Coupling microcosm experiments to modeling in order to understand ecological impact of stressors

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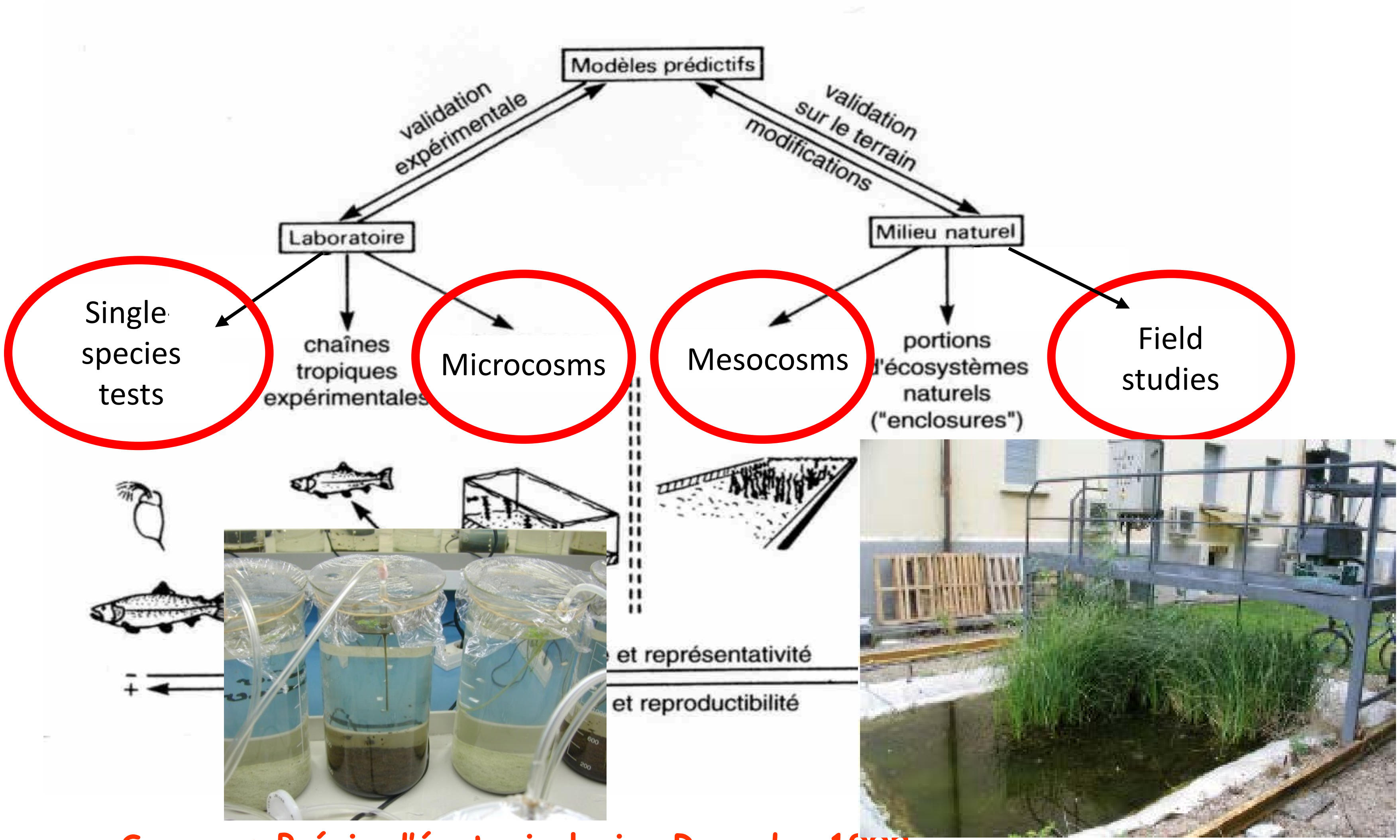
Outline

- Ecotoxicological risk assessment using laboratory microcosms
- The LEHNA’s microcosm (Clément and coll.)
- Why modeling ?
- How modeling ?
- Some results: modeling of the 3-species microcosm under toxic pressure
- Discussion
- Future work and perspectives

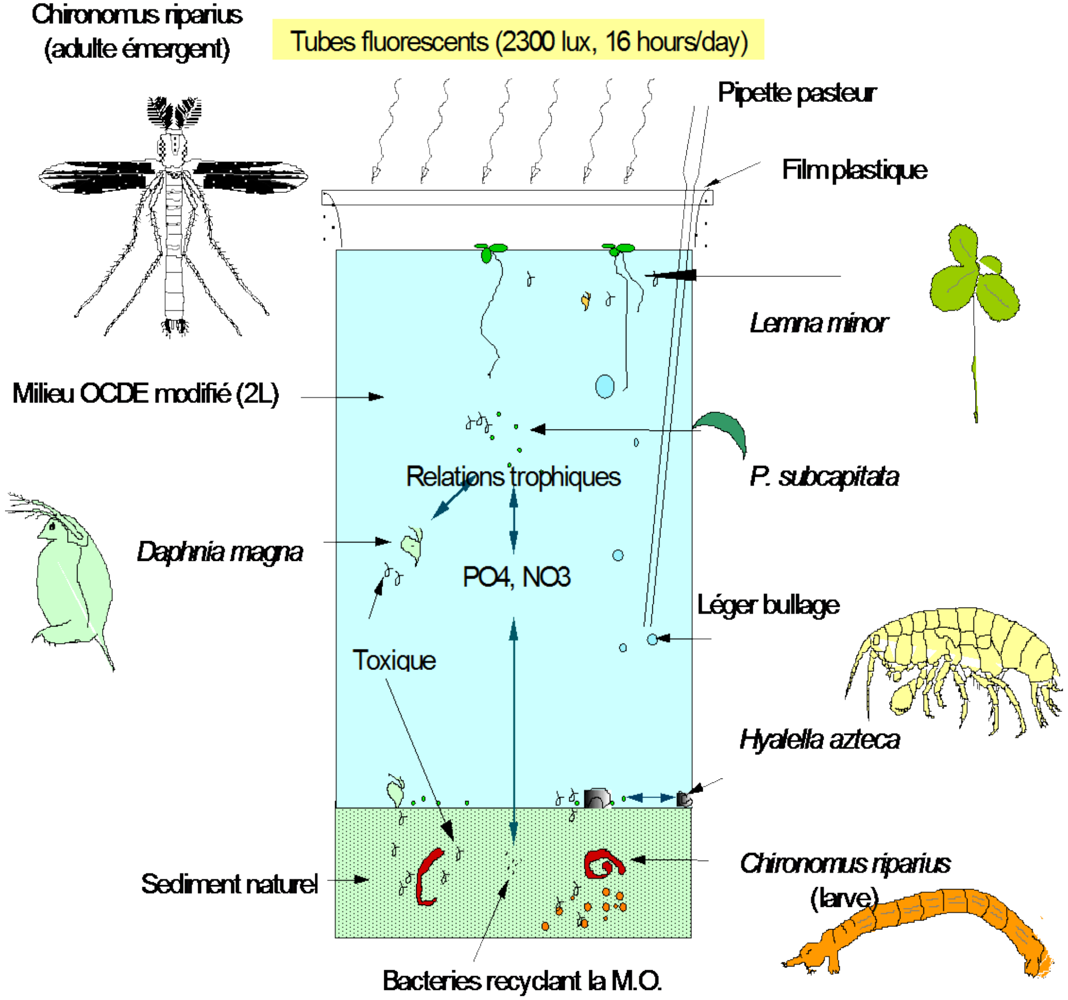
Ecotoxicological risk assessment using laboratory microcosms



Source : Précis d'écotoxicologie, Ramade, 1992

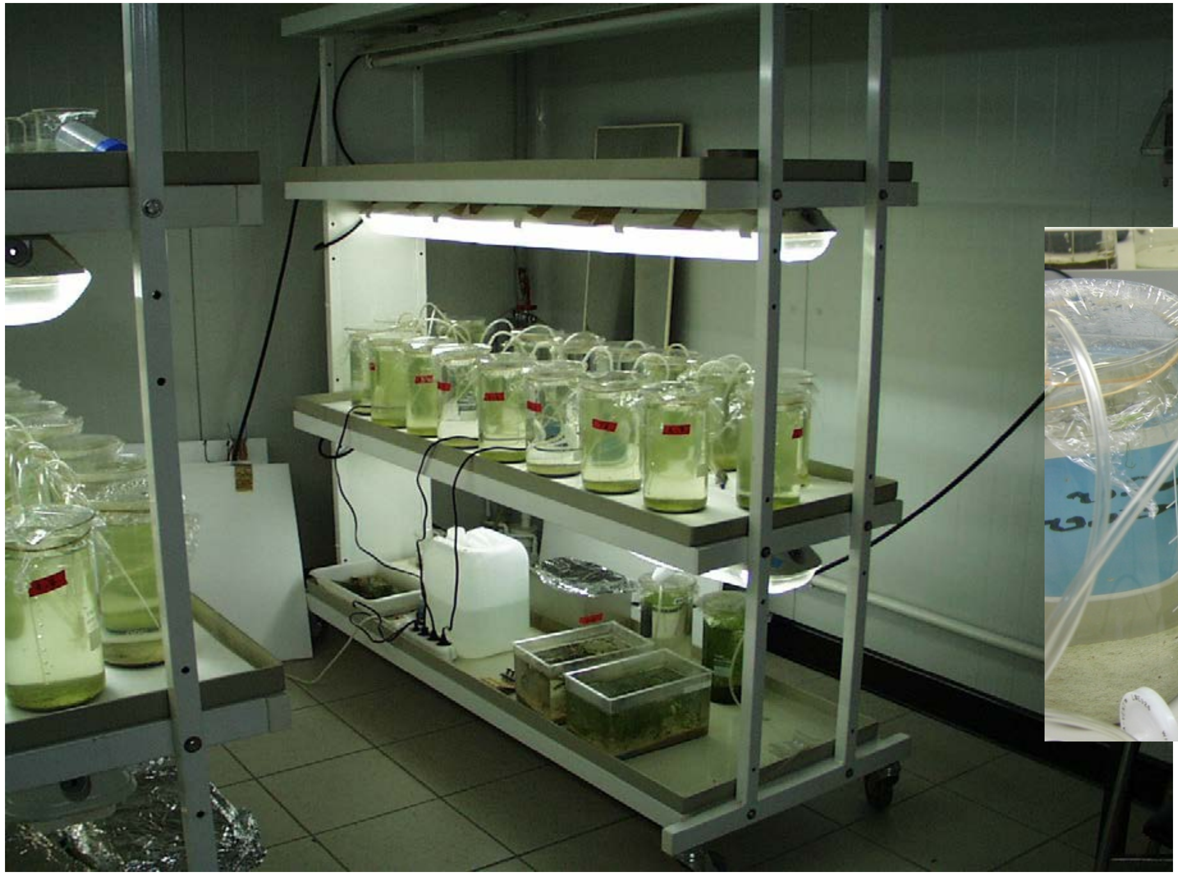
The LEHNA microcosms (Clément and coll.)

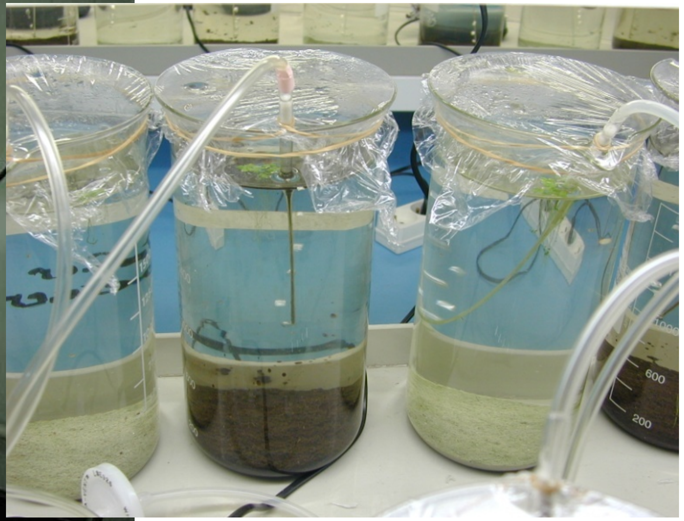
Volume: 2 L



The LEHNA microcosms (Clément and coll.)

Volume: 2 L





The LEHNA microcosms (Clément and coll.)

Volume : 2 L, static or dynamic

STATIC (batch)

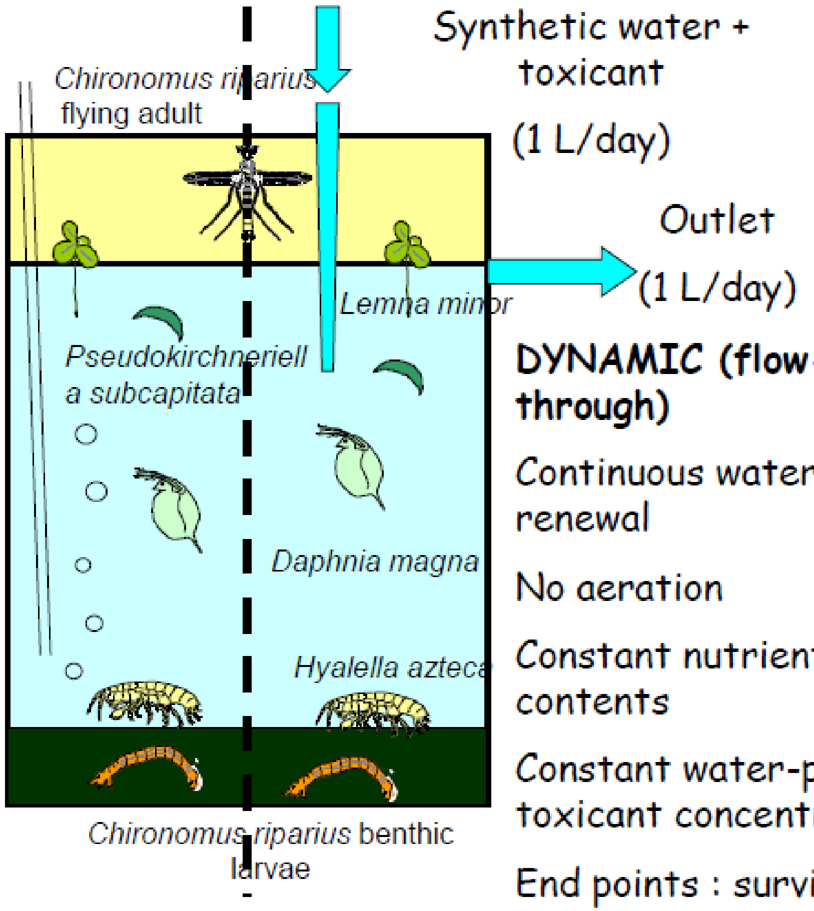
No water renewal

Continuous aeration

Consumption of nutrients

One-spot contamination

End points : survival, growth, emergence, reproduction



DYNAMIC (flow-through)

Continuous water renewal

No aeration

Constant nutrient contents

Constant water-phase toxicant concentration

End points : survival, growth, emergence, reproduction

The LEHNA microcosms (Clément and coll.)

Applications

Study of the ecotoxicity of PAH (mixture Phe/Flu/BkFlu; Pyr) spiked sediments

CLEMENT B. (2012). Bioavailability of Polycyclic Aromatic Hydrocarbons Studied Through Single-Species Ecotoxicity Tests and Laboratory Microcosm Assays, in Organic Pollutants Ten Years After the Stockholm Convention - Environmental and Analytical Update, Edited by: Tomasz Puzyn and Aleksandra Mostrag-Szlichtyng, ISBN 978-953-307-917-2, Publisher: InTech

Study of the ecotoxicity of percolates or leachates from various wastes

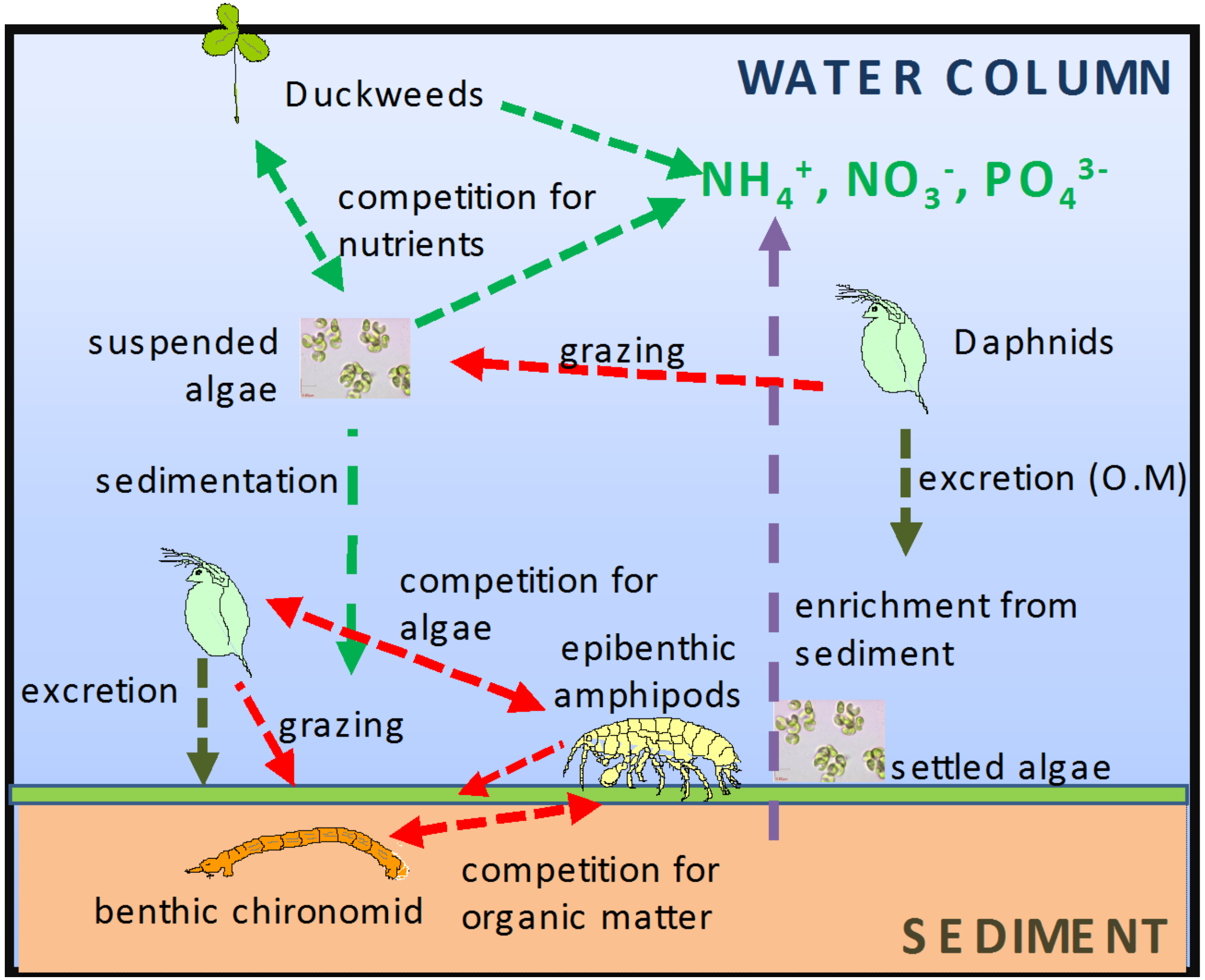
TRIFFAULT-BOUCHET G., CLEMENT B., BLAKE G. (2005). Ecotoxicological assessment of pollutant flux released from bottom ash reused in road construction, Aquatic Ecosystem Health Management 8 : 405-414.

Risk assessment of various storage or valorization scenarios of dredged sediments (from canals or sea harbours) or road sediments.

CLEMENT B., GUILLEN B., XU J., PERRODIN Y. (2014). Ecotoxicological risk assessment of a quarry filling with seaport sediments using laboratory freshwater aquatic microcosms, J Soils Sediments, Vol. 14, Issue 1, 183-195.

Why modeling ?

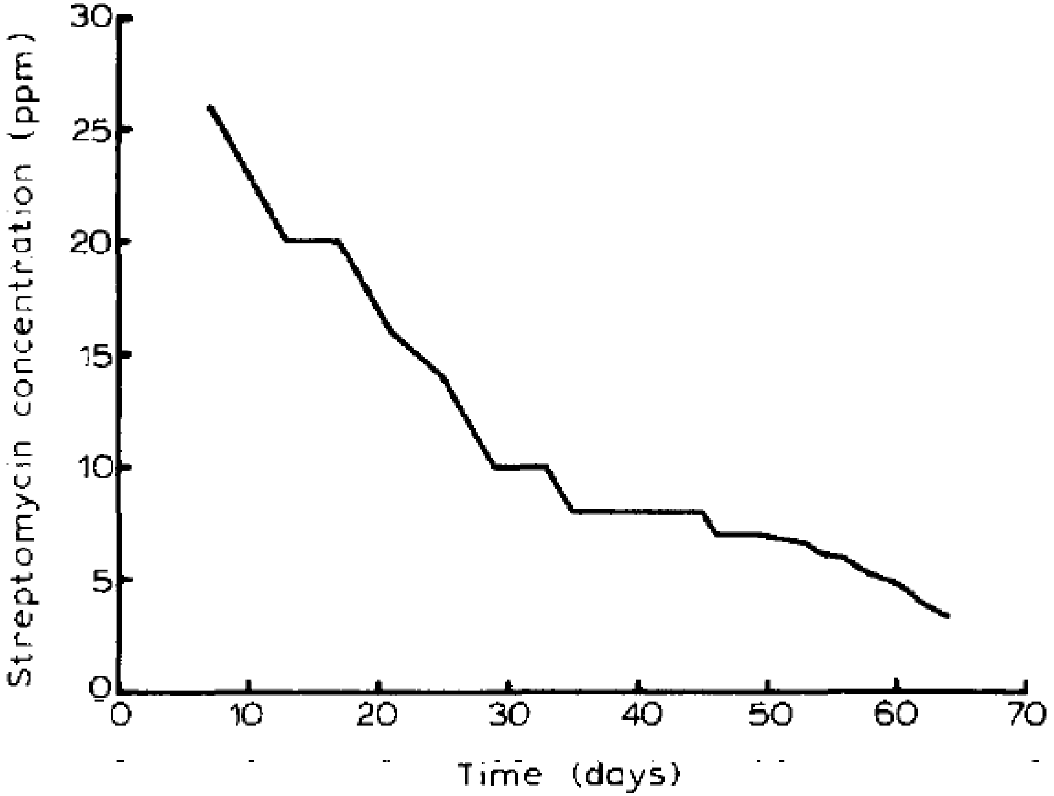
Ecological complexity

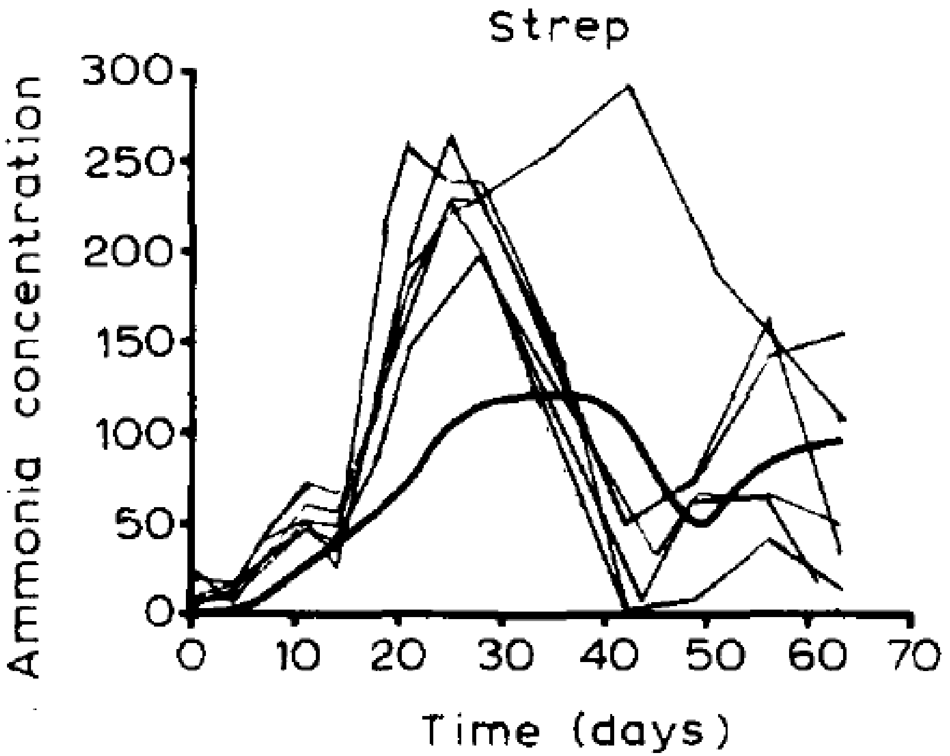


Why modeling ?

Time-varying processes

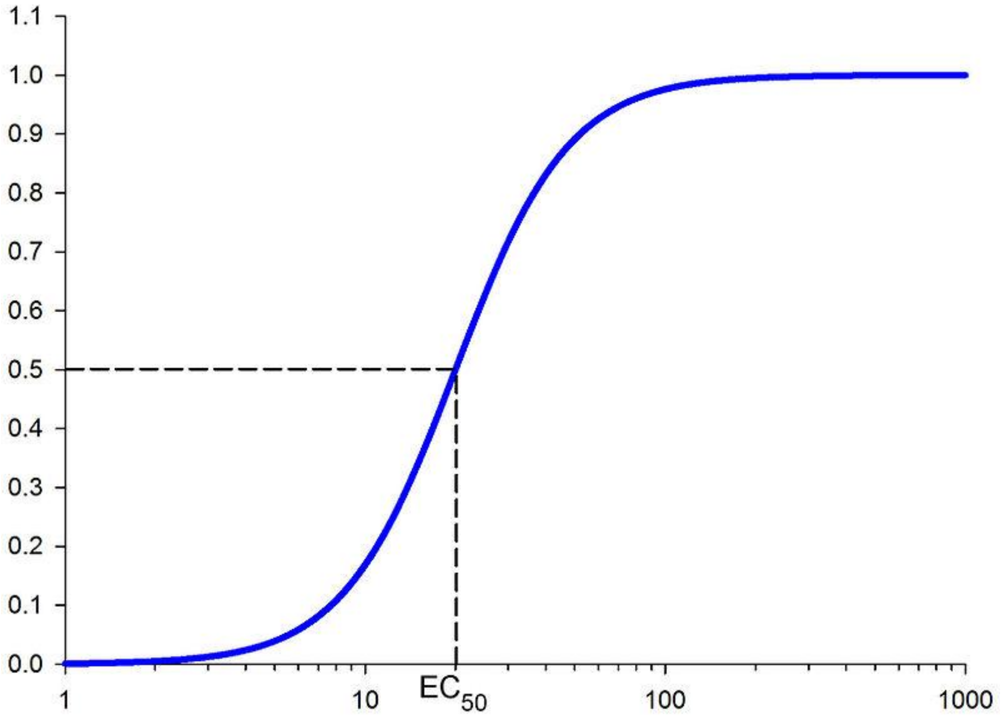
Swartzmann *et al.*, 1989





Interpretation of effects

Single-species test: direct link between effect and concentration

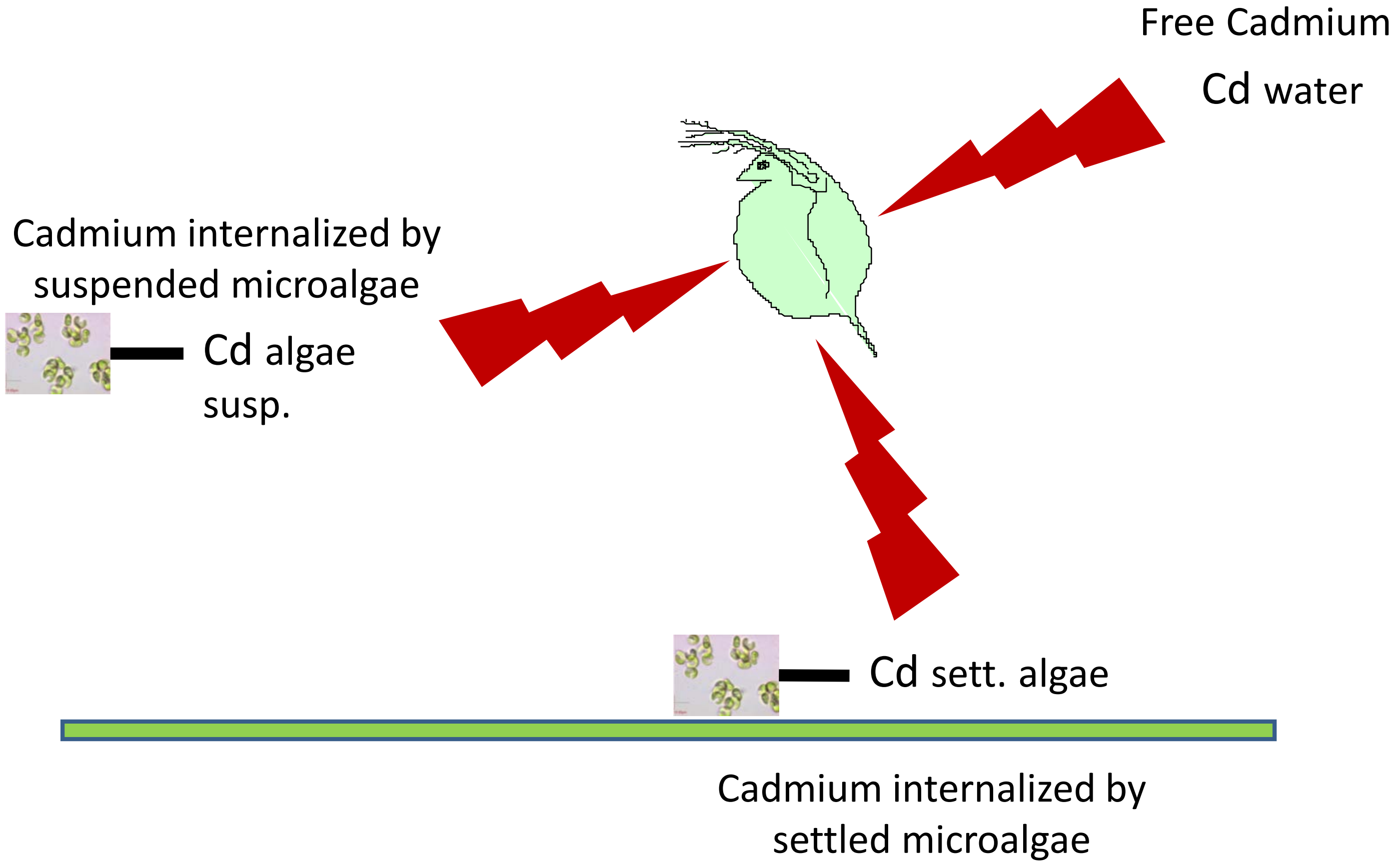


https://commons.wikimedia.org/wiki/File:Concentration-response_curve.jpg

Why modeling ?

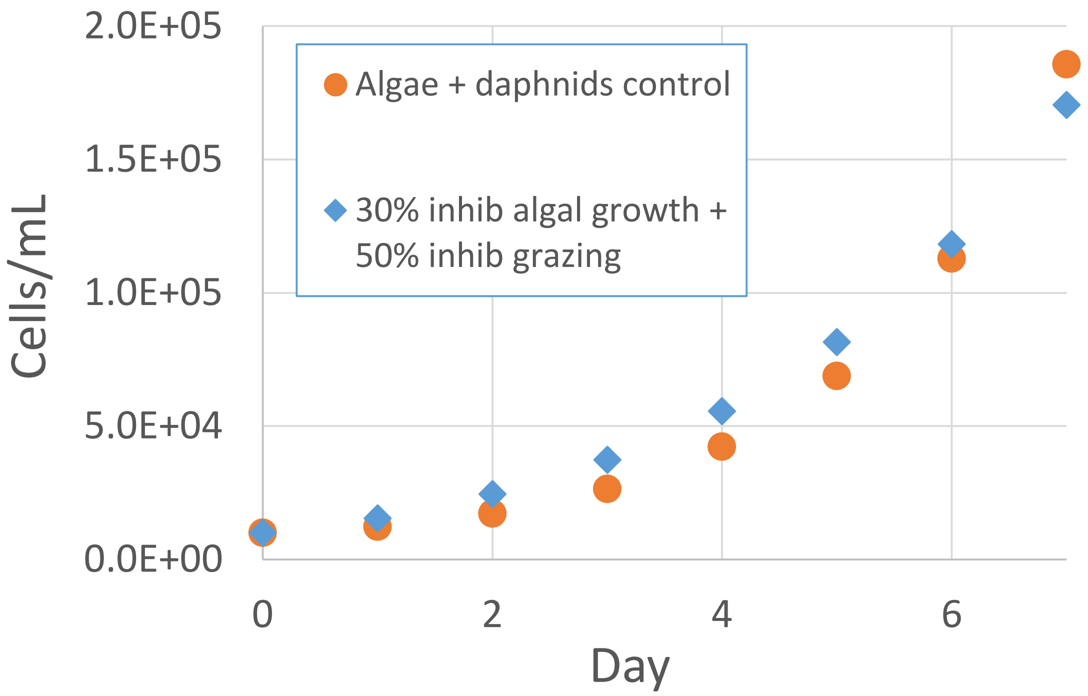
Interpretation of effects

Microcosm assays: possible multiple exposure of one given species



Interpretation of effects

Microcosm assays: similar observations can be the results of different combinations of effects



Algae + daphnid controls : no effect on algal growth and daphnid grazing, the algal density curve is the result of normal algal growth and grazing

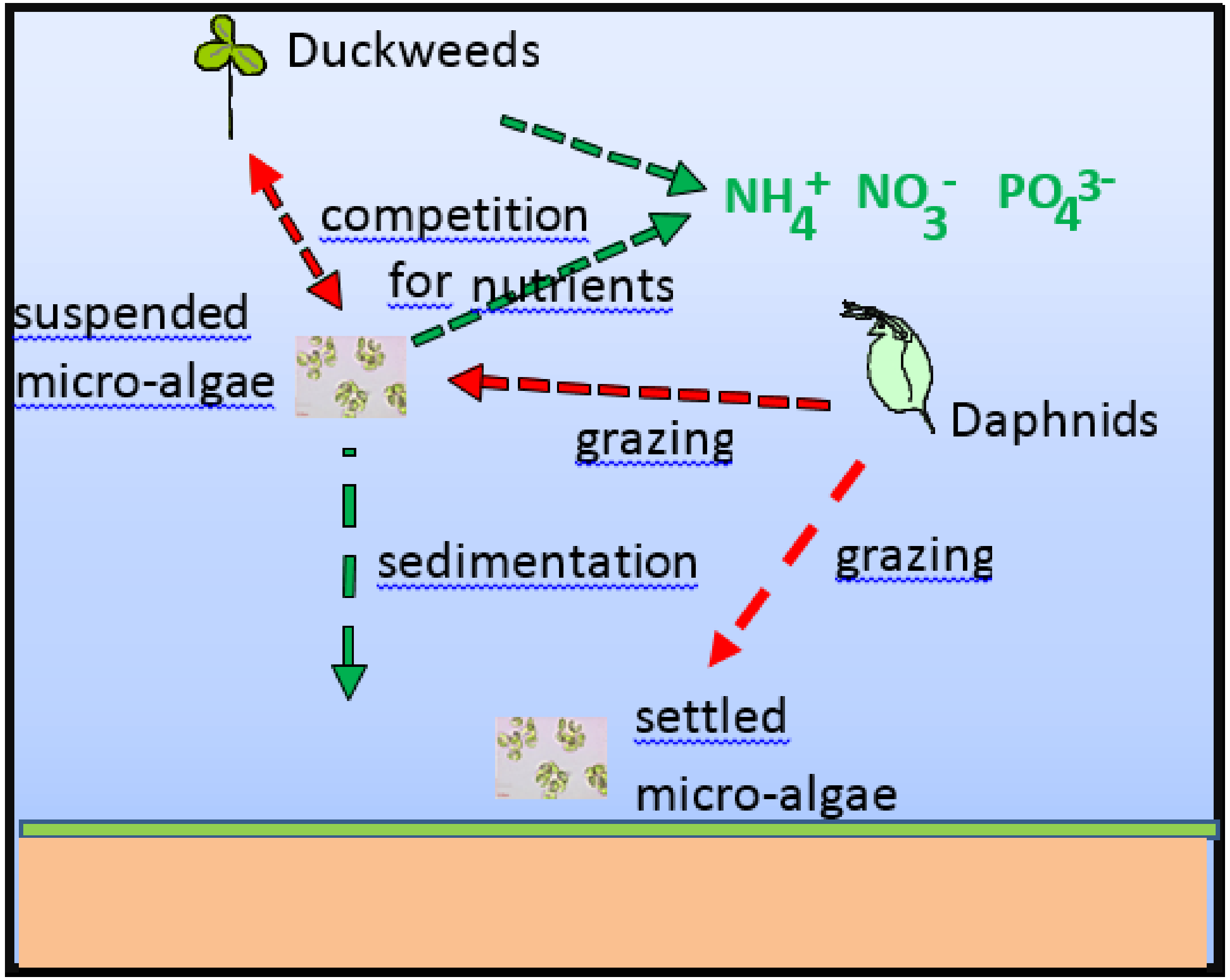
30% inhib algal growth + 50% inhib grazing : the algal density is the result of an effect on both processes

Why modeling ?

Benefits of modeling

- ➔ Better understanding of the functioning of the microecosystem and of the observed effects
- ➔ Interpretation of experimental observations through parameters values (output)
- ➔ Simulations to extrapolate and build new scenarios

Structure of the model of a sub-system



Processes considered and differential equations (algae + daphnids, no cadmium)

- Logistic growth of micro-algae in the water column (N1) and on the sediment (N2)

$$\begin{cases} \dfrac{dN_1(t)}{dt} = r_1 N_1(t)\left(1 - \dfrac{N_1(t)}{K_1(t)}\right) \\ \dfrac{dN_2(t)}{dt} = r_2 N_2(t)\left(1 - \dfrac{N_2(t)}{K_2}\right) \end{cases}$$

ri = growth rate

Ki = carrying capacity

- Settling of algal cells (exponential decay)

$$\frac{dN_1(t)}{dt} = -sN_1(t)$$

Processes considered and differential equations (algae + daphnids, no cadmium)

Daphnid survival, growth and grazing

$$S(t) = \exp(-ht)$$

Exponential decay of survival rate with time (h: mortality rate)

$$D_s(t) \sim \mathcal{B}\left(\frac{S(t)}{S(t-1)}, D_s(t-1)\right)$$

Number of alive daphnids in the system at time t (binomial model)

$$L(t) = L_\infty - (L_\infty - L_0)\exp(-kt)$$

Von Bertalanffy growth model

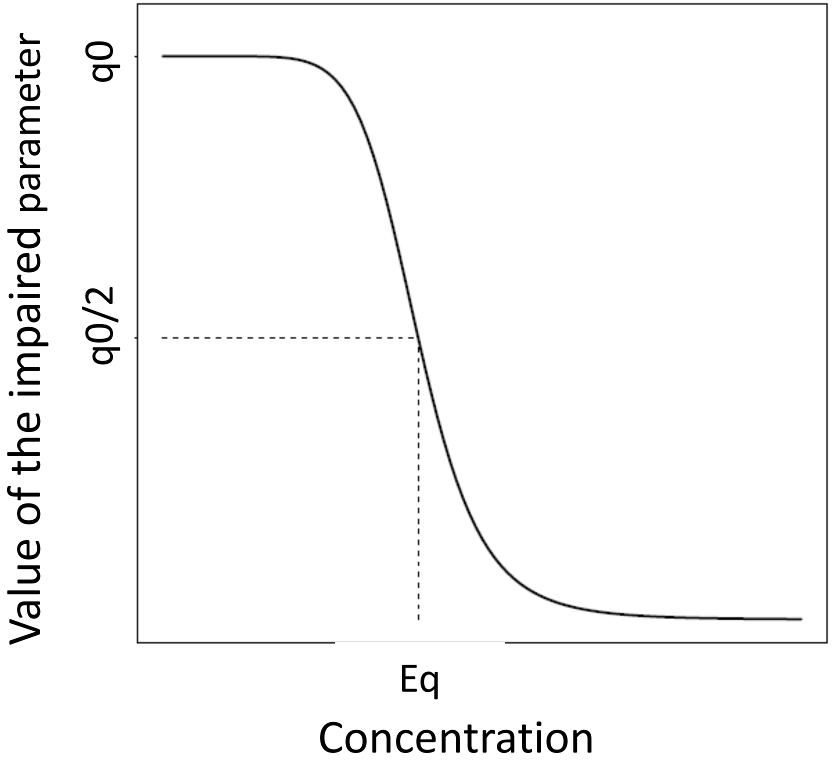
$$g_1(t) = \begin{cases} f(t) \times \frac{N_1(t)}{V_1(0)} & \text{if} \quad 0 < \frac{N_1(t)}{V_1(0)} \leq I_{\text{lim}} \\ f(t) \times I_{\text{lim}} & \text{if} \quad \frac{N_1(t)}{V_1(0)} > I_{\text{lim}} \end{cases}$$

$$f(t) = \alpha L(t)^\gamma$$

Ingestion rate gi(t) product of filtering rate f(t) and algal density (i=1 water, i=2 sediment)
f(t) function of daphnid size

Processes considered and differential equations (algae + daphnids + cadmium)

Same equations as without cadmium but variables depend on time *and* on Cd concentration



Growth rate (micro-algae, daphnids, duckweeds) and intensity of competition follow a three-parameter log-logistic function :

$$q(C_j) = \frac{q_0}{1 + \left(\frac{C_j}{E_q}\right)^{b_q}}$$

Eq = EC50

Processes considered and differential equations (algae + duckweeds + cadmium)

Competition between microalgae and duckweeds taken into account through a Lotka-Volterra type I model; competition intensity supposed affected by Cd

$$\begin{cases} \frac{dN_1(t,C_k)}{dt} = \frac{r_{a0}}{1+\left(\frac{C_k}{Er_a}\right)^{br_a}} N_1(t,C_k)\left(1 - \frac{N_1(t,C_k)}{K_1(0)\exp(-st)}\right) - sN_1(t,C_k) - \frac{\eta_0}{1+\left(\frac{C_k}{E_\eta}\right)^{b_\eta}} N_1(t,C_k)N_d(t,C_k) \\ \frac{dN_2(t,C_k)}{dt} = \frac{r_{a0}}{1+\left(\frac{C_k}{Er_a}\right)^{br_a}} N_2(t,C_k)\left(1 - \frac{N_2(t,C_k)}{K_2}\right) + sN_1(t,C_k) \\ \frac{dN_d(t,C_k)}{dt} = \frac{r_{d0}}{1+\left(\frac{C_k}{Er_d}\right)^{br_d}} N_d(t,C_k)\left(1 - \frac{N_d(t,C_k)}{K_d}\right) - \frac{\beta_0}{1+\left(\frac{C_k}{E_\beta}\right)^{b_\beta}} N_d(t,C_k)N_1(t,C_k) \end{cases}$$

Processes considered and differential equations (algae + duckweeds + daphnids + cadmium)

Growth rate of daphnids depends on Cd concentration, daphnid survival expressed using the No Effect Concentration (NEC)

$$
\begin{cases}
\frac{dN_1(t,C_j)}{dt} = r_a(C_j) \times N_1(t,C_j) \times \left(1 - \frac{N_1(t,C_j)}{K_1(0)\exp(-s\times t)}\right) - s \times N_1(t,C_j) - D_1(t,C_j) \times g_1(t,C_j) \\
\frac{dN_2(t,C_j)}{dt} = r_a(C_j) \times N_2(t,C_j) \times \left(1 - \frac{N_2(t,C_j)}{K_2}\right) + s \times N_1(t,C_j) \\
-(D_s(t,C_j) - D_1(t,C_j)) \times g_2(t,C_j) \\
\frac{dN_d(t,C_j)}{dt} = r_d(C_j) \times N_d(t,C_j) \times \left(1 - \frac{N_d(t,C_j)}{K_d}\right) - \beta(C_j) \times N_d(t,C_j) \times N_1(t,C_j) \\
L(t,C_j) = L_\infty - (L_\infty - L_0) \times \exp(-k(C_j) \times t) \\
S(t,C_j) = \exp(-(m_0 + k_s \times \max(0, C_j - NEC)) \times t)
\end{cases}
$$

Use of Bayesian inference for the solving of equations

$Y = f(\theta)$

Y = data (observations, eg algal density, and variables (eg time, Cd concentration, …)

θ = parameters to estimate (eg growth rate, survival rate, …)

Aim : to find $P(\theta|Y)$ **the *a posteriori* distribution of** θ **when data are known**

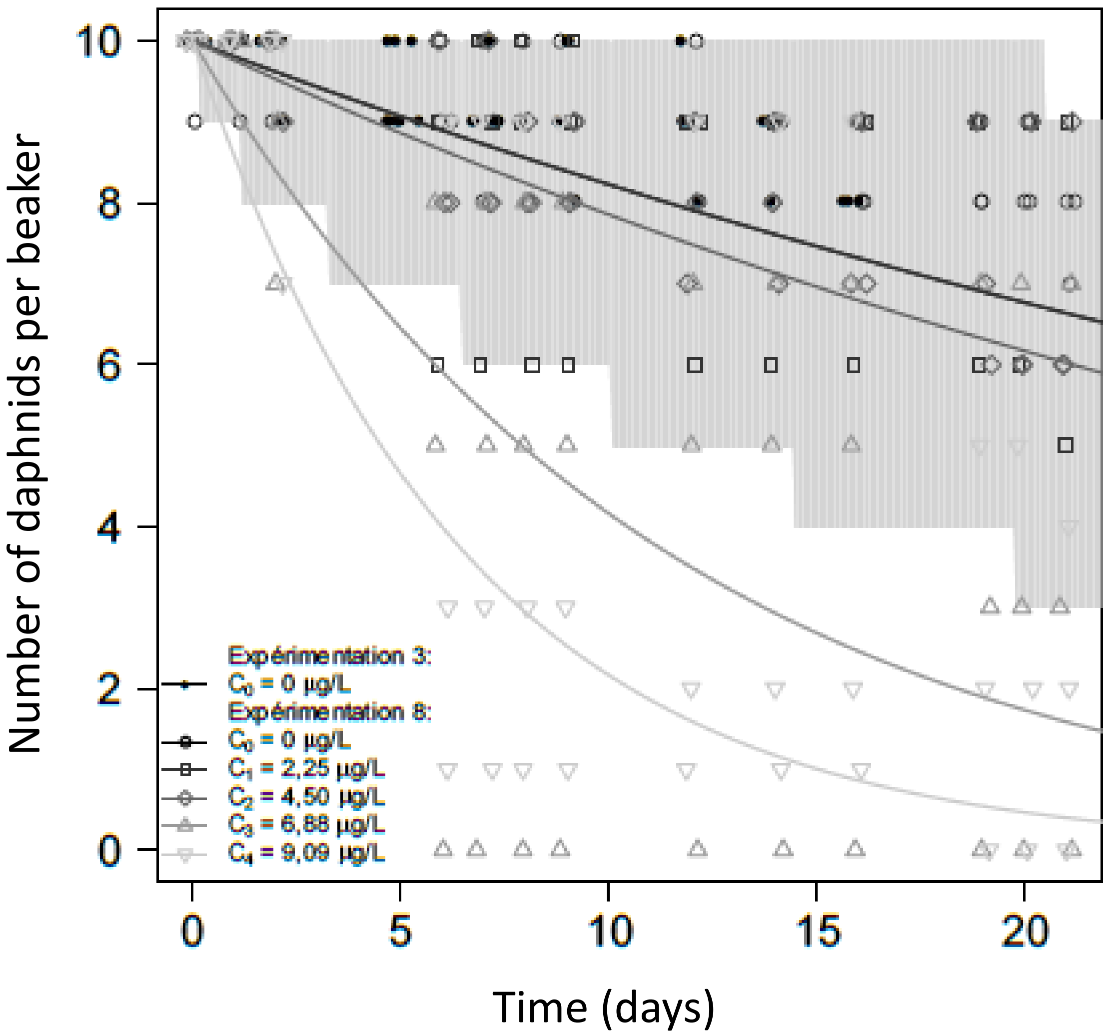
Bayes theorem : $P(\theta) \times P(Y|\theta) \sim P(\theta|Y)$

$P(\theta)$ = *a priori* distribution of θ , what is known on parameters before knowing data

$P(Y|\theta)$ = likelyhood of data under model assumption

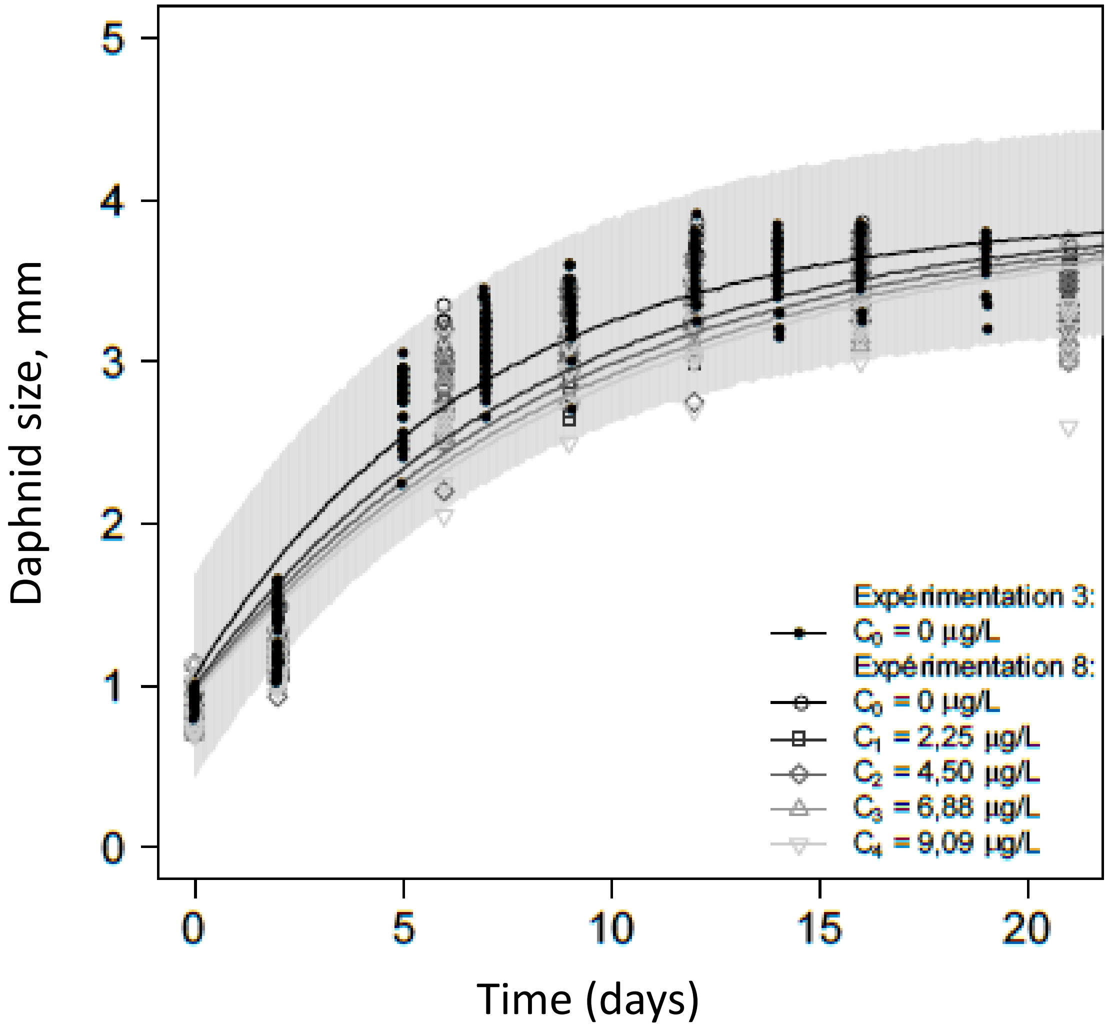
Computation : Monte Carlo Markov Chains (MCMC) + software JAGSS and library rjags of R

Some results: modeling of the 3-species microcosm



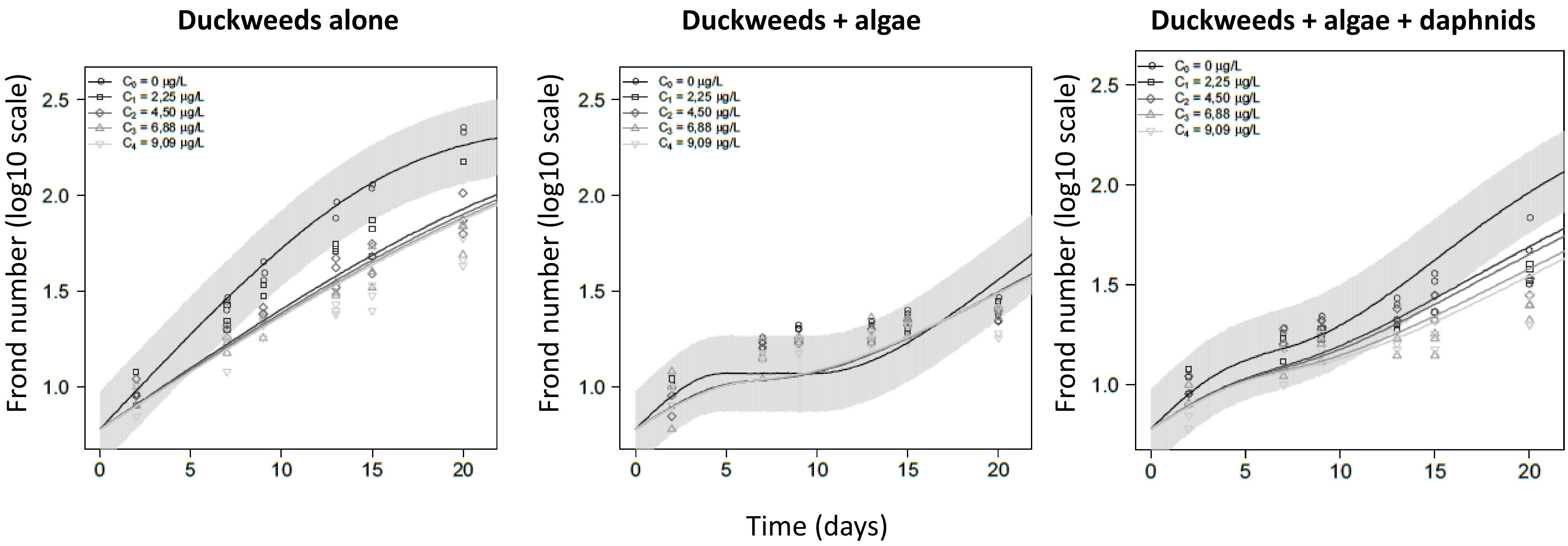
Daphnid survival under Cd exposure: observed data, quantiles at 50% of simulated data (curves), 95%-credibility bands of control

Some results: modeling of the 3-species microcosm



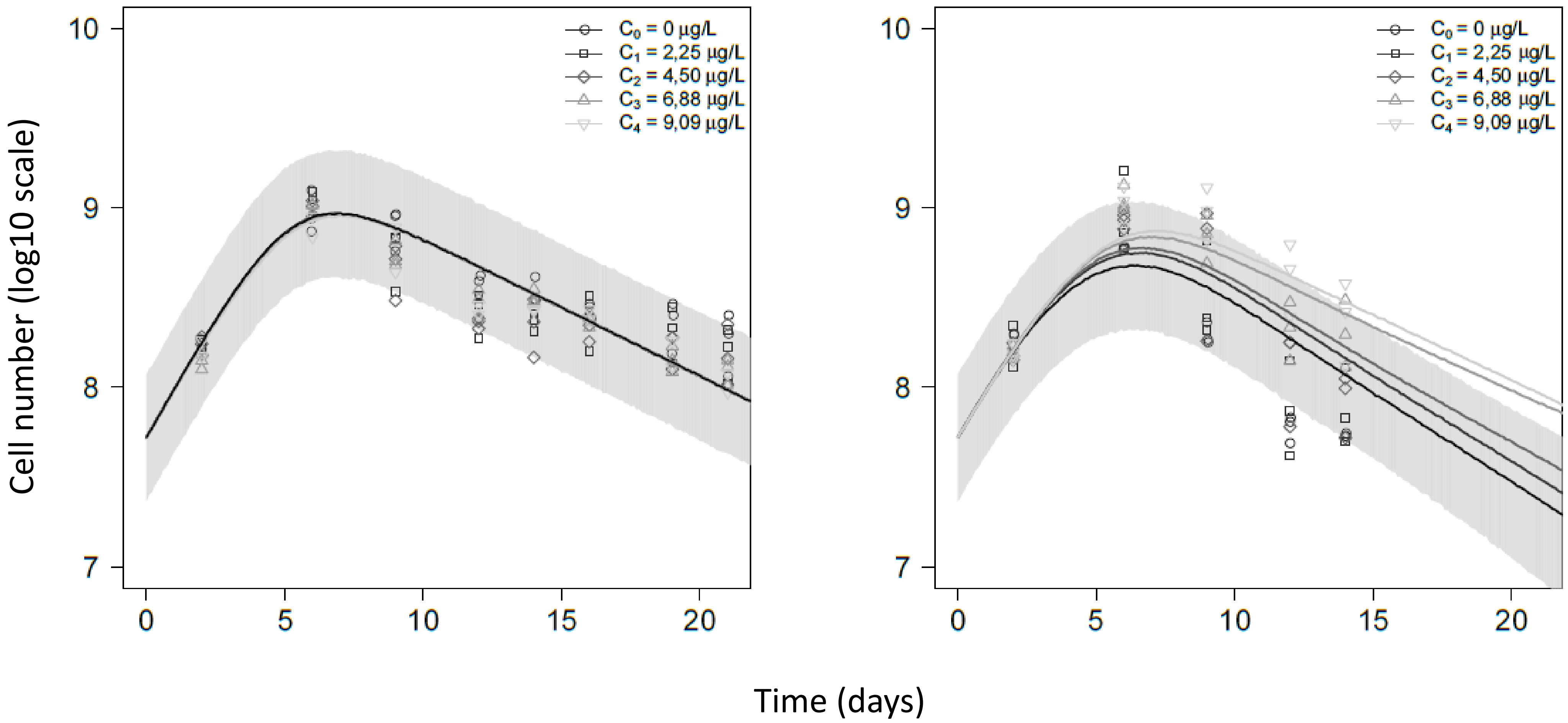
Daphnid size under Cd exposure: observed data, quantiles at 50% of simulated data (curves)

Some results: modeling of the 3-species microcosm



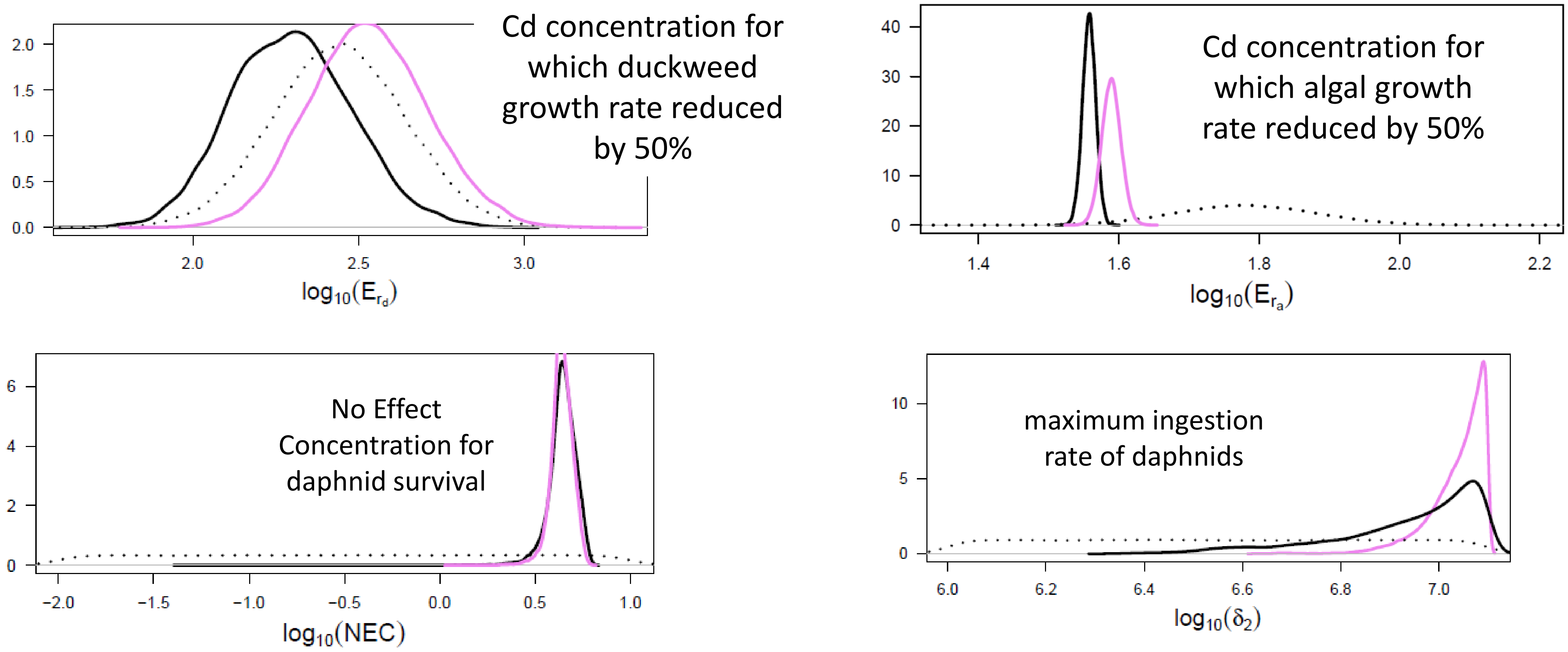
Dynamics of duckweeds alone, with algae and with algae and daphnids: observed data, quantiles at 50% of simulated data (curves), 95%-credibility bands of control

Some results: modeling of the 3-species microcosm



Dynamics of algae with duckweeds and with duckweeds and daphnids: observed data, quantiles at 50% of simulated data (curves), 95%-credibility bands of control

Some results: modeling of the 3-species microcosm



A priori **(dotted line) and** ***a posteriori*** **(models I and II) distributions of some parameters (out of 31) estimated using all available data**

Discussion

Positive points:

- microcosm functioning and interactions under Cd pressure sucessfully modeled
- critical effect concentrations and their uncertainties determined
- modeling improves understanding of microcosm response
- coupling experiments and modeling by iterative process ➔ improvement of assay protocols, of experimental design

Limits and difficulties:

- variability of microcosm assays (inter and intra)
- some processes not easily described: daphnid grazing activity for example

Future work and perspectives

- Continuing modeling of the whole microcosm
- Taking into account daphnid reproduction
- Integrating processes such as nutrient dynamics, chemical speciation, uptake of chemical by organisms.

Main references

BILLOIR E., DELHAYE H., CLÉMENT B., DELIGNETTE-MULLER M. L., CHARLES S., « Bayesian modelling of daphnid responses to time-varying cadmium exposure in laboratory aquatic microcosms », *Ecotoxicology and Environmental Safety*, n° 74, p. 693-702, 2011.

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THANK YOU FOR YOUR ATTENTION