

# ToxLim : Incorporating Ecological Data and Uncertainty in Bioaccumulation Modeling

Frederik de Laender  
Ghent University  
Belgium

Karline Soetaert  
NIOO-CEME  
The Netherlands

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## Abstract

Rpackage **ToxLim** (De~Laender and Soetaert 2010) contains the OMEGA model to estimate the estimates the bioaccumulation of a nonbiotransforming chemical through a food web.

It also contains several food web examples.

The methodology was described in the paper by (De~Laender, Van~Oevelen, Middelburg, and Soetaert 2009). Please cite this paper when using this package.

*Keywords:*~ toxicity, food webs, linear inverse models, R .

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## 1. Introduction

R-package **ToxLim** , accompanying the paper (De~Laender *et al.* 2009) models the bioaccumulation of a nonbiotransforming chemical through a food web.

It contains an implementation of the **OMEGA** model (Hendriks, van~der Linde, Cornelissen, and Sijm 2001), as extended for multiple food sources by (De~Laender *et al.* 2009), and three food web examples: the pelagic food web of the Barents Sea, and two food webs of freshwater (lake) enclosures.

For background on inverse modelling, we refer to the documents of the **LIM** package (van Oevelen, van~den Meersche, Meysman, Soetaert, Middelburg, and Vezina 2010), or the **lim-Solve** package (Soetaert, den Meersche, and van Oevelen 2009).

Also see (Van~den Meersche, Soetaert, and Van~Oevelen 2009) for running a constrained monte carlo.

The **LIM** package also contains many other food web examples.

## 2. The example food webs

Three food webs are included in the package.

### 2.1. LIMbarents

The Barents Sea food web was published in (De~Laender, Van~Oevelen, Middelburg, and Soetaert 2010a) and the bioaccumulation model applied to it in (De~Laender, Van~Oevelen, S, Middelburg, and Soetaert 2010b).

It consists of the linear inverse model specification for the Southern Barents Sea.

The food web compartments for the area are dissolved organic carbon (DOC), detritus, bacteria, heterotrophic flagellates and ciliates, phytoplankton (pico- and nanoplankton, diatoms and *Phaeocystis* sp.), mesozooplankton (copepods), macrozooplankton (krill and chaetognaths), cod (*Gadus morhua*), herring (*Clupea harengus*) and capelin (*Mallotus villosus*). Adult cod ( $> 3$  yrs) and young cod ( $< 3$  yrs) were considered as two different populations.

First the food web is solved:

```
> plotweb(Flowmatrix(LIMbarents),main="Barents Sea Food Web",
+   sub="gC/m2/day")
```

Then the ranges of flows and variables are calculated and plotted:

```
> pm <- par(mfrow=c(1,2))
> Plotranges(LIMbarents,lab.cex=0.7,xlab="gC/m2/d",
+   main="Flows")
> #
> Plotranges(LIMbarents,type="V",lab.cex=0.7,xlab="gC/m2/d",
+   main="variables")
> mtext(outer=TRUE,"Southern Barents Sea food web",side=3,line=-1,cex=1.5)
> par(mfrow=pm)
```

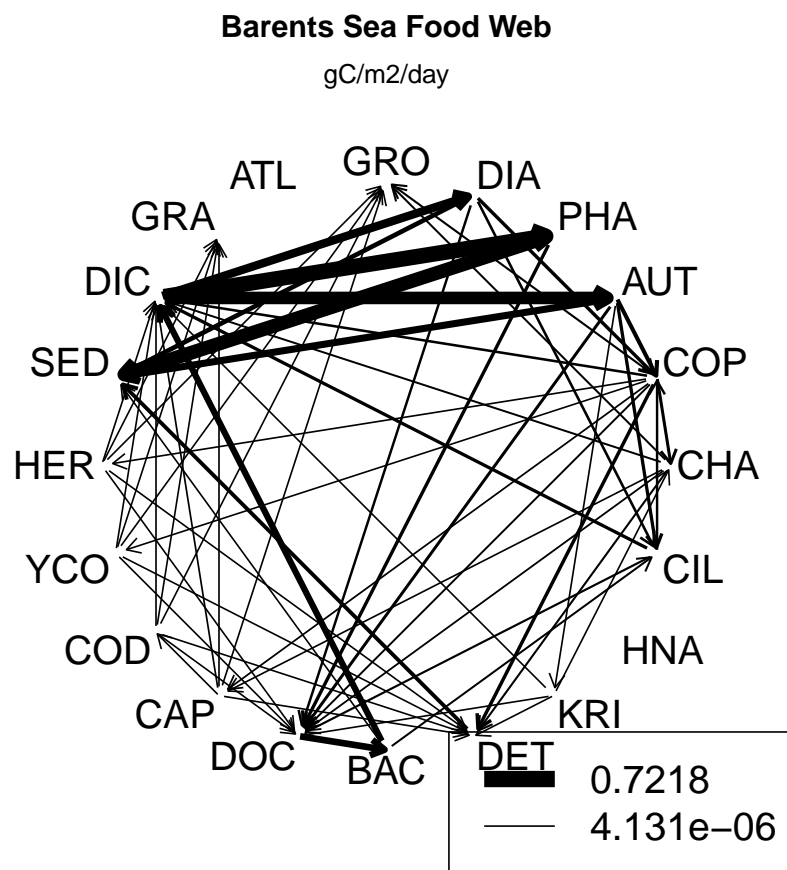


Figure 1: The Barents Sea food web

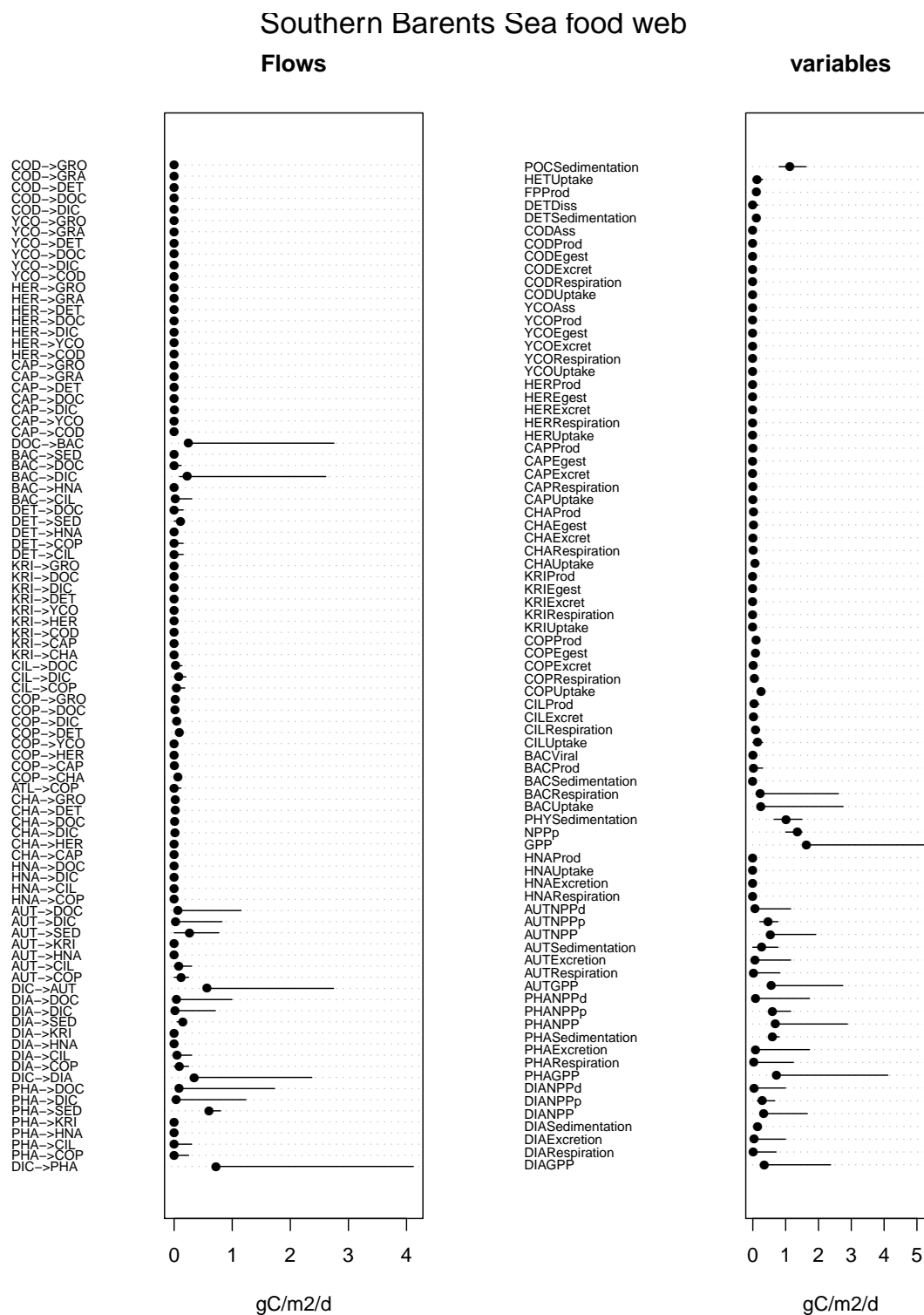


Figure 2: The Barents Sea food web ranges of flows and variables

## 2.2. LIMlake and LIMlakeFish

This includes the Linear inverse model specification for two freshwater lake enclosures (Lac Croche, Canada), (Ridal, Mazumder, and Lean 2001), used as demonstration example in (De Laender *et al.* 2009).

Food web compositions in the enclosures were manipulated by additions of planktivorous fish and/or nutrients giving four types of food webs: planktonic, planktonic with nutrient addition, planktonic with planktivorous fish, and planktonic with planktivorous fish and nutrient additions. The trophic links in the mass-balances of each LIM are identical, except that the fish compartment is only present in F and FN.

LIMlake is the linear inverse model for the food web without fish and without nutrient addition. LIMlakeFish has fish, but also no nutrients were added.

First the food web is solved:

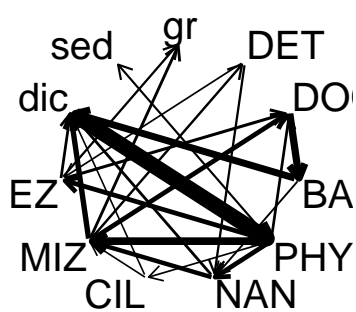
```
> pm <- par(mfrow=c(1,2))
> lake <- Flowmatrix(LIMlake)
> plotweb(lake,main="Lake enclosure food web",sub="gC/m2/day")
> plotweb(Flowmatrix(LIMlakeFish),main="Lake enclosure food web + FISH",
+   sub="gC/m2/day")
```

Then the ranges of flows and variables are calculated and plotted:

```
> # ranges of flows
> Plotranges(LIMlake,lab.cex=0.7,xlab="gC/m2/d",
+   main="Flows")
> # ranges of variables
> Plotranges(LIMlake,type="V",lab.cex=0.7,xlab="gC/m2/d",
+   main="variables")
> mtext(outer=TRUE,"Lake enclosure food web",side=3,line=-1,cex=1.5)
> par(mfrow=pm)
```

**Lake enclosure food web**

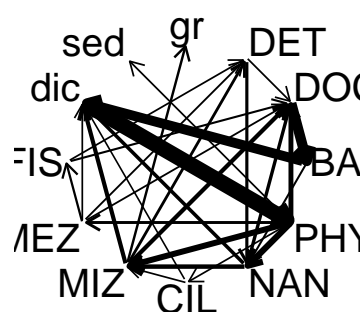
gC/m2/day



<b>—</b>	0.09068
—	0.00014748

**Lake enclosure food web + FISH**

gC/m2/day



<b>—</b>	0.057219
—	0.00016062

Figure 3: The Limlake food web with and without fish

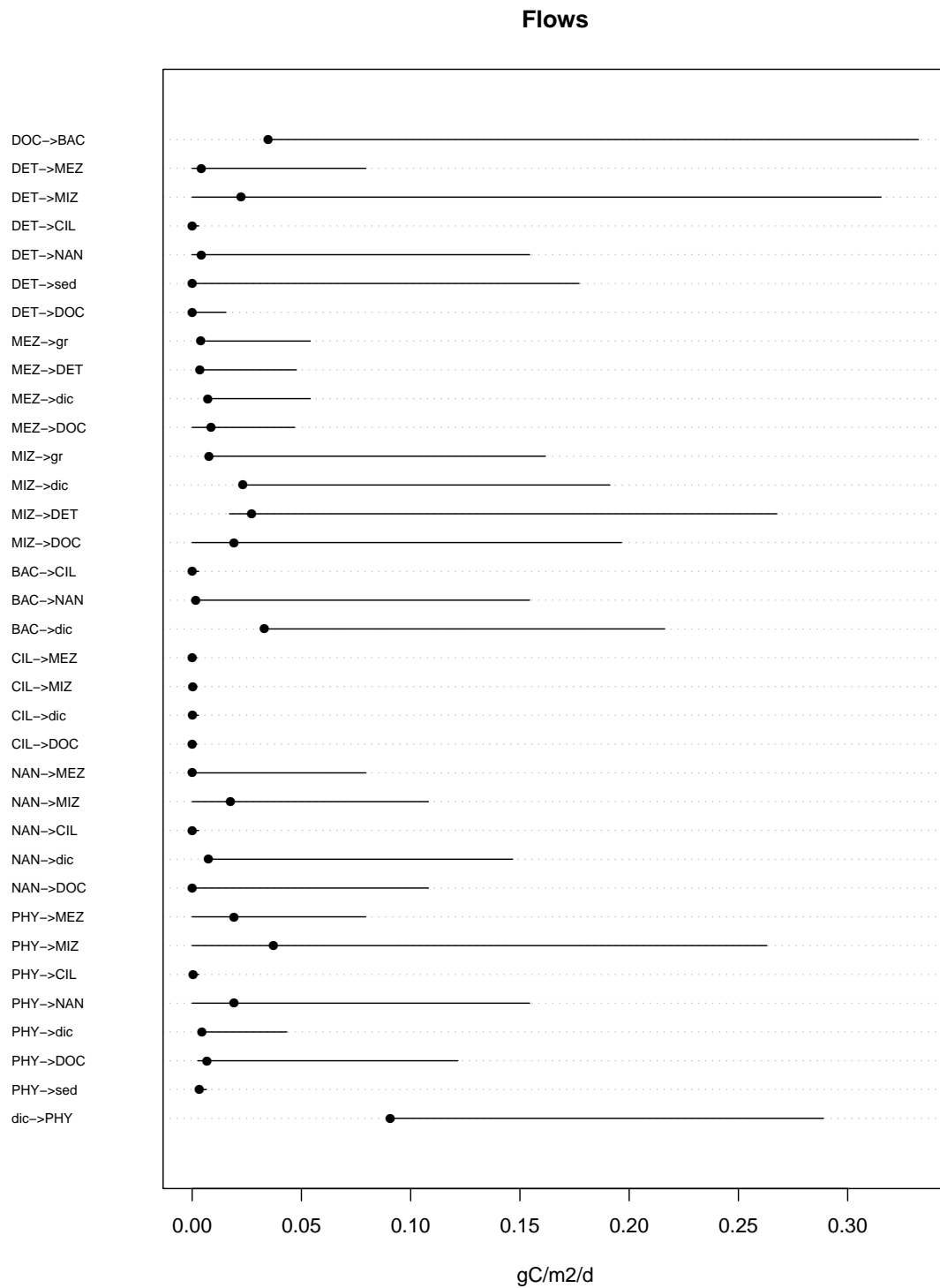


Figure 4: The Limlake food web ranges of flows and variables

### 3. The LimOmega function

The OMEGA model (Hendriks *et al.* 2001) estimates the rate of change of the concentration  $C_i$  of a nonbiotransforming chemical in compartment  $i$  by taking into account the chemical uptake rates through feeding and directly from water, the chemical dilution rate through production and the rates of egestion with faeces and excretion to water.

While OMEGA initially was developed to represent food chains, it was extended with multiple food sources in (De~Laender *et al.* 2009).

The set of differential equations for all  $m$  compartments in a food web was cast in matrix notation as:

$$\frac{dC}{dt} = K_{up,food} \cdot C + K_{up,water} \cdot C_{water} - K_{out+dil} \cdot C$$

where  $C$  is the internal concentration vector,  $\frac{dC}{dt}$  is the rate of change of the internal concentration vector,  $K_{up,food}$  is a  $m \times m$  matrix with chemical uptake rates through feeding ( $d^{-1}$ ), containing elements  $k_{up,food,ji}$  on row  $i$ , column  $j$ ,  $K_{up,water}$  the uptake rates directly from water ( $L \cdot kg^{-1} \cdot d^{-1}$ ) is a column vector with  $m$  elements and  $K_{out+dil}$  the chemical dilution rate through production, the rates of egestion with faeces and excretion to water ( $d^{-1}$ ), a  $m \times m$  diagonal matrix with elements  $k_{out,eg,i} + k_{dil,pr,i} + k_{out,water,i}$ .

Expressions for rate coefficients ( $k_{up,food,ji}$ ;  $k_{up,water,i}$ ;  $k_{out,eg,i}$ ;  $k_{dil,pr,i}$ ;  $k_{out,water,i}$ ) that regulate chemical uptake and loss processes and how these relate to the carbon flows predicted by the LIM framework can be found in Table S1 of the Supporting Information (SI) of (De~Laender *et al.* 2009).

Internal concentrations in small particles such as microzooplankton, phytoplankton, detritus, protozoa, and bacteria (collectively termed INST in this package), are assumed to be in rapid equilibrium with the water phase and may be calculated as

$$C_{INST}^* = C_{water} \cdot OC_{INST} \cdot K_{OC}$$

where  $C_{inst}^*$  denotes the concentration vector for model compartments that are in instant equilibrium with the surrounding water (microg kg<sup>-1</sup> wet weight),  $OC_{inst}$  their organic carbon fraction (-), and  $K_{OC}$ , the organic carbon-water partition coefficient ( $L \cdot kg^{-1}$ ), calculated as 0.41KOW, with KOW the octanol-water partition coefficient.

#### 3.1. The bioaccumulation model applied to the three example food webs

First we apply the bioaccumulation model to the three food webs, and using the default values (e.g. a logKow of 6):

The lake food web,

```
> LimOmega (lim = LIMlake,
+           INST=c("DET", "DOC", "BAC", "PHY", "NAN", "CIL", "MIZ"),
+           KINE= "MEZ", EXP0=c("sed", "gr"),
+           DOC="DOC", DET="DET", DIC="dic",
+           WW_KINE=7.596535e-08, SS_KINE=0.079508)
```



```
$BAF_LC
      MEZ
1073583
```

```
$BCF_OC
      DET      DOC      BAC      PHY      NAN      CIL      MIZ
410000 410000 410000 410000 410000 410000 410000
```

The lake food web with fish:

```
> LimOmega (lim = LIMlakeFish,
+           INST=c("DET", "DOC", "BAC", "PHY", "NAN", "CIL", "MIZ"),
+           KINE=c("MEZ", "FIS"), EXPO=c("sed", "gr"),
+           DOC="DOC", DET="DET", DIC="dic",
+           WW_KINE=c(1.85e-08, 1.7e-3),
+           SS_KINE=c(0.00514800, 0.26))
```

```
$BAF_LC
      MEZ      FIS
943609 1051809
```

```
$BCF_OC
      DET      DOC      BAC      PHY      NAN      CIL      MIZ
410000 410000 410000 410000 410000 410000 410000
```

The Barents Sea example:

```
> LimOmega (lim = LIMbarents,
+           INST=c("DIA", "PHA", "AUT", "CIL", "HNA", "DET", "BAC"),
+           KINE=c("COP", "CHA", "KRI", "CAP", "COD", "YCO", "HER"),
+           EXPO=c("SED", "GRA", "GRO"),
+           DOC="DOC", DET="DET", DIC="DIC",
+           WW_KINE=c(0.000001, 8e-05, 0.00006, 10e-3, 3, 1, 20e-3),
+           LIPID_KINE=c(0.01, 0.01, 0.01, 0.03, 0.03, 0.03, 0.03),
+           LIPID_INST=0.04,
+           SS_KINE=c(1.79, 0.6965, 0.003, 0.38, 0.053, 0.006, 0.055))
```

```
$BAF_LC
      COP      CHA      KRI      CAP      COD      YCO      HER
887935.9 1003297.5 467057.2 958170.3 1657017.9 780377.1 1160962.6
```

```
$BCF_OC
      DIA      PHA      AUT      CIL      HNA      DET      BAC
410000 410000 410000 410000 410000 410000 410000
```

### 3.2. A monte carlo run on food web structure

First we take `niter` random samples from all possible solutions using a Markow Chain Monte Carlo approach (Van den Meersche *et al.* 2009)

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```
> X0      <- Lsei(LIMlake)$X
> niter <- 50
> SolXS   <- Xsample(LIMlake, iter=niter, type = "mirror",
+                   jmp=NULL, x0=X0, fulloutput = FALSE)
> BAFlc_all <- NULL
```

Then, for each of these samples the flowmatrix is created and LimOmega applied:

```
> for (i in 1:niter) {
+   flowmat <- Flowmatrix(LIMlake, SolXS[i,])
+   LO<- LimOmega (flowmatrix=flowmat,
+                 INST=c("DET","DOC","BAC","PHY","NAN","CIL","MIZ"),
+                 KINE=c("MEZ"), EXP0=c("sed","gr"),
+                 DOC="DOC", DET="DET", DIC="dic",
+                 WW_KINE=7.596535e-08, SS_KINE=0.079508,
+                 Growth=0, k=0.25, Q=1)
+   BAFlc_all <- c(BAFlc_all,LO$BAF_LC)
+ }
```

Show results

```
> hist(BAFlc_all)
```

Now the same food web structure is used with different chemical parameters:

```
> niter <- 100
```

We create a normally distributed sample of log kow:

```
> lkw <- rnorm(niter,mean=6,sd=0.4)
> BAFlc_all <- NULL
> BCFoc_all <- NULL
```

We also use the LIMlake foodweb:

```
> flowmat <- Flowmatrix(LIMlake)
```

and run the LimOmega model for each value of log kow:

```
> for (i in 1:niter) {
+   LO<- LimOmega (flowmatrix=flowmat,
+                 INST=c("DET","DOC","BAC","PHY","NAN","CIL","MIZ"),
+                 KINE=c("MEZ"), EXP0=c("sed","gr"),
+                 DOC="DOC", DET="DET", DIC="dic",
+                 WW_KINE=7.596535e-08, SS_KINE=0.079508,
+                 Growth=0, k=0.25, Q=1, logKow = lkw[i])
+   BAFlc_all <- c(BAFlc_all,LO$BAF_LC)
+   BCFoc_all <- c(BCFoc_all,LO$BCF_OC[1])
+ }
```

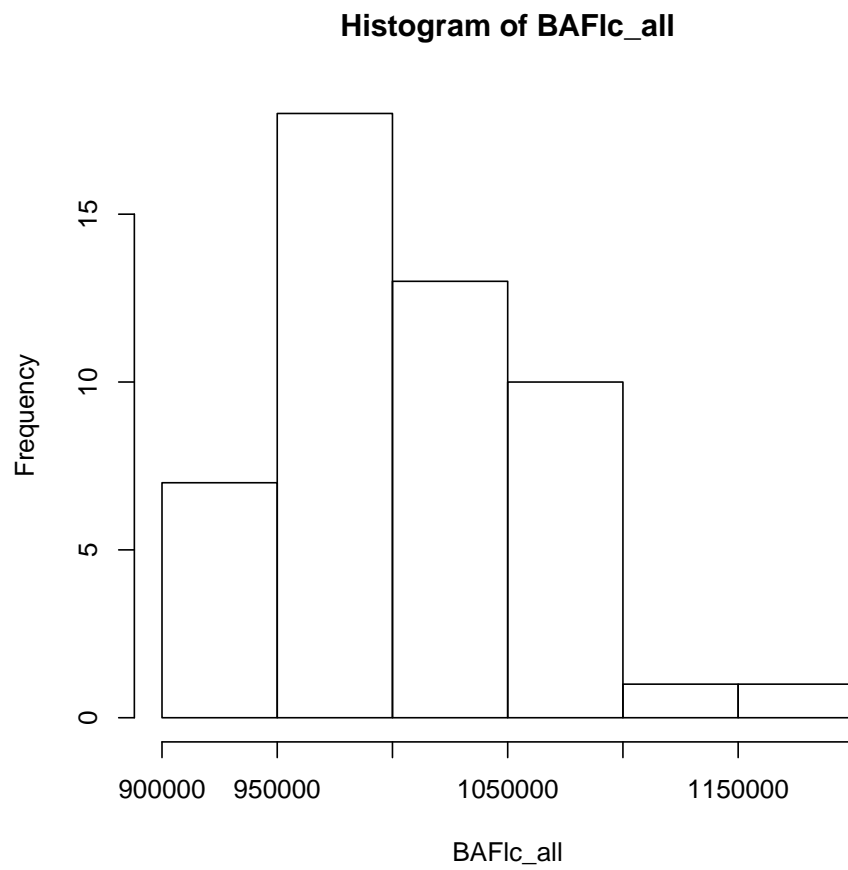


Figure 5: The LimOmega model, applied 50 times, to the lake food web

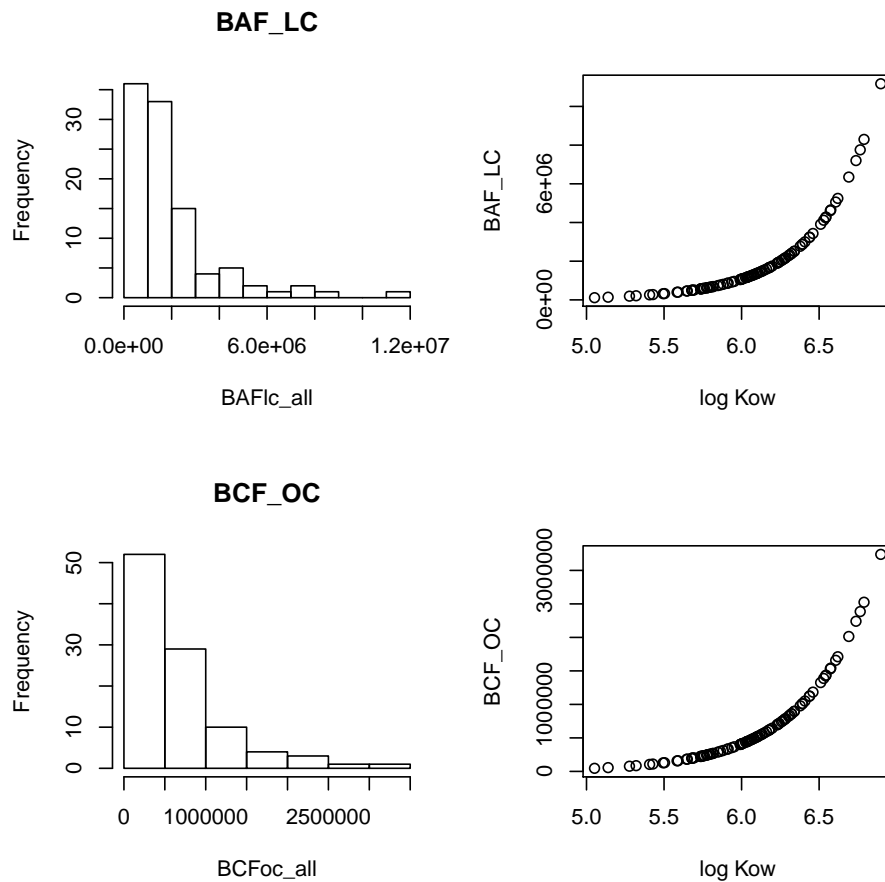


Figure 6: The LimOmega model, applied with different values of log kow

Finally, we plot the results:

```
> pm <- par(mfrow=c(2,2))
> hist(BAFlc_all,main="BAF_LC")
> plot(lkw,BAFlc_all,xlab="log Kow",ylab="BAF_LC")
> hist(BCFoc_all,main="BCF_OC")
> plot(lkw,BCFoc_all,xlab="log Kow",ylab="BCF_OC")
> par(mfrow=pm)
```

## 4. Finally

This vignette was made with Sweave ([Leisch 2002](#)).

## References

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## Affiliation:

Frederik De Laender  
Laboratory of Environmental Toxicology and Aquatic Ecology  
Ghent University  
Plateaustraat 22

9000 Ghent

Belgium

E-mail: [frederik.delaender@ugent.be](mailto:frederik.delaender@ugent.be)

Karline Soetaert

Centre for Estuarine and Marine Ecology (CEME)

Netherlands Institute of Ecology (NIOO)

4401 NT Yerseke, Netherlands

E-mail: [k.soetaert@nioo.knaw.nl](mailto:k.soetaert@nioo.knaw.nl)

URL: <http://www.nioo.knaw.nl/users/ksoetaert>