A Bayesian approach to estimate biodynamic model parameters: bioaccumulation of PCB 153 by the freshwater crustacean Gammarus fossarum

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Introduction

To date, biodynamic models generally take into account only one exposure route. Furthermore, estimating biodynamic model parameters is done through a frequentist approach in two steps.

Aims:
• To compare two PCB153 exposure routes (spiked leaves and sediment) by a crustacean, *Gammarus fossarum*;
• To propose a Bayesian framework to simulttaneously estimate all the parameters of a biodynamic model by considering accumulation and depuration data together.

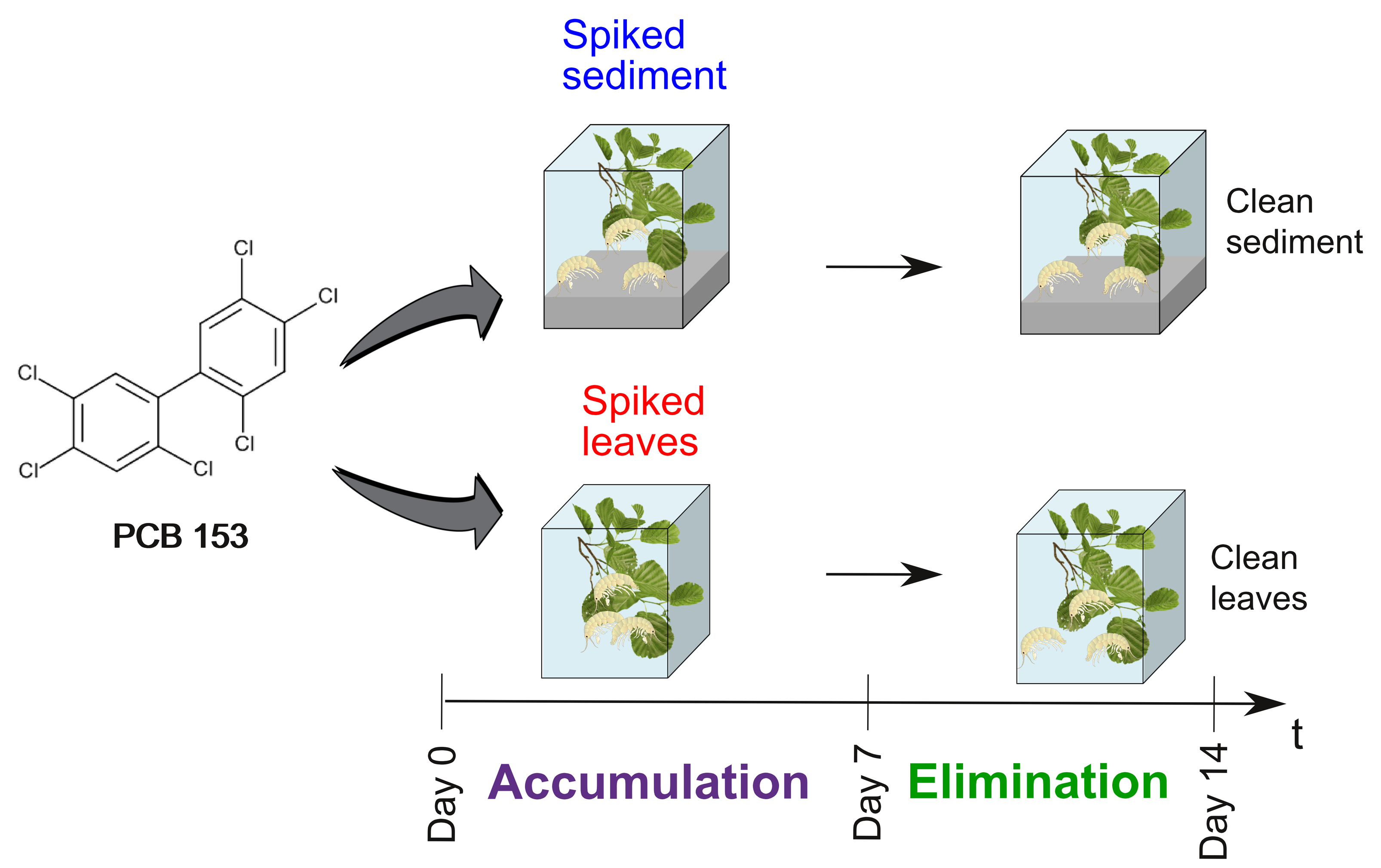
Materials and methods

Experimental design

Gammarus fossarum

Controlled conditions
12°C ;16:8h light:dark

PCB153 analyses
GC/µECD



Nominal concentration: 75 ng.g^{-1} ww

Bayesian framework

Biodynamic model in spiked leaves condition:

$$\frac{dC(t)}{dt} = [k_l.C_{ol}] - [k_e.C(t)]$$

Biodynamic model in spiked sediment condition:

$$\frac{dC(t)}{dt} = [k_l.C_{ol}] + [k_s.C_{os}] - [k_e.C(t)]$$

Accumulation ways — Elimination

C(t): PCB153 concentration in gammarids (µg.kg^{-1} ww) at time t (days); k_s: uptake rate from sediment (d^{-1}); C_{os}: PCB153 concentration in sediment (µg.kg^{-1} dw); k_l: uptake rate from leaves (d^{-1}); C_{ol}: PCB153 concentration in leaves (µg.kg^{-1} dw); k_e: elimination rate (d^{-1}).

Model implementation with JAGS and R (package 'rjags').
The convergence of the 3 chains MCMC was monitored using Gelman criteria[1].
For prior distributions, see **Table 2** (Results and discussion).

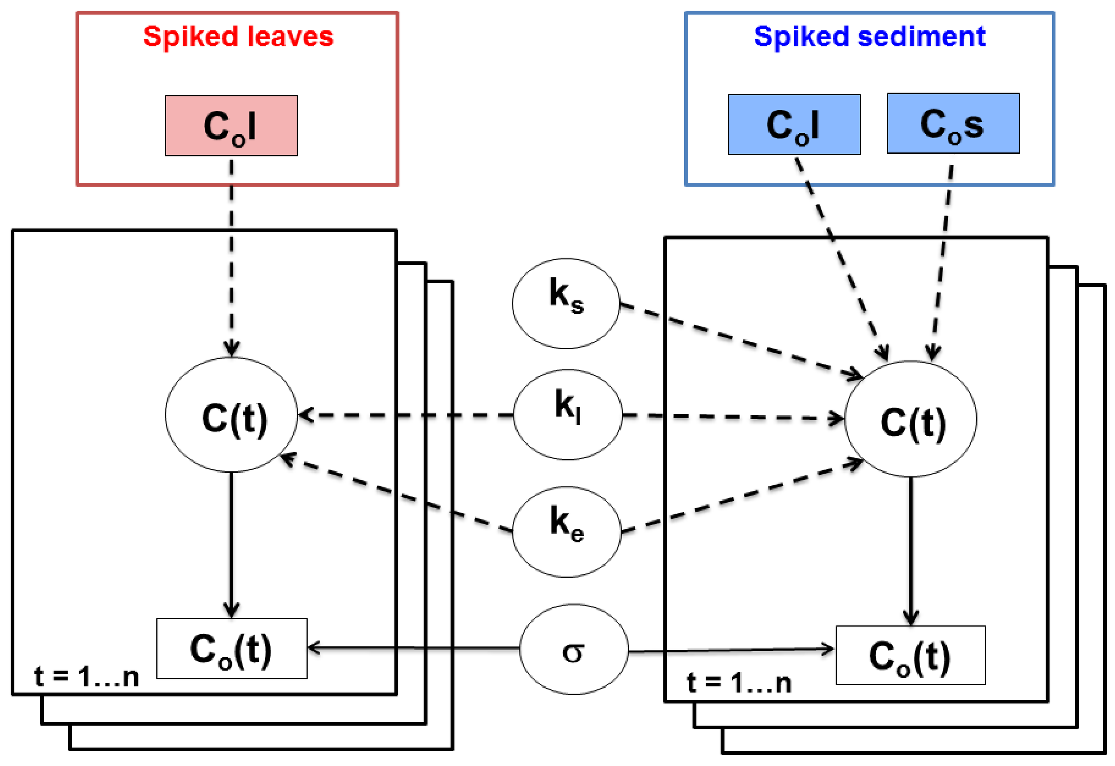


Figure 1. Directed Acyclic Graph (DAG) for the model on *G.fossarum* exposed to PCB153. Rectangle nodes represent observed data and circular nodes represent predicted data. Plain and dotted arrows represent respectively stochastic and deterministic links between nodes.

Results and discussion

Table 1. Measured PCB153 concentrations in different matrices (sediment, leaves and water) for both conditions.

Condition	Sediment (ng.g^{-1}dw)	Leaves (ng.g^{-1}dw)	Dissolved water (ng.L^{-1})
Spiked leaves	-	252.2	0.2
Spiked sediment	45.9	44.9	0.1

Spiked leaves *versus* spiked sediment conditions
PCB153 in leaves = **x5** PCB153 in sediment or leaves

Table 2. Summary of prior probability density functions and posteriors estimates for model parameters.

Parameter	Priors	Mean	Quantiles 2.5%	97.5%
k_l	LogUnif (-5,2)	0.01327	0.01029	0.01649
k_s	LogUnif (-5,2)	0.06792	0.05372	0.08369
k_e	LogUnif (-5,2)	0.18695	0.13721	0.24111
σ	Gamma (0.001,0.001)	1.57990	1.14493	2.21420

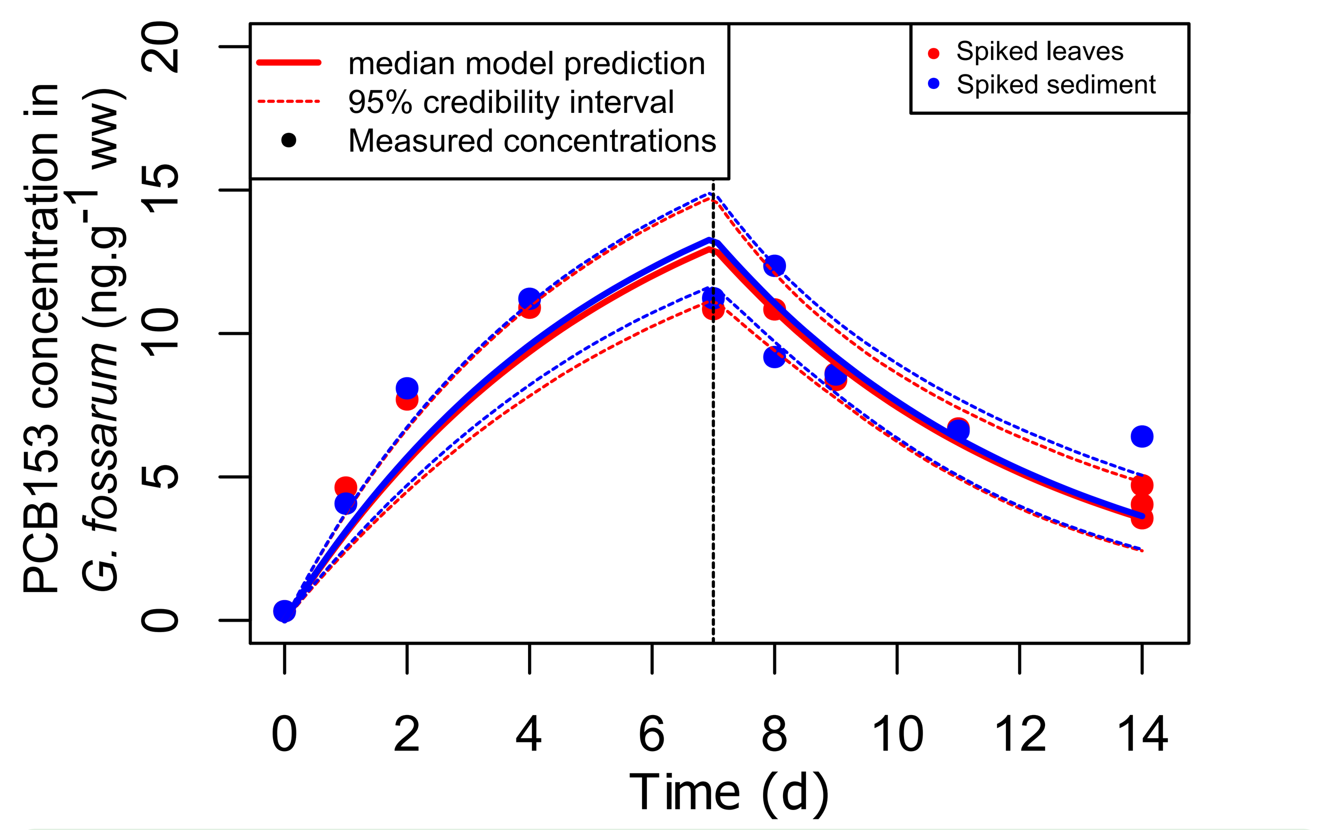


Figure 2. Measured and predicted PCB153 concentrations (ng.g^{-1} ww) in gammarids.

Conclusion

•Model predictions fit well with data; the inference process quickly converged and thin posterior distributions were obtained for all parameters. We demonstrated the ability of Bayesian inference to quantify the uncertainty of model parameters and variability of model predictions.

•Dissolved water route of exposure is negligible. Identical models are obtained with all data (leaves and sediment conditions) or without leaves data in spiked sediment condition. We showed that the accumulation by sediment is the major exposure route in spiked sediment condition.

1- Gelman, A., Carlin, JB., Stern, HS., Rubin, DB. (1995). "Bayesian Data Analysis". Chapman and Hall. New York, NY, USA.

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