Exploring the influence of environmental and ecological dynamics on exposure predictions: a modelling approach

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1. Introduction

❖ Current approaches for **ecological risk assessment** (ERA): exposure modelled assuming constant emissions and static environmental/ecological parameters

❖ **Spatio-temporal variations** of exposure levels related to pulsed emissions, environmental heterogeneity and biomass, POC (particulate organic carbon) and DOC (dissolved organic carbon) dynamics

❖ Need to increase the **ecological realism** of the modelling approaches used in ERA procedures

3. Materials and Methods

3.1 Model formulation

❖ Based on the dynamic fugacity model DynA[1] (water + sediment)

❖ 2 new compartments exchanging with water: **phytoplankton** and **macrophytes**; exchanges computed by means of K_{OW}-dependent rate constants

❖ **TSP** (total suspended particles) and **DOM** (dissolved organic matter): water sub-compartments; POC and DOC are fractions of TSP and DOM, respectively

❖ Vertical discretization of sediment compartment (layers)

❖ Chemical mass balance: an ordinary differential equation (ODE) for each comparment; ODE system solved numerically[2]

❖ **Spatial discretization**: connection of two or more model units (**Fig. 1a**) to create a system of water bodies (**Figs. 1b,c**). Connection through water flow, computed with a 1-D hydrological module

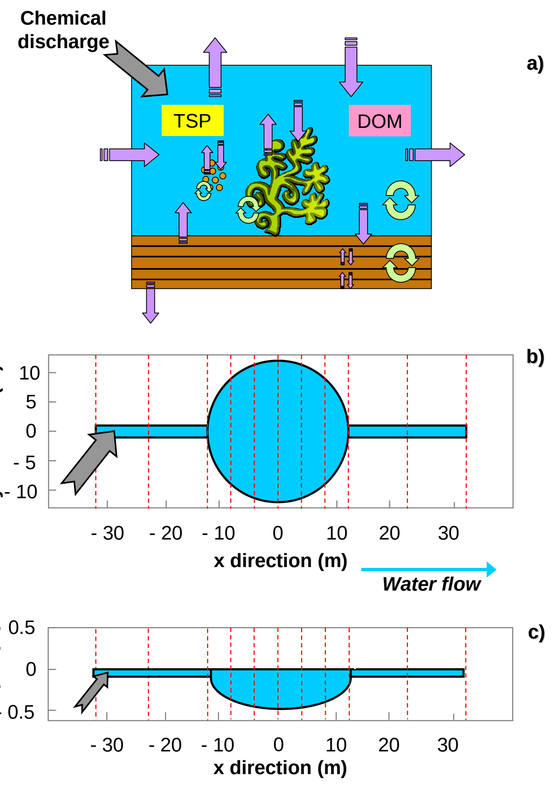

Figure 1. (a) ChimERA fate model unit; (b) top view and (c) side view of the environmental system simulated in the model illustration.

Table 1. Physical-chemical properties and environmental half-lives at 25 °C of the modelled compounds.

Property	Atrazine	PCB 1	Pyrene	PCB 153
MW (g/mol)	215.7	188.7	202.3	360.9
MP (°C)	175.8	34	156	103
VP (Pa)	3.85E-05	2.04	6E-04	1.19E-04
WS (g/m³)	33	5.5	0.132	1E-03
log K_{OW}	2.5	4.3	5.18	6.9
HL_{Wat} (d)	55	229	70	2292
HL_{Sed} (d)	200	708	2292	2292
HL_{Mf} (d)	55	229	70	2292

2. Objectives

❖ New spatially-resolved dynamic fate model (**ChimERA fate**) for aquatic lentic systems: dynamics of emissions, environmental parameters, primary producer biomass and POC/DOC concentrations (**Fig. 1**)

❖ Model evaluation against field data

❖ Model illustration → potential **spatio-temporal variability of bioavailable concentrations** in a system composed of a pond and its inflow and outflow streams (**Figs. 1b,c**)

3.2 Model parameterization

❖ **Macrophyte-dominated systems** (i.e., no phytoplankton). For simulations with phytoplankton see poster **MO 345**

❖ **Model evaluation**: lambda-cyhalothrin applied to ditch enclosures[3]. Comparison between measured and predicted concentrations in water, macrophytes and sediment

❖ **Model illustration**: one-year simulations, 4 chemicals (**Table 1**) emitted to the inflow stream (**Figs. 1b,c**). Pulsed chemical emission, dynamic macrophyte biomass and POC/DOC concentrations (**Fig. 2a**) + dynamic water temperature (**Fig. 2b**)

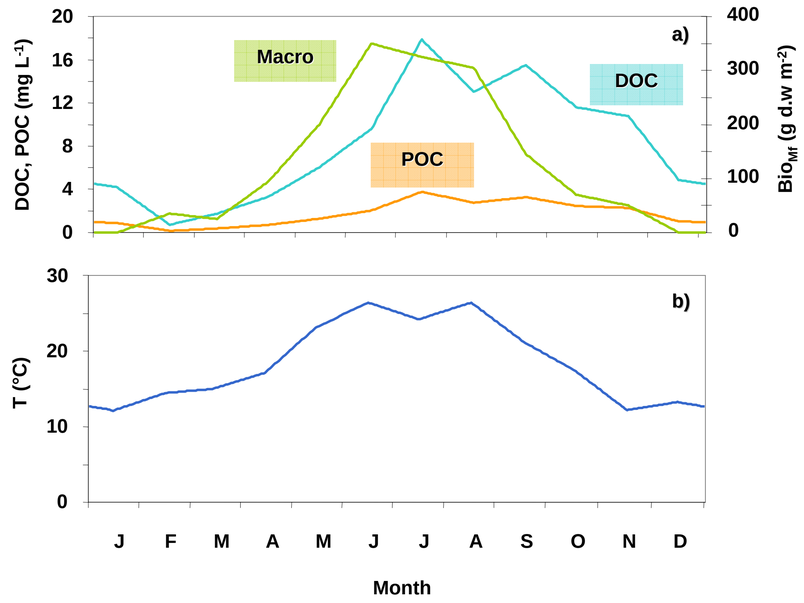

Figure 2. (a) Macrophyte biomass density, POC and DOC concentration and (b) water temperature profiles during the simulation period.

4. Results and Discussion

4.1 Model evaluation

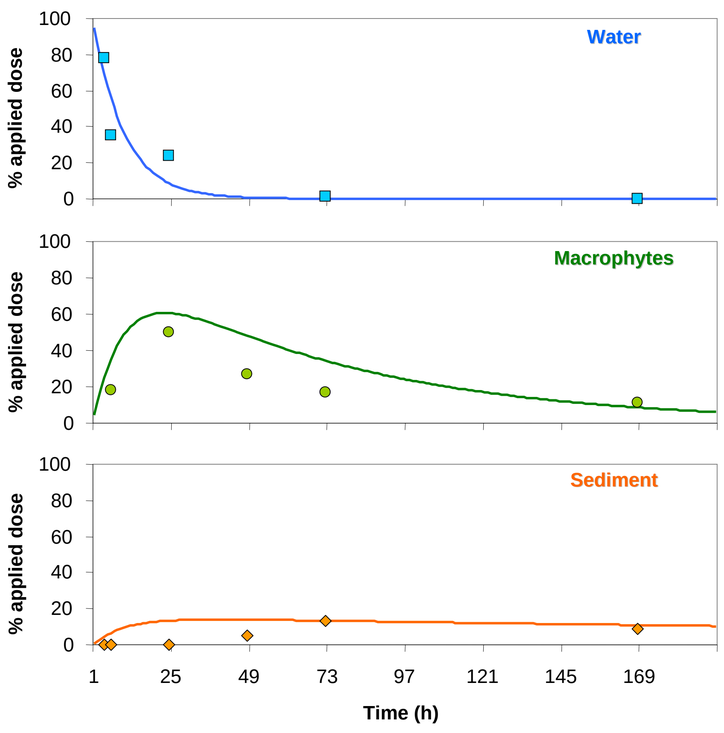

Figure 3. Comparison between measured (markers) and predicted (lines) concentrations in water, macrophytes and sediment.

❖ Model predictions were generally **within an order of magnitude** with respect to measures (**Fig. 3**)

❖ Agreement was better for another case study (azinphos-methyl), with predictions **within a factor of 2 or less** with respect to observations

4.2 Model illustration

Temporal variability

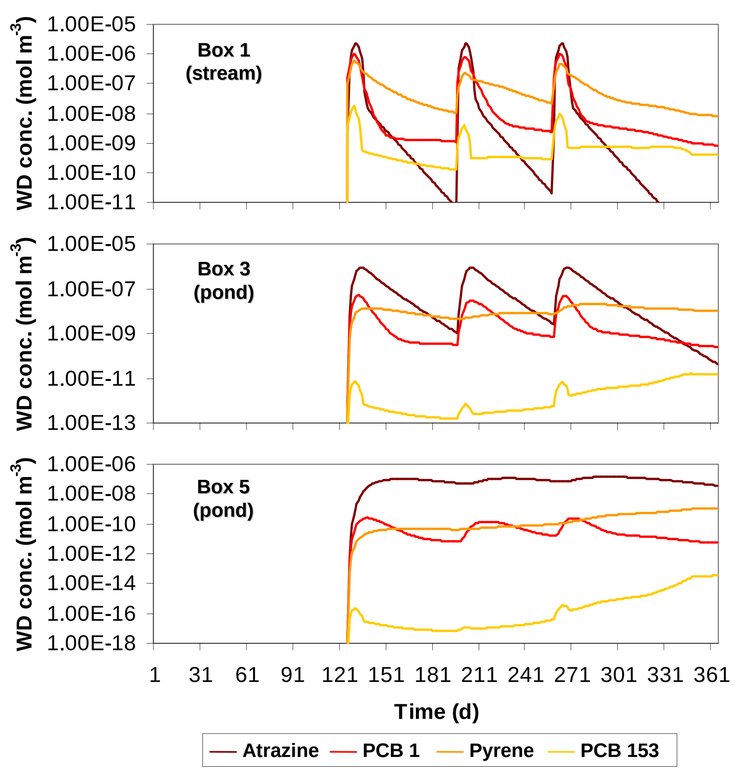

Figure 4. Water-dissolved (WD) concentrations of the 4 modelled chemicals in 3 locations of the investigated system: Box 1 (stream, where emission occurred), Box 3 (1st box of the pond) and Box 5 (middle box of the pond). 3 emission pulses.

❖ Different degrees of temporal variability according to physical-chemical properties

❖ **Hydrophobic chemicals** (i.e., pyrene and PCB 153) were more affected by changes in organic phases (**Fig. 4**)

Spatial variability

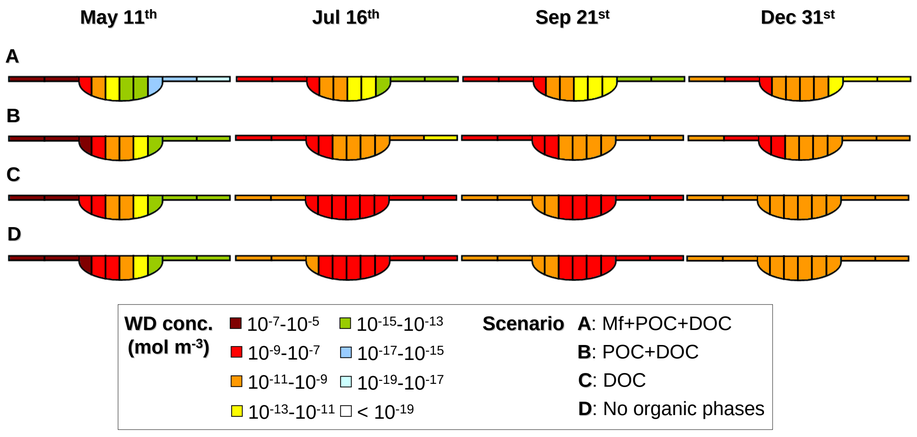

Figure 5. Spatial distribution of **pyrene** water-dissolved (WD) concentrations during (May 11th) and after the emission peak (1 emission pulse). Water flux was from left to right.

❖ Variations in water-dissolved concentrations of **several orders of magnitude** for all chemicals (only **pyrene** was reported in **Fig. 5**)

❖ Movement of the more hydrophobic chemicals with water slowed down by the presence of the organic phases

5. Conclusions

❖ **ChimERA fate model**: vital tool to investigate exposure in natural systems, where changes in properties often occur on short temporal and spatial scales

❖ More field data are needed to properly parameterize and "validate" the model

[1]Di Guardo et al. (2006) *Environ Sci & Pollut Res* 13(1), 50-58
[2]Semplice et al. (2012) *Environ Sci Technol* 46, 1616-1623
[3]Leistra et al. (2003) *Pest Manag Sci* 60, 75-84

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