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

EPOC

Aude Ratier¹, Christelle Lopes², H el ene Budzinski³, Pierre Labadie³, Olivier Geffard¹, Marc Babut¹.¹Irstea, UR RIVERLY, centre de Lyon-Villeurbanne, 5 rue de la Doua, CS 20244, 69625 Villeurbanne Cedex, France.²Univ Lyon, Universit  Lyon 1, CNRS, Laboratoire de Biom trie et Biologie Evolutive UMR5558, F-69622 Villeurbanne, France.³Universit  Bordeaux 1, Environnements et Pal oenvironnements Oc aniques et Continentaux (EPOC), UMR 5805 CNRS, Laboratoire de Physico- et Toxicochimie de l'environnement (LPTC), 351 cours de la Lib ration, 33405 Talence, France.

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Introduction

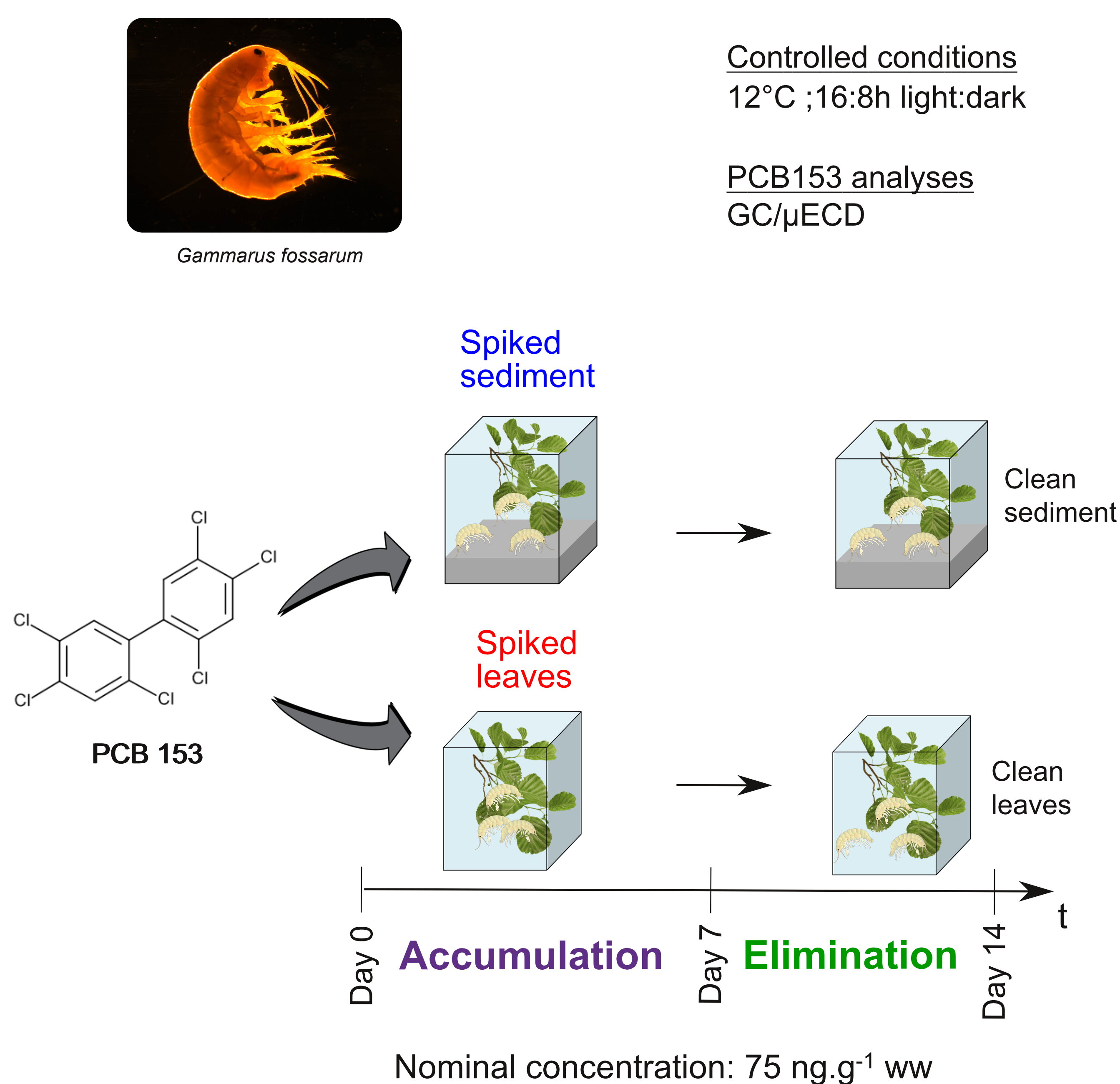
To date, biodynamic models generally take into account only one exposure route. Furthermore, estimating biodynamic model parameters is done through a frequentist approach in two steps.

Aims:

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

Materials and methods

Experimental design



Bayesian framework

$$\text{Biodynamic model in spiked leaves condition: } \frac{dC(t)}{dt} = ([k_l \cdot C_{o,l}] - [k_e \cdot C(t)])$$

$$\text{Biodynamic model in spiked sediment condition: } \frac{dC(t)}{dt} = ([k_l \cdot C_{o,l}] + [k_s \cdot C_{o,s}] - [k_e \cdot C(t)])$$

Accumulation ways Elimination

$C(t)$: PCB153 concentration in gammarids ($\mu\text{g}\cdot\text{kg}^{-1}$ ww) at time t (days); k_s : uptake rate from sediment (d^{-1}); $C_{o,s}$: PCB153 concentration in sediment ($\mu\text{g}\cdot\text{kg}^{-1}$ dw); k_l : uptake rate from leaves (d^{-1}); $C_{o,l}$: PCB153 concentration in leaves ($\mu\text{g}\cdot\text{kg}^{-1}$ 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).

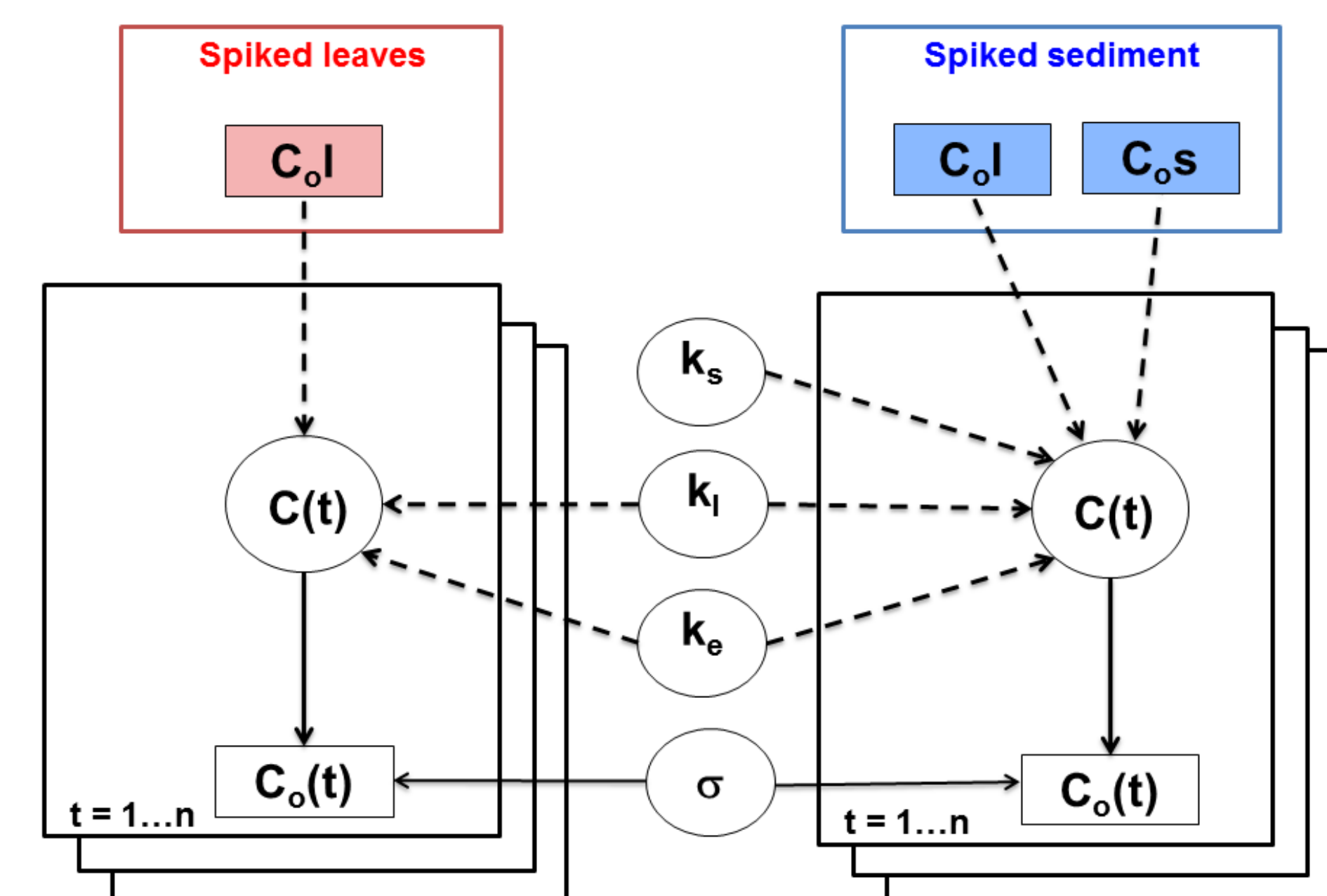


Figure 1. Directed Acyclic Graph (DAG) for the model on *G. fossarum* exposed to PCB153. Rectangle nodes represent observed data and circular nodes represent predicted data. Plain and dotted arrows represent respectively stochastic and deterministic links between nodes.

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

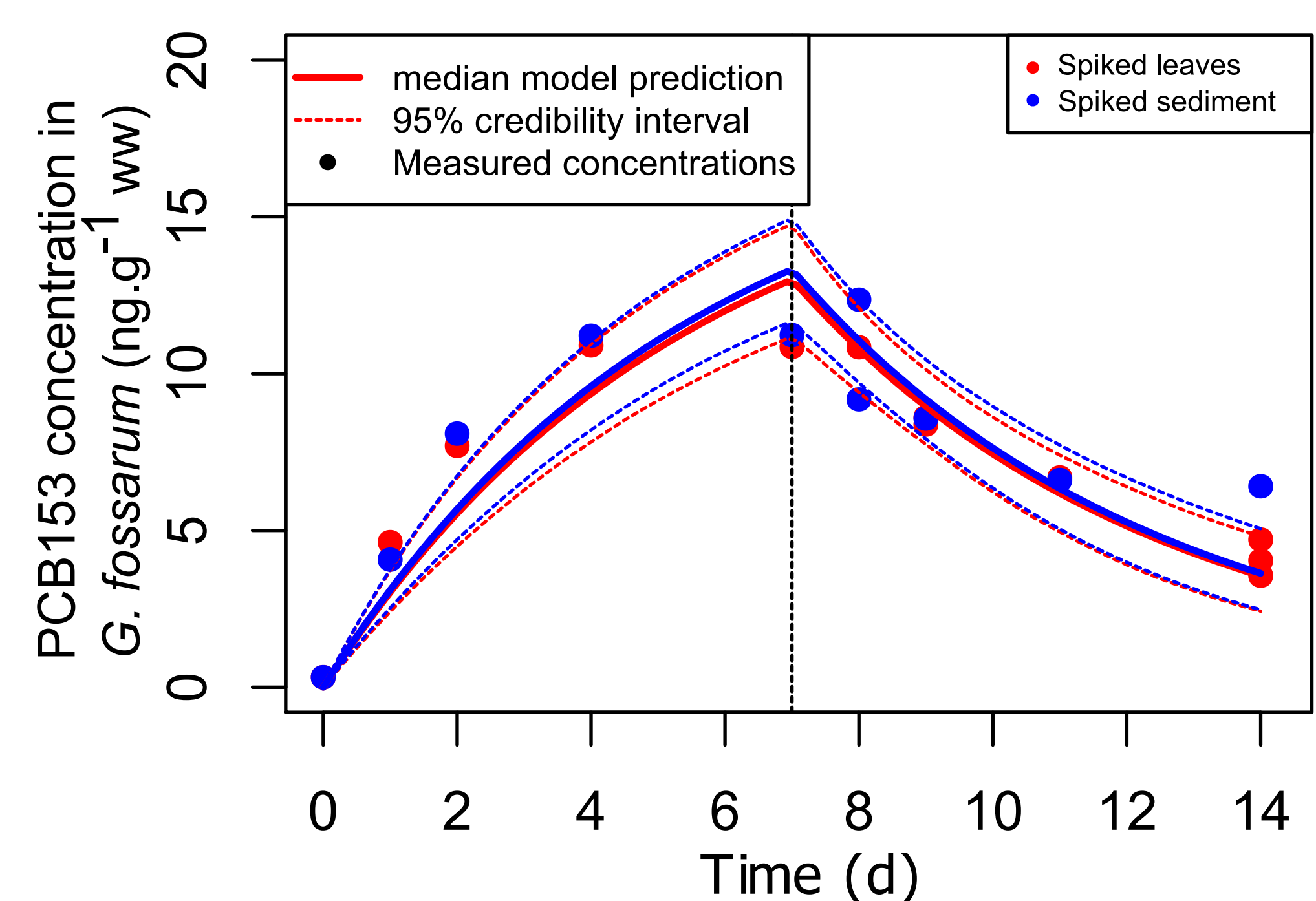


Figure 2. Measured and predicted PCB153 concentrations ($\text{ng}\cdot\text{g}^{-1}$ ww) in gammarids.

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.