

# MOSAIC<sub>bioacc</sub> REPORT

2021-06-03

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This report is provided by the MOSAIC<sub>bioacc</sub> application available here:  
<https://mosaic.univ-lyon1.fr/bioacc>

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MOSAIC<sub>bioacc</sub> uses the JAGS (version 4.3.0) and R (version 4.0.2) software, and in particular packages RJags (version 4.10), jagsUI (version 1.5.1) and Shiny (version 1.6.0).

The MOSAIC<sub>bioacc</sub> application is a turn-key web tool providing bioaccumulation factors (BCF/BSAF/BMF) from a toxicokinetic (TK) model fitted to accumulation-depuration data. It is designed to fulfil the requirements of regulators when examining applications for market authorization of active substances.

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## Data summary

File used: Daphnia\_anthracene\_24h\_Wang2021\_body-without-gut-food.txt

Exposure: 59.745  $\mu\text{g}\cdot\text{g}^{-1}$

Accumulation phase duration: 24 hours

Number of replicates: 3

Times: 0, 0.5, 2, 5, 10, 24, 26, 29, 34, 48, 72

Exposure routes: food

Elimination routes: excretion

## Bayesian inference

Three MCMC chains were used to estimate model parameters.

Number of iterations: 18730

Thin: 5

## TK Model

The TK model used for these calculations was:

$$\frac{dC_p(t)}{dt} = k_{uf} \times c_f - (k_{ee}) \times C_p(t) \quad \text{for } 0 \leq t \leq t_c$$

$$\frac{dC_p(t)}{dt} = - (k_{ee}) \times C_p(t) \quad \text{for } t > t_c$$

with:

$t$ : time (expressed in hours )

$t_c$ : duration of the accumulation phase (expressed in hours )

$C_p(t)$ : internal concentration of the parent compound at time (expressed in  $\mu g.g^{-1}$ )

$k_{ee}$ : elimination rates of excretion (expressed per hours  $^{-1}$ )

$c_f$ : exposure concentration of food route (expressed in  $\mu g.g^{-1}$ )

$k_{uf}$ : uptake rate of food exposure (expressed per hours  $^{-1}$ )

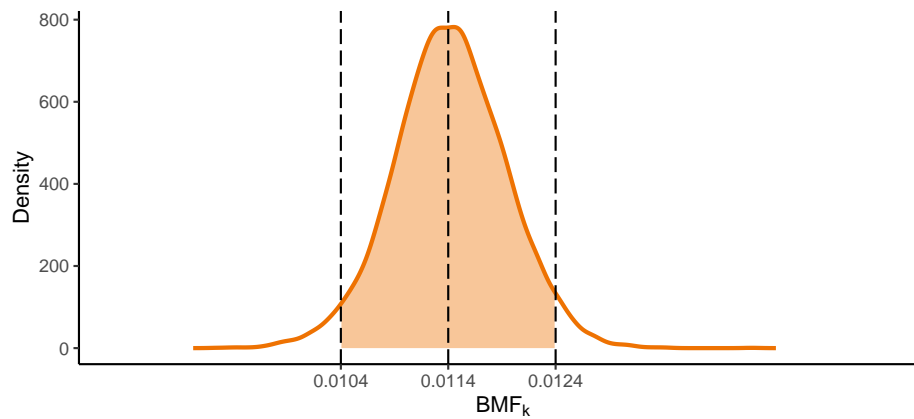
## Bioaccumulation factor calculation

### Calculations

$$BMF_k = \frac{k_{uf}}{k_{ee}}$$

$$BMF_{ss} = \frac{C_p(t_c)}{c_f}$$

### BMF<sub>k</sub> plot

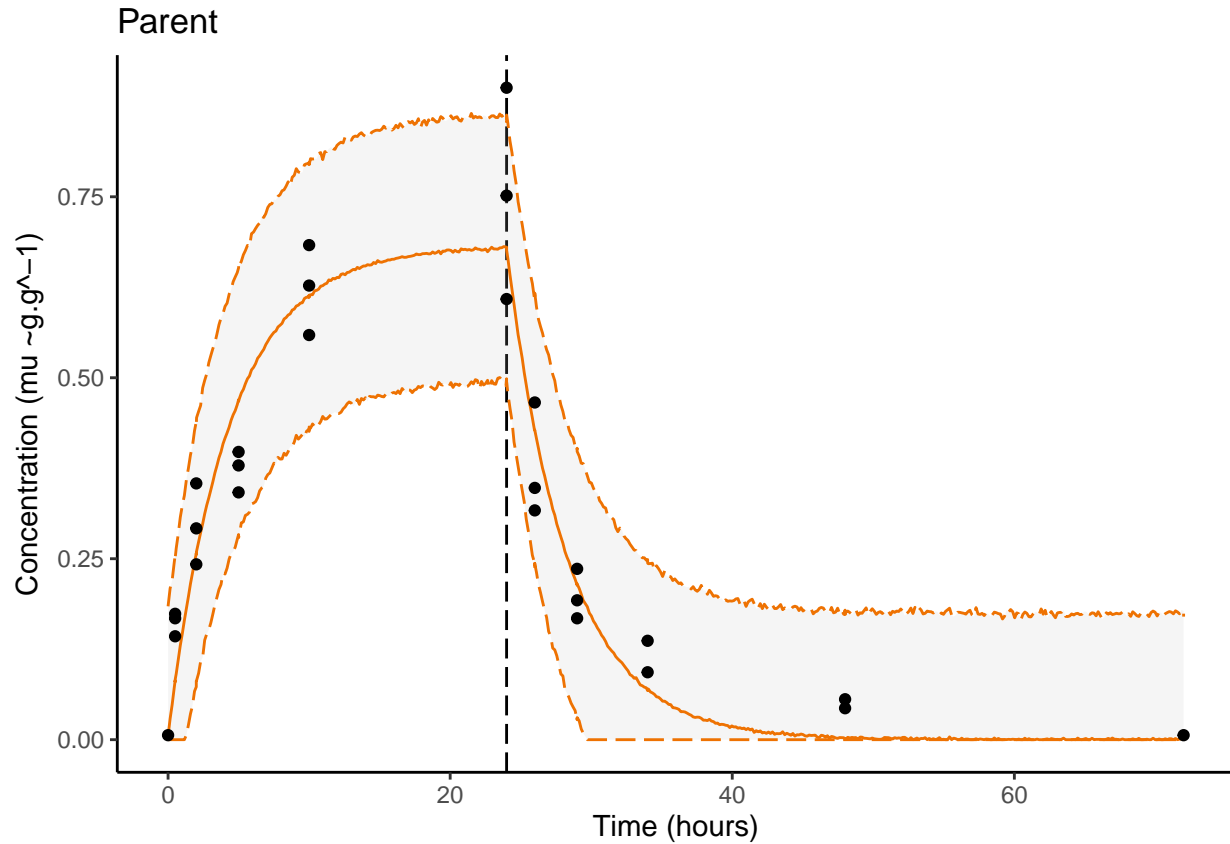


### BMF summary

	2.5%	50%	97.5%	CV
BMFk	0.0104	0.0114	0.0124	0.044

## Fitting results

### Fit plot



### Quantiles of estimated parameters

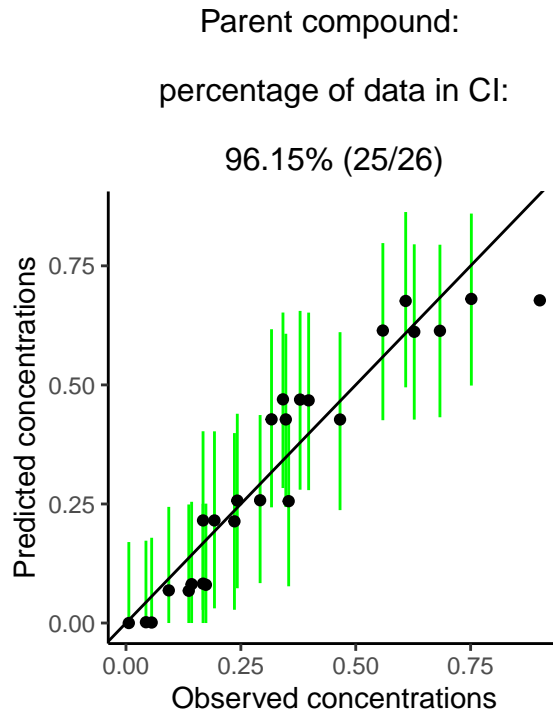
	2.5%	50%	97.5%	
$k_{uf}$	0.002088	0.002638	0.003269	$h^{-1}$
$k_{ee}$	0.184	0.2307	0.2895	$h^{-1}$
$\sigma_p$	0.06543	0.08545	0.1191	$\mu g.g^{-1}$

## Goodness-of-fit criteria

### Posterior Predictive Check

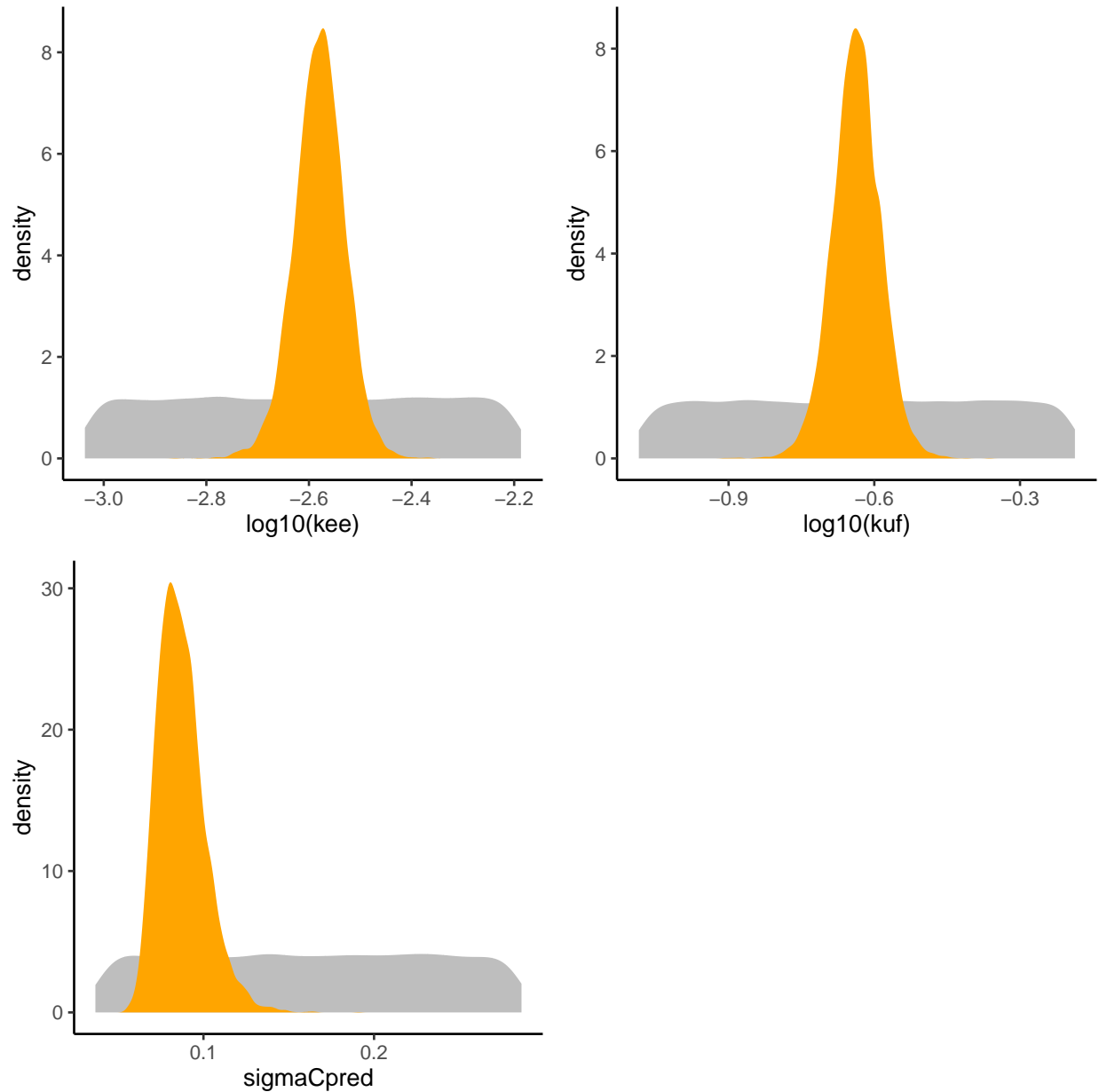
The PPC shows the observed values against their corresponding estimated predictions (black dots), along with their 95% credible interval (vertical segments). If the fit is correct, we expect to see 95% of the data within the intervals. Ideally observations and predictions should coincide, so we would expect to see black dots along the first bisector  $y = x$  (plain black line). The 95% credible intervals are colored in green if they

overlap this line, in red otherwise.



### Priors and posteriors

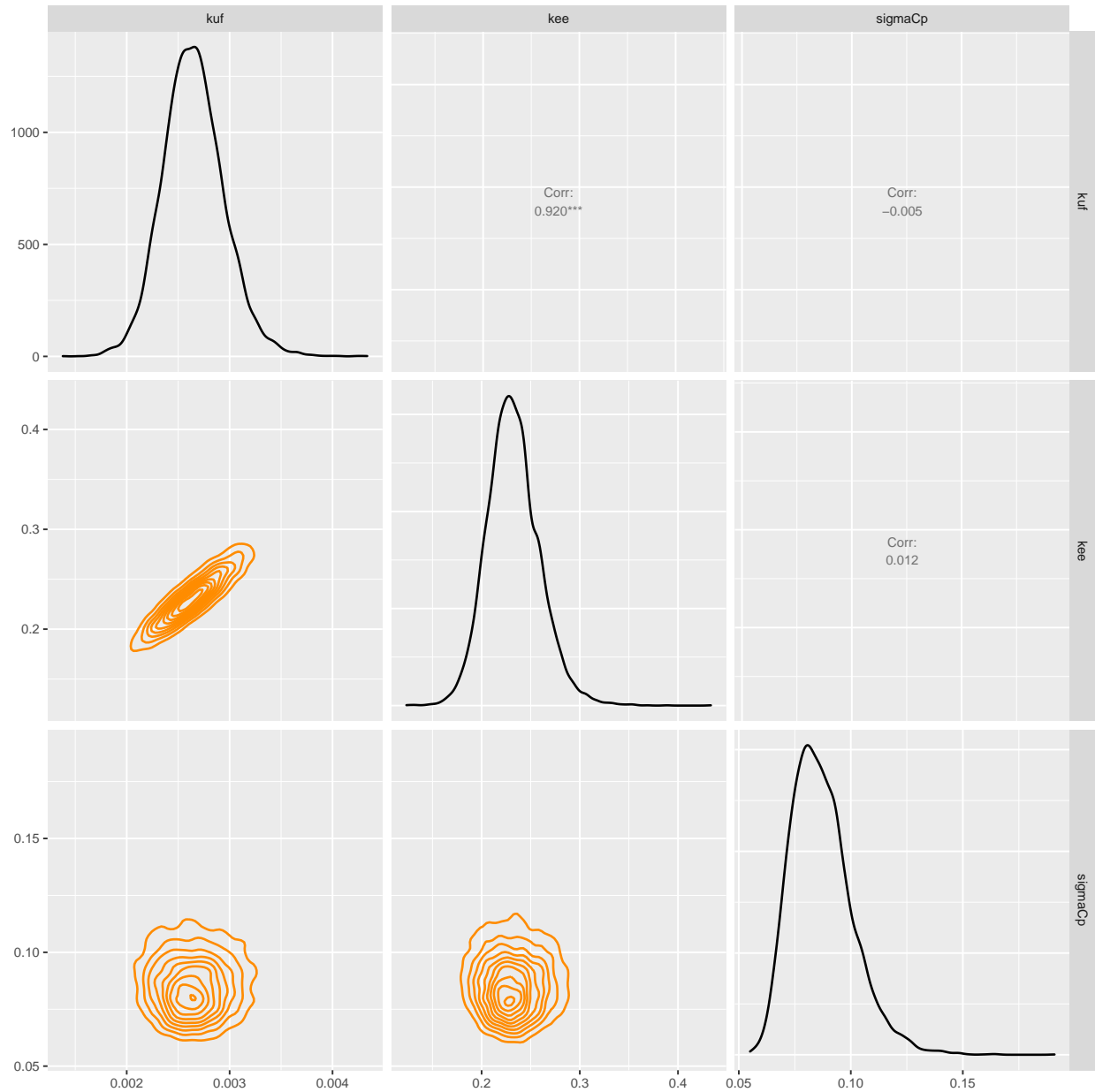
The prior distribution is represented by the gray area and the posterior distribution by the orange area. The accuracy of the model parameter estimation can be visualized by comparing prior and posterior distributions: the overall expectation is to get a narrower posterior distribution compared to the prior one, what reflects that data contributed enough to precisely estimate parameters.



### Correlation between parameters

If you want to see the coloured matrix giving a summary of parameter correlations, you need to import the corresponding figure directly from the application, page bottom, section “Downloads”, then choose Download an output and select “GOF” then “parameter correlation”. You can select the output format you prefer.

Correlations between parameters are visualized by projecting the joint posterior distribution in a plot matrix with planes of parameter pairs (lower triangular elements), marginal posterior distribution of each model parameter (diagonal), and Pearson correlation coefficients (upper triangular elements). Correlations are expected to be low (reflected by “potatoid” shapes of density lines in orange); a leaning elliptical shape translates high correlations (positive if leaning to the right, negative if leaning to the left).



### Potential Scale Reduction Factors

Convergence of the MCMC chains can be checked with the Gelman-Rubin diagnostic expressed with the potential scale reduction factor (PSRF). Approximate convergence is diagnosed when the PSRF is below 1.01.

	PSRF
kuf	1.000728
kee	1.000757
sigmaCpred	1.001729

### Watanabe–Akaike information criterion

Information criteria offer a computationally appealing way of estimating the generalization performance of the model. A fully Bayesian criterion is the widely applicable information criterion (WAIC) by Watanabe a penalized deviance statistics accounting for the uncertainty in the parameters and can be used also for singular models. WAIC is widely used in model comparison for a same dataset (e.g., with or without  $k_{ee}$ ). Sub-models with lower WAIC values will be preferred.

$$\text{WAIC} = -51.7$$

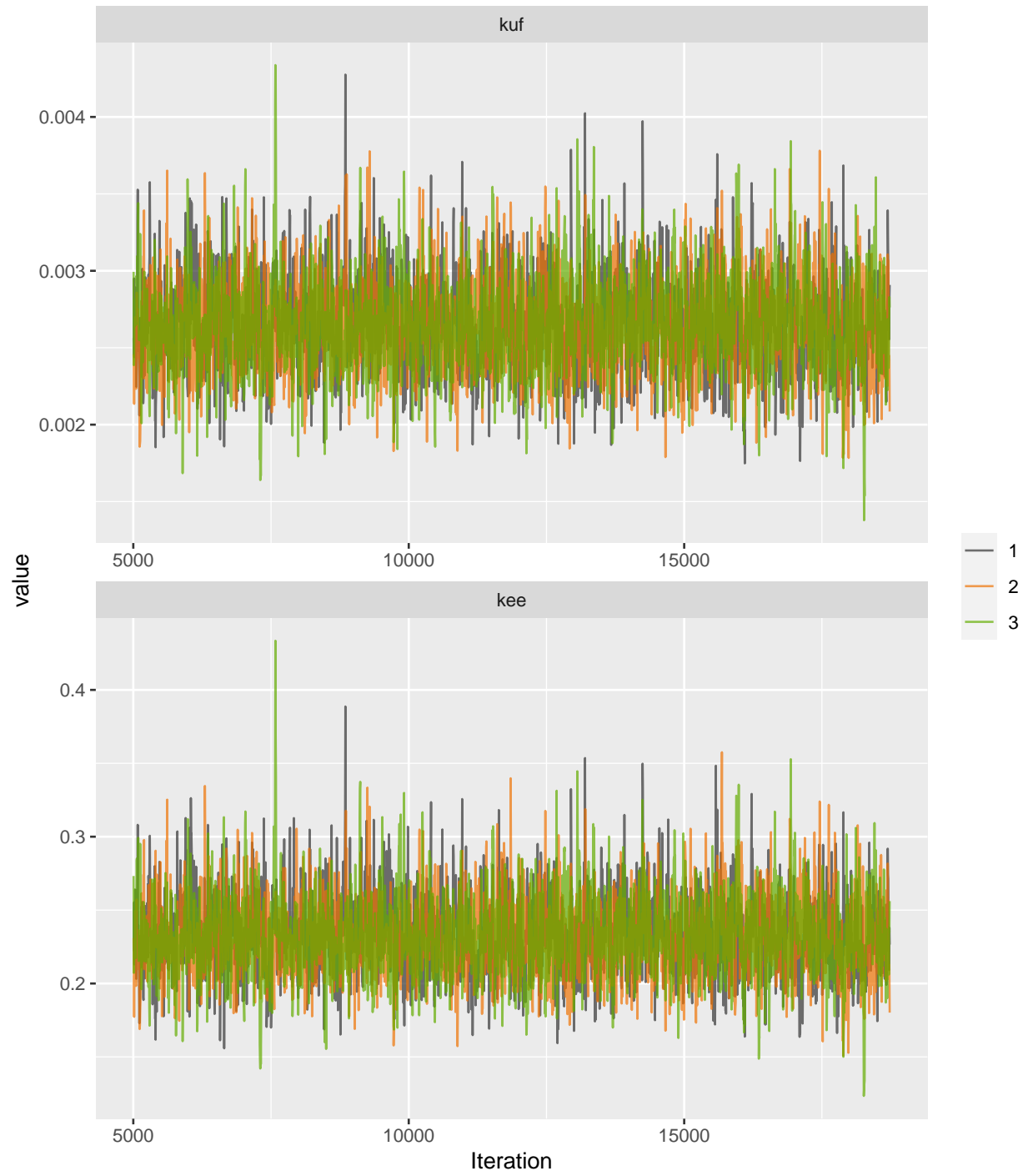
### Deviance Information Criterion

This criteria, denoted DIC, is a penalized deviance statistics accounting for the number of parameters for use in model comparison for a same dataset (e.g., with or without  $k_{ee}$ ). Sub-models with lower DIC values will be preferred.

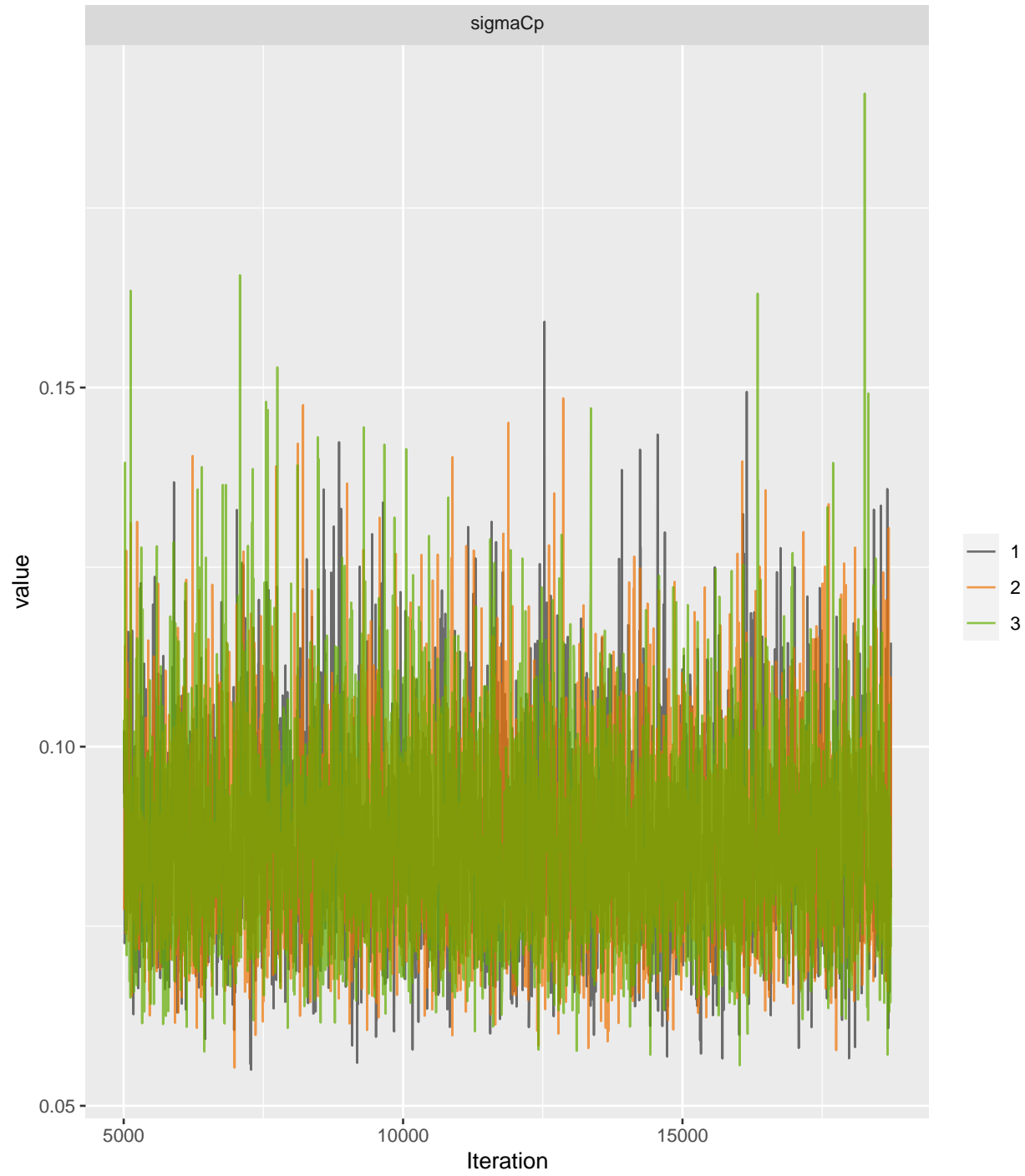
$$\text{DIC} = -50.82373$$

### Traces of MCMC iterations

A traceplot is an essential plot for assessing convergence and diagnosing of MCMC chains. It shows the time series of the sampling process leading to the posterior distribution. Different colors are used for each of the chains (here 3) to assess within-chain convergence.







## Data Table

time	conc	expf	replicate
0.0	0.00621118	59.745	1
0.5	0.14285714	59.745	1
0.5	0.17391304	59.745	2
0.5	0.16770186	59.745	3
2.0	0.24223602	59.745	1
2.0	0.29192547	59.745	2
2.0	0.35403727	59.745	3
5.0	0.34161491	59.745	1
5.0	0.37888199	59.745	2
5.0	0.39751553	59.745	3
10.0	0.55900621	59.745	1
10.0	0.62732919	59.745	2
10.0	0.68322981	59.745	3
24.0	0.75155280	59.745	1
24.0	0.90062112	59.745	2
24.0	0.60869565	59.745	3
26.0	0.46583851	59.745	1
26.0	0.34782609	59.745	2
26.0	0.31677019	59.745	3
29.0	0.23602484	59.745	1
29.0	0.19254658	59.745	2
29.0	0.16770186	59.745	3
34.0	0.13664596	59.745	1
34.0	0.09316770	59.745	2
48.0	0.05590062	59.745	1
48.0	0.04347826	59.745	2
72.0	0.00621118	59.745	1