a, a schematic representation of the model unit is provided. Moreover, the temperature dependence of properties and degradation rates was included, as explained in Text S1. Details concerning model development and parameterization are presented in the following sections and in the SI. A complete list of *Z*- and *D*-values can be found in Tables S1 and S2.

2.1. Model background

ChimERA fate was grounded on the DynA Model (Di Guardo et al., 2006), developed to investigate the fate of organic chemicals in dynamic water–sediment systems. In DynA, time-varying chemical emissions and environmental parameters (e.g., water temperature and fluxes) can be specified, and model output (chemical concentrations and fluxes) is provided on an hourly basis. Suspended solids are modelled as a water sub-compartment (in equilibrium with water), and POC is simulated by specifying the organic fraction of suspended solids. In the original DynA Model, the presence of DOC is neglected. The model was calibrated and validated for herbicides in rice paddy scenarios, but no vegetation compartment was simulated (Infantino et al., 2008). More recently, an organism compartment was included and the model was applied to simulate uptake of DDTs by fish in an Italian sub-alpine

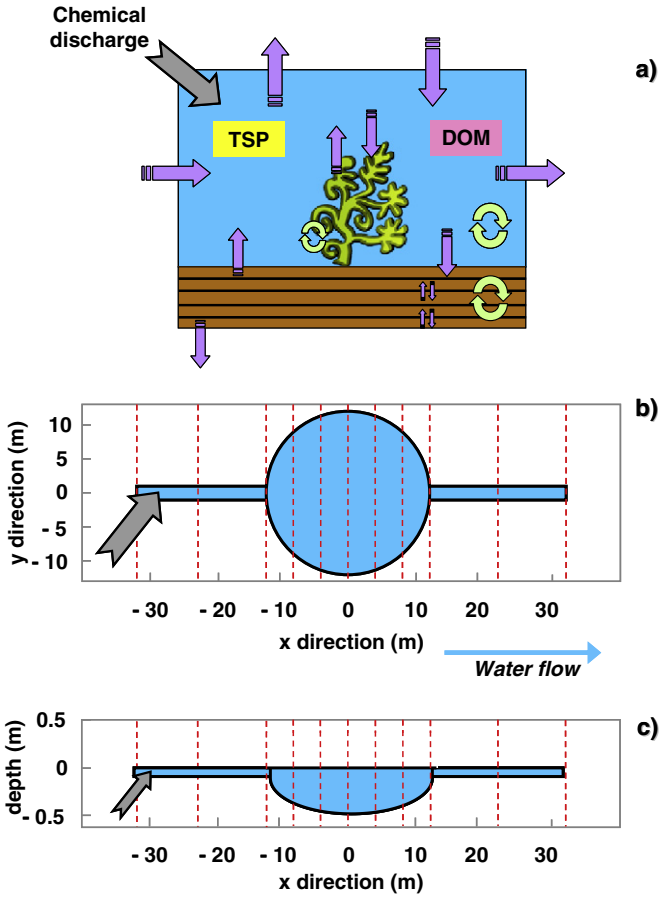

Fig. 1. Schematic representation of (a) the ChimERA fate model unit, with purple arrows indicating chemical fluxes between compartments or accessing/leaving the system and circular green arrows indicating degradation processes; (b) top-view and (c) side-view (b) of the environmental system simulated in the model illustration. TSP is total suspended particles while DOM is dissolved organic matter.