Applications of toxico-kinetic (TK) models on freshwater invertebrates in a regulation perspective

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Introduction and objectives

Polycyclic Aromatic Hydrocarbons (PAHs) regulation

- To predict a threshold concentration in sediment that would lead to a concentration in biota below the EQS_{biota} , both for the parent compound and for the metabolites
- To explore the influence of sediment organic carbon content on the threshold concentration in sediment

Materials & Methods

Experimental data collected
Schuler et al., 2003. ETC, 22.

TK model
for $0 < t < t_c$

Hyalella azteca

$$\frac{dC_p(t)}{dt} = k_s \times C_s - k_{e,p} \times C_p(t)$$

Chironomus tentans

$$\frac{dC_p(t)}{dt} = k_s \times C_s - (k_{e,p} + k_m) \times C_p(t)$$

$$\frac{dC_m(t)}{dt} = k_m \times C_p(t) - k_{e,m} \times C_m(t)$$

t_c : time at the end of the uptake phase (d)

C_p : BaP concentration in biota ($ng\ g^{-1}\ ww$)

C_m : metabolites concentration in biota ($ng\ g^{-1}\ ww$)

k_s : uptake rate from sediment (d^{-1})

C_s : BaP concentration in sediment ($ng\ g^{-1}\ dw$)

$k_{e,p}$: elimination rate for BaP (d^{-1})

k_m : biotransformation rate (d^{-1})

$k_{e,m}$: elimination rate for metabolites (d^{-1})

Bayesian inference

Baye's Theorem

$$P(\theta|Y) \propto P(\theta) \times P(Y|\theta)$$

parameters	units	median	95% credibility intervals
<i>C. tentans</i>			
k_s	d^{-1}	0.732	[0.468-1.09]
$k_{e,p}$	d^{-1}	2.18	[0.600-4.22]
k_m	d^{-1}	1.65	[1.38-2.03]
$k_{e,m}$	d^{-1}	0.758	[0.648-0.890]
<i>H. azteca</i>			
k_s	d^{-1}	0.152	[0.127-0.181]
$k_{e,p}$	d^{-1}	0.488	[0.363-0.637]

Predictions

Variation of exposure time (t_c)
---> Steady state

Variation of exposure concentration (C_s)
---> $[BaP]_{biota} \leq EQS_{biota}$

Variation of the total organic carbon (TOC)
---> $C_{s,TOC} = C_s / TOC$

$C_{s,max}$ predicted to obtain $C_{biota} < EQS_{biota}$

Chironomus tentans

Predictions for
 $C_{s,max} = 23.5\ ng\ g^{-1}\ dw$

- $C_{BaP,biota} < EQS_{biota}$
- $C_{metabolites,biota} > EQS_{biota}$

Figure 1. Predictions for *C. tentans* exposed to BaP spiked sediment ($C_{s,max} = 23.5\ ng\ g^{-1}\ dw$) for 3 days in order to be under the EQS_{biota} .

Extended exposure time to reach steady state:
 $t_c = 10\ d$

Figure 2. Predictions for *C. tentans* exposed to BaP spiked sediment ($C_{s,max} = 11.3\ ng\ g^{-1}\ dw$) for 10 days in order to be under the EQS_{biota} .

Predictions for
 $C_{s,max} = 11.3\ ng\ g^{-1}\ dw$

- $C_{BaP,biota} < EQS_{biota}$
- $C_{metabolites,biota} < EQS_{biota}$

Hyalella azteca

Predictions for $C_{s,max} = 14.0\ ng\ g^{-1}\ dw$

Extended exposure time to reach steady state $t_c = 10\ d$ (instead of 3 d)

- No metabolites detected
- H. azteca* less sensitive than chironomids

Figure 3. Predictions for *H. azteca* exposed to BaP spiked sediment ($C_{s,max} = 14.0\ ng\ g^{-1}\ dw$) for 10 days in order to be under the EQS_{biota} .

TOC and its influence on $C_{s,max}$

Chironomus tentans

Predictions for
 $C_{s,max} = 23.5\ ng\ g^{-1}\ dw$

TOC = 1%
and
TOC = 2%

Figure 4. Predictions for *C. tentans* exposed to BaP spiked sediment ($C_{s,max} = 23.5\ ng\ g^{-1}\ dw$) for 3 days for TOC = 1% (green) and 2% (blue).

Table 1. Predictions of $C_{s,max}$ according to the TOC value for *C. tentans* and *H. azteca*.

Organism	Condition of predictions	$C_{s,max}$ ($ng\ g^{-1}\ dw$) TOC = 1%	$C_{s,max}$ ($ng\ g^{-1}\ dw$) TOC = 2%
<i>C. tentans</i>	$[BaP]_{biota} < EQS_{biota}$	23.5	47.0
	$[BaP]_{biota} < EQS_{biota}$ $[metabolites]_{biota} < EQS_{biota}$	11.3	22.5
<i>H. azteca</i>	$[BaP]_{biota} < EQS_{biota}$	14.0	28.5

Conclusions

- The results raised the issue of taking into account metabolites in regulation, where their concentrations in the organism could exceed the EQS_{biota} defined for the parent compound.
- When exposed to BaP spiked sediment, the higher % TOC, the lower the concentration in biota. Thus, more the TOC is high, higher is the threshold concentration in sediment.
- A new on-line tool **MOSAIC_{Bioacc}** (presented at the poster 3.02P.13) can easily performed these kinds of TK analyzes (<https://scharles-univlyon1.shinyapps.io/MOSAICbioacc/>).

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