

R Package **FME** : Inverse Modelling, Sensitivity, Monte Carlo – Applied to a Steady-State Model

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Abstract

Rpackage **FME** (Soetaert and Petzoldt 2010) contains functions for model calibration, sensitivity, identifiability, and Monte Carlo analysis of nonlinear models.

This vignette, (`vignette("FMEsteady")`), applies **FME** to a partial differential equation, solved with a steady-state solver from package **rootSolve**

A similar vignette (`vignette("FMEdyna")`), applies the functions to a dynamic simulation model, solved with integration routines from package **deSolve**

A third vignette (`vignette("FMEother")`), applies the functions to a simple nonlinear model

`vignette("FMEcmc")` tests the Markov chain Monte Carlo (MCMC) implementation

Keywords: steady-state models, differential equations, fitting, sensitivity, Monte Carlo, identifiability, R.

1. A steady-state model of oxygen in a marine sediment

This is a simple model of oxygen in a marine (submersed) sediment, diffusing along a spatial gradient, with imposed upper boundary concentration oxygen is consumed at maximal fixed rate, and including a monod limitation.

See (Soetaert and Herman 2009) for a description of reaction-transport models.

The constitutive equations are:

$$\begin{aligned}\frac{\partial O_2}{\partial t} &= -\frac{\partial Flux}{\partial x} - cons \cdot \frac{O_2}{O_2 + k_s} \\ Flux &= -D \cdot \frac{\partial O_2}{\partial x} \\ O_2(x=0) &= upO2\end{aligned}$$

```
> par(mfrow=c(2,2))  
> require(FME)
```

First the model parameters are defined...

```
> pars <- c(upO2=360, # concentration at upper boundary, mmolO2/m3  
+          cons=80,   # consumption rate, mmolO2/m3/day
```

```
+          ks=1,          # O2 half-saturation ct, mmolO2/m3
+          D=1)           # diffusion coefficient, cm2/d
```

Next the sediment is vertically subdivided into 100 grid cells, each 0.05 cm thick.

```
> n <- 100                                # nr grid points
> dx <- 0.05    #cm
> dX <- c(dx/2,rep(dx,n-1),dx/2) # dispersion distances; half dx near boundaries
> X <- seq(dx/2,len=n,by=dx)      # distance from upper interface at middle of box
```

The model function takes as input the parameter values and returns the steady-state condition of oxygen. Function `steady.band` from package **rootSolve** ((Soetaert 2009)) does this in a very efficient way (see (Soetaert and Herman 2009)).

```
> O2fun <- function(pars)
+ {
+   derivs<-function(t,O2,pars)
+   {
+     with (as.list(pars),{
+
+       Flux <- -D* diff(c(upO2,O2,O2[n]))/dX
+       dO2 <- -diff(Flux)/dx-cons*O2/(O2+ks)
+
+       return(list(dO2,UpFlux = Flux[1],LowFlux = Flux[n+1]))
+     })
+   }
+
+   # Solve the steady-state conditions of the model
+   ox <- steady.band(y=runif(n),func=derivs,parms=pars,nspec=1,positive=TRUE)
+   data.frame(X=X,O2=ox$y)
+ }
```

The model is run

```
> ox<-O2fun(pars)
```

and the results plotted...

```
> plot(ox$O2,ox$X,ylim=rev(range(X)),xlab="mmol/m3",
+       main="Oxygen", ylab="depth, cm",type="l",lwd=2)
```

2. Global sensitivity analysis : Sensitivity ranges

The sensitivity of the oxygen profile to parameter `cons`, the consumption rate is estimated. We assume a normally distributed parameter, with mean = 80 (`parMean`), and a variance=100 (`parCovar`). The model is run 100 times (`num`).

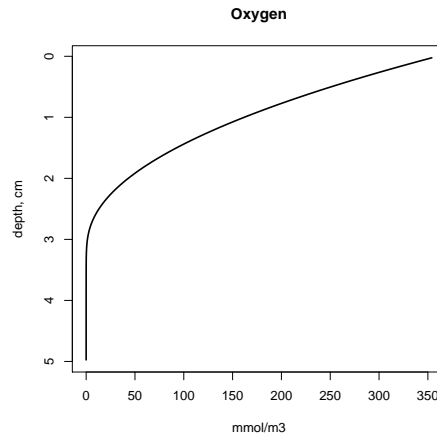


Figure 1: The modeled oxygen profile - see text for R-code

```
> print(system.time(
+   Sens2 <- sensRange(parms=pars,func=O2fun,dist="norm",
+                     num=100,parMean=c(cons=80),parCovar=100)
+ ))
```

```
user  system elapsed
1.62   0.00   1.62
```

The results can be plotted in two ways:

```
> par(mfrow=c(1,2))
> plot(Sens2,xyswap=TRUE,xlab= "O2",
+       ylab="depth, cm",main="Sensitivity runs")
> plot(summary(Sens2),xyswap=TRUE,xlab= "O2",
+       ylab="depth, cm",main="Sensitivity ranges")
> par(mfrow=c(1,1))
```

3. Local sensitivity analysis : Sensitivity functions

Local sensitivity analysis starts by calculating the sensitivity functions

```
> O2sens <- sensFun(func=O2fun,parms=pars)
```

The summary of these functions gives information about which parameters have the largest effect (univariate sensitivity):

```
> summary(O2sens)
```

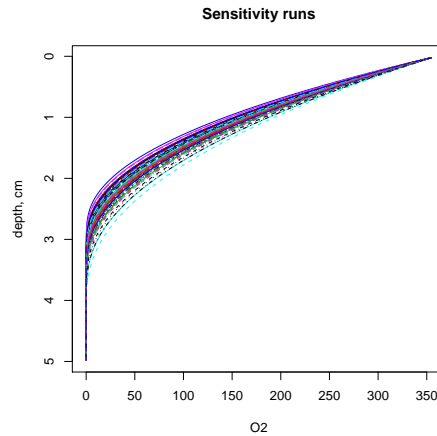


Figure 2: Results of the sensitivity run - left: all model runs, right: summary - see text for R-code

	value	scale	L1	L2	Mean	Min	Max	N
up02	360	360	7.0	0.88	7.0	1.0e+00	13.4176	100
cons	80	80	8.1	1.14	-8.1	-2.2e+01	-0.0084	100
ks	1	1	2.2	0.37	2.2	1.2e-04	9.6137	100
D	1	1	8.1	1.14	8.1	8.4e-03	22.0312	100

In bivariate sensitivity the pair-wise relationship and the correlation is estimated and/or plotted:

```
> pairs(O2sens)
```

```
> cor(O2sens[,-(1:2)])
```

	up02	cons	ks	D
up02	1.0000000	-0.9787945	0.8375806	0.9787945
cons	-0.9787945	1.0000000	-0.9317287	-1.0000000
ks	0.8375806	-0.9317287	1.0000000	0.9317287
D	0.9787945	-1.0000000	0.9317287	1.0000000

Multivariate sensitivity is done by estimating the collinearity between parameter sets (Brun, Reichert, and Kunsch 2001).

```
> Coll <- collin(O2sens)
```

```
> Coll
```

	up02	cons	ks	D	N	collinearity
1	1	1	0	0	2	7.7
2	1	0	1	0	2	2.9

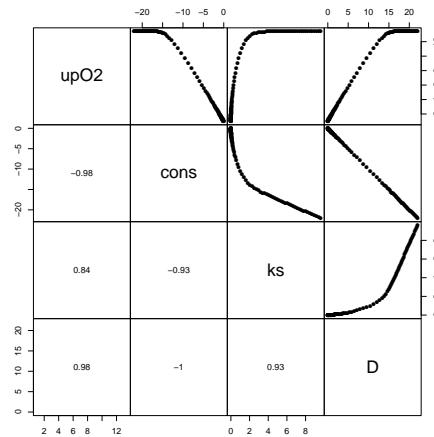


Figure 3: pairs plot - see text for R-code

3	1	0	0	1	2	7.7
4	0	1	1	0	2	4.4
5	0	1	0	1	2	25364766.4
6	0	0	1	1	2	4.4
7	1	1	1	0	3	25.5
8	1	1	0	1	3	96597623.3
9	1	0	1	1	3	25.5
10	0	1	1	1	3	169544791.3
11	1	1	1	1	4	NaN

```
> plot(Coll, log="y")
```

4. Fitting the model to the data

Assume both the oxygen flux at the upper interface and a vertical profile of oxygen has been measured.

These are the data:

```
> O2dat <- data.frame(x=seq(0.1,3.5,by=0.1),
+   y = c(279,260,256,220,200,203,189,179,165,140,138,127,116,
+   109,92,87,78,72,62,55,49,43,35,32,27,20,15,15,10,8,5,3,2,1,0))
> O2depth <- cbind(name="O2",O2dat)      # oxygen versus depth
> O2flux <- c(UpFlux=170)                # measured flux
```

First a function is defined that returns only the required model output.

```
> O2fun2 <- function(pars)
+ {
```

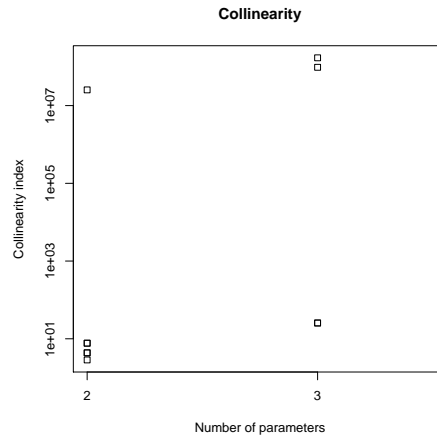


Figure 4: collinearity - see text for R-code

```
+ derivs<-function(t,02,pars)
+ {
+   with (as.list(pars),{
+
+     Flux <- -D*diff(c(up02,02,02[n]))/dx
+     d02 <- -diff(Flux)/dx-cons*02/(02+ks)
+
+     return(list(d02,UpFlux = Flux[1],LowFlux = Flux[n+1]))
+   })
+ }
+
+ ox <- steady.band(y=runif(n),func=derivs,parms=pars,nspec=1,
+                   positive=TRUE,rtol=1e-8,atol=1e-10)
+
+ list(data.frame(x=X,02=ox$y),
+       UpFlux=ox$UpFlux)
+ }
```

The function used in the fitting algorithm returns an instance of type `modCost`. This is created by calling function `modCost` twice. First with the modeled oxygen profile, then with the modeled flux.

```
> Objective <- function (P)
+ {
+   Pars <- pars
+   Pars[names(P)]<-P
+   mod02 <- 02fun2(Pars)
+
+   # Model cost: first the oxygen profile
+   Cost <- modCost(obs=02depth,model=mod02[[1]],x="x",y="y")
+ }
```

```

+
+   # then the flux
+   modF1 <- c(UpFlux=mod02$UpFlux)
+   Cost  <- modCost(obs=02flux,model=modF1,x=NULL,cost=Cost)
+
+   return(Cost)
+ }

```

We first estimate the identifiability of the parameters, given the data:

```

> print(system.time(
+   sF<-sensFun(Objective,parms=pars)
+ ))

   user  system elapsed
   0.21    0.00    0.20

> summary(sF)

      value scale  L1  L2 Mean      Min  Max  N
up02   360   360 4.25 0.97 4.25   0.5069 13.3 36
cons    80    80 3.68 0.99 -3.65 -15.3722  0.5 36
ks       1     1 0.40 0.14 0.40  -0.0069  3.1 36
D        1     1 3.68 0.99 3.68   0.0342 15.4 36

> collin(sF)

      up02 cons ks D N collinearity
1         1    1 0 0 2             8.6
2         1    0 1 0 2             3.1
3         1    0 0 1 2             8.7
4         0    1 1 0 2             4.2
5         0    1 0 1 2            50.6
6         0    0 1 1 2             4.2
7         1    1 1 0 3            14.2
8         1    1 0 1 3            50.8
9         1    0 1 1 3            14.7
10        0    1 1 1 3            50.6
11        1    1 1 1 4            51.0

```

The collinearity of the full set is too high, but as the oxygen diffusion coefficient is well known, it is left out of the fitting. The combination of the three remaining parameters has a low enough collinearity to enable automatic fitting. The parameters are constrained to be >0

```

> collin(sF,parset=c("up02","cons","ks"))

      up02 cons ks D N collinearity
1         1    1 1 0 3             14

```

```

> print(system.time(
+   Fit<-modFit(p=c(up02=360,cons=80,ks=1),
+               f=Objective,lower=c(0,0,0))
+ ))

      user  system elapsed
      1.3      0.0      1.3

> (SFit<-summary(Fit))

Parameters:
      Estimate Std. Error t value Pr(>|t|)
up02   292.937      2.104 139.242  <2e-16 ***
cons    49.686      2.367  20.991  <2e-16 ***
ks       1.297      1.363   0.951    0.348
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 4.401 on 33 degrees of freedom

Parameter correlation:
      up02   cons    ks
up02 1.0000 0.5791 0.2976
cons 0.5791 1.0000 0.9013
ks   0.2976 0.9013 1.0000

```

We next plot the residuals

```

> plot(Objective(Fit$par),xlab="depth",ylab="",main="residual",legpos="top")

and show the best-fit model

> Pars <- pars
> Pars[names(Fit$par)]<- Fit$par
> mod02 <- O2fun(Pars)

> plot(O2depth$y,O2depth$x,ylim=rev(range(O2depth$x)),pch=18,
+      main="Oxygen-fitted", xlab="mmol/m3",ylab="depth, cm")
> lines(mod02$O2,mod02$X)

```

5. Running a Markov chain Monte Carlo

We use the parameter covariances of previous fit to update parameters, while the mean squared residual of the fit is use as prior fo the model variance.

```

> Covar <- SFit$cov.scaled * 2.4^2/3
> s2prior <- SFit$modVariance

```

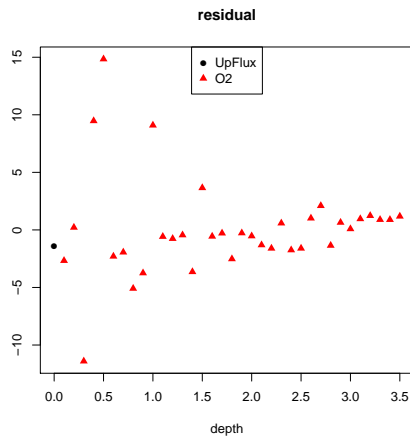



Figure 5: residuals - see text for R-code

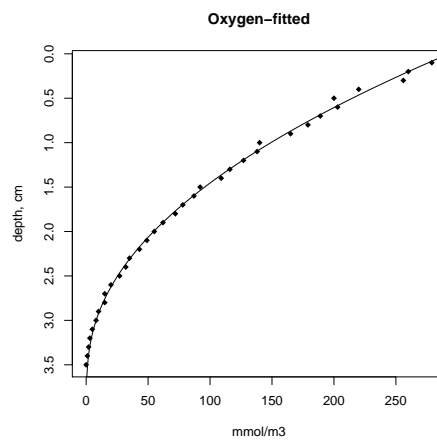


Figure 6: Best fit model - see text for R-code

We run an adaptive Metropolis, making sure that ks does not become negative...

```
> print(system.time(
+   MCMC <- modMCMC(f=Objective,p=Fit$par,jump=Covar,niter=1000,ntrydr=2,
+                   var0=s2prior,wvar0=1,updatecov=100,lower=c(NA,NA,0))
+ ))
```

number of accepted runs: 698 out of 1000 (69.8%)

```
   user  system elapsed
50.80    0.00   50.91
```

```
> MCMC$count
```

```
      dr_steps      Alfasteps  num_accepted num_covupdate
        669          2007         698           9
```

Plotting the results is similar to previous cases.

```
> plot(MCMC,Full=TRUE)
```

```
> hist(MCMC,Full=TRUE)
```

```
> pairs(MCMC,Full=TRUE)
```

or summaries can be created:

```
> summary(MCMC)
```

```
      up02      cons      ks      var_model
mean 293.594179 53.298575 4.132597 444.679881
sd    3.553676  6.048711 4.515856 5275.951590
min   279.370835 45.009287 0.059529  1.834255
max   310.219627 88.540390 30.415083 92818.691178
q025  291.794391 49.803378 1.524003  12.030316
q050  293.307724 51.831071 2.836307  28.434950
q075  295.008611 54.325024 4.755834  75.127592
```

```
> cor(MCMC$pars)
```

```
      up02      cons      ks
up02 1.0000000 0.5959491 0.3364385
cons 0.5959491 1.0000000 0.9249786
ks    0.3364385 0.9249786 1.0000000
```

Note: we pass to sensRange the full parameter vector (**parms**) and the parameters sampled during the MCMC (**parInput**).

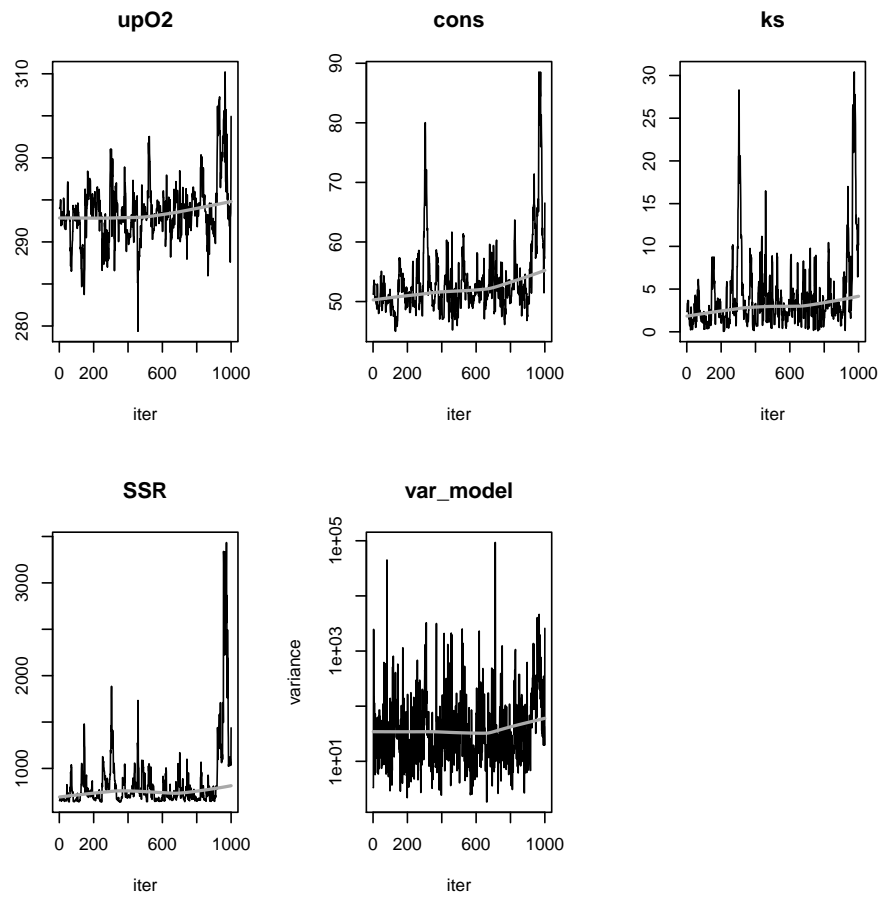


Figure 7: MCMC plot results - see text for R-code

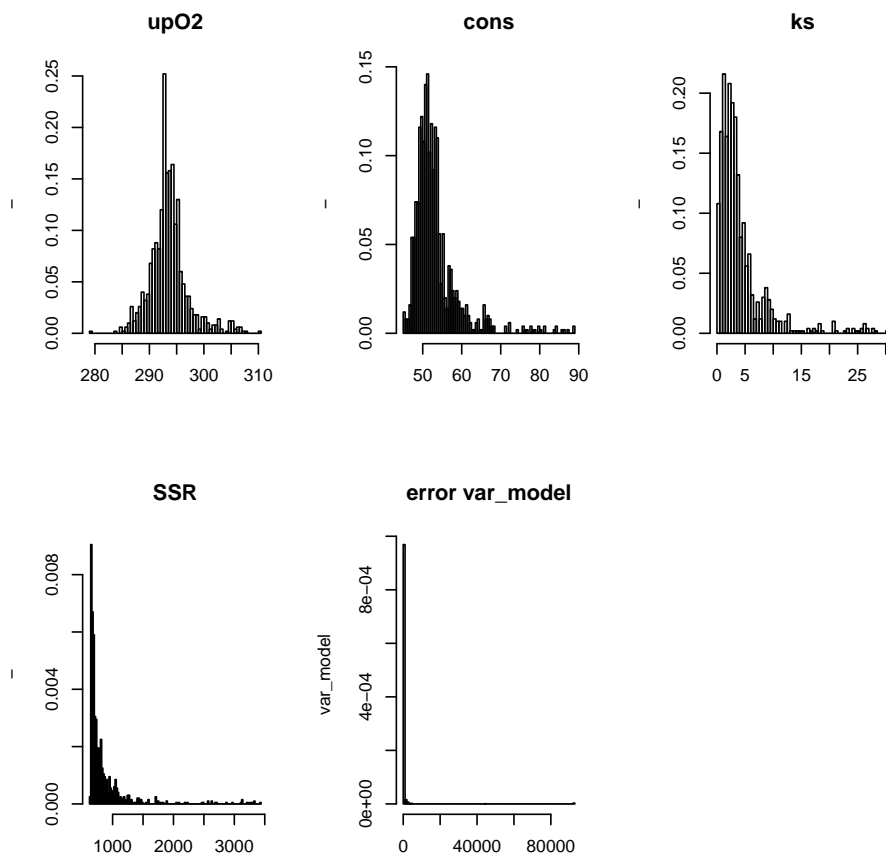


Figure 8: MCMC histogram results - see text for R-code

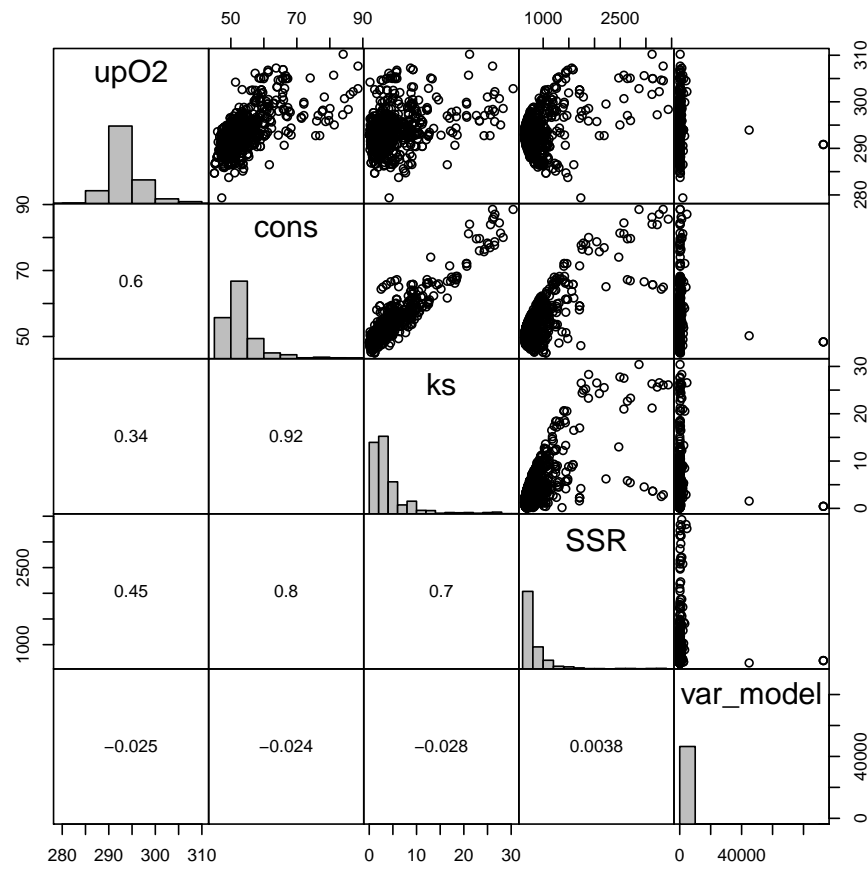


Figure 9: MCMC pairs plot - see text for R-code

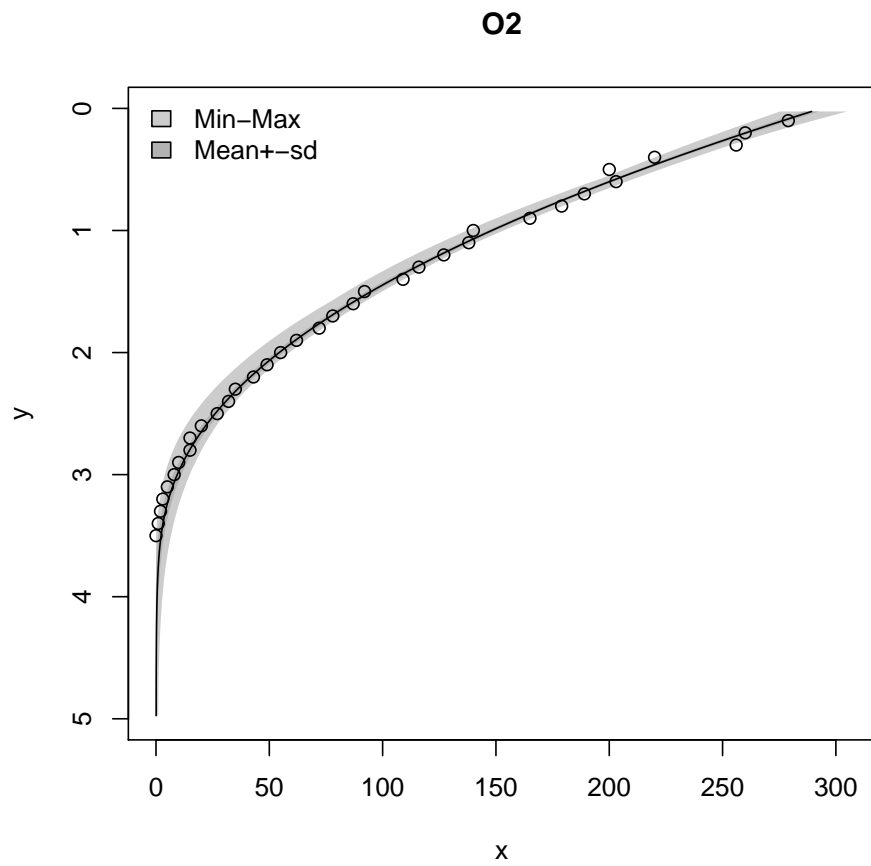


Figure 10: MCMC range plot - see text for R-code

```
> plot(summary(sensRange(parms=pars,parInput=MCMC$par,f=O2fun,num=500)),
+       xyswap=TRUE)
> points(O2depth$y,O2depth$x)
```

6. Finally

This vignette is made with Sweave (Leisch 2002).

References

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