



**National
Oceanography Centre**
NATURAL ENVIRONMENT RESEARCH COUNCIL

UNIVERSITY OF
Southampton

Using R to Model Complex Biogeochemical Systems

Chris Wood

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Introduction to the science

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- Why are we interested in sediments?
 - 71% of Earth's surface (335,258,000 km²)

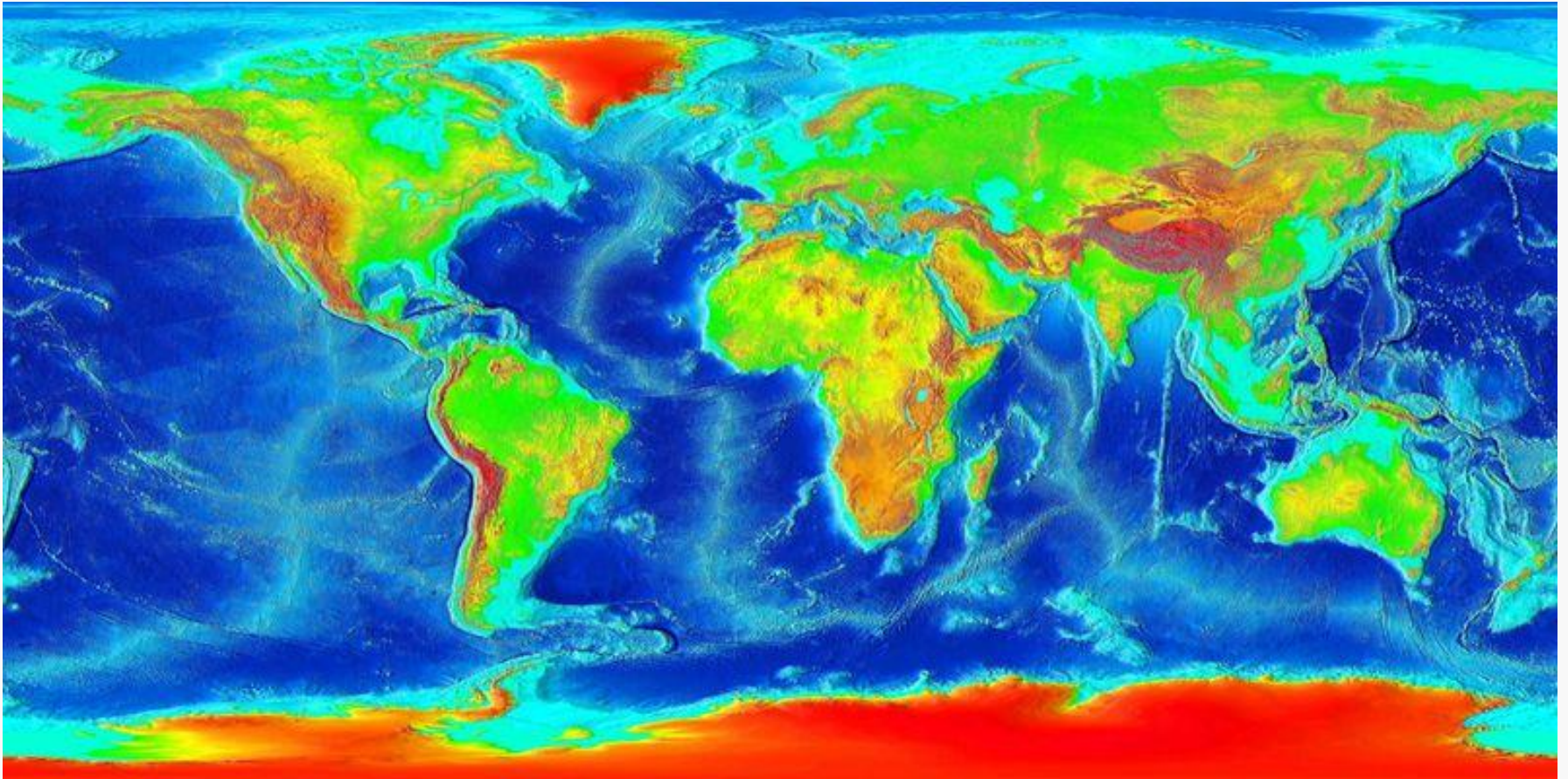
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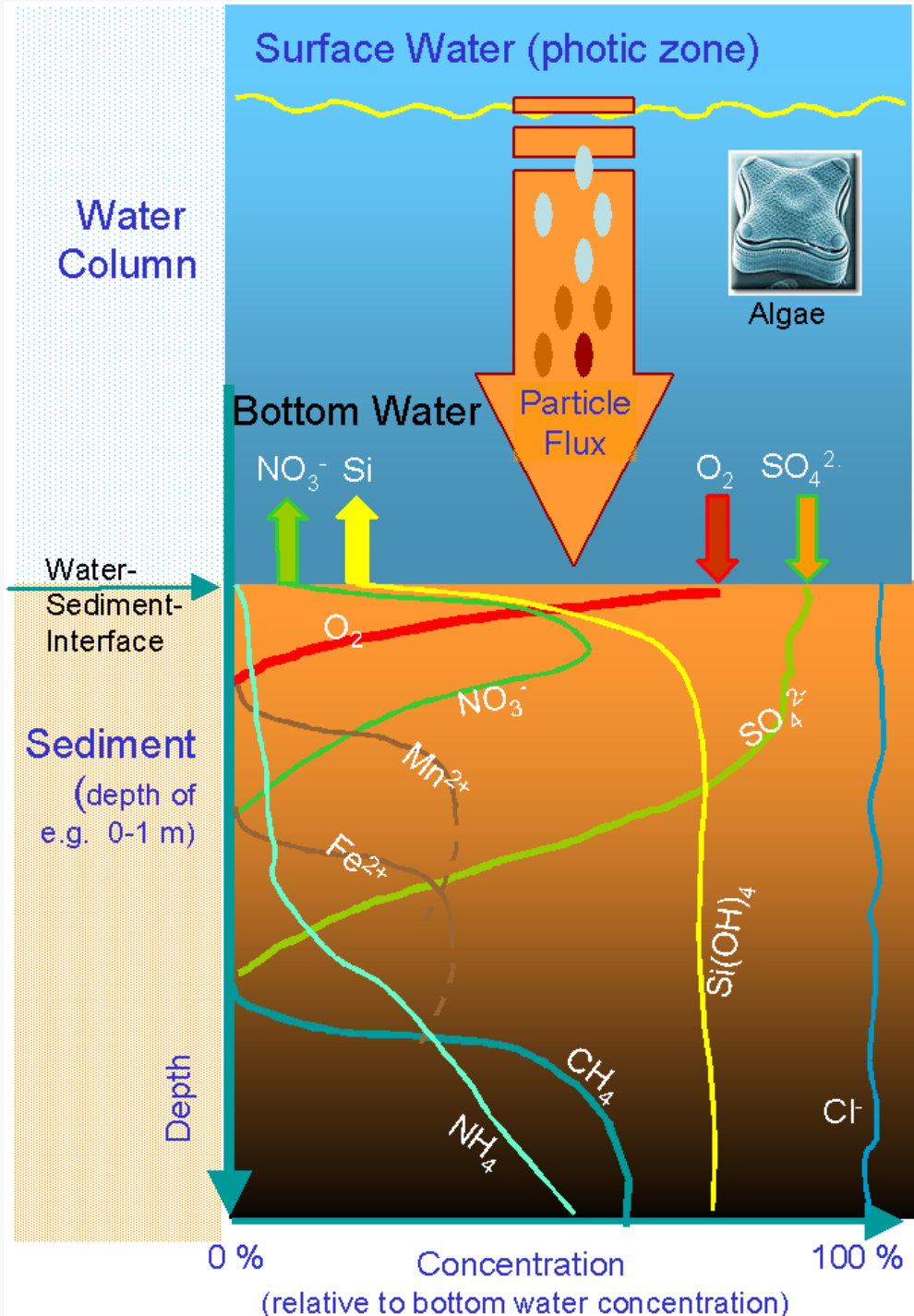


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 - High rates of primary productivity



The maths...

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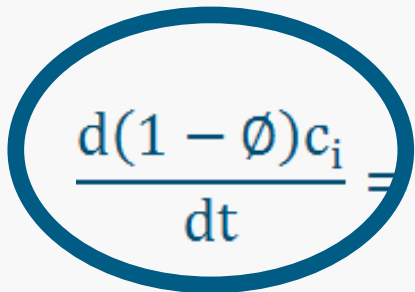
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$$\frac{d(1 - \emptyset)c_i}{dt} = \frac{\partial \left((1 - \emptyset)D_b \frac{\partial c_i}{\partial x} - \omega(1 - \emptyset)c_i \right)}{\partial x}$$

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The diagram shows a mass balance equation for a chemical species i in a porous medium. The equation is:

$$\frac{d(1 - \phi)c_i}{dt} = \frac{\partial}{\partial x} \left((1 - \phi)D_b \frac{\partial c_i}{\partial x} - \omega(1 - \phi)c_i \right)$$

Annotations in the diagram include:

- A blue oval around the left-hand side term $\frac{d(1 - \phi)c_i}{dt}$ with an arrow pointing to the text "Change in concentration of i".
- A blue oval around the $(1 - \phi)D_b$ term in the numerator of the right-hand side, with an arrow pointing to the text "Transport of chemical species".
- A blue oval around the $\omega(1 - \phi)c_i$ term in the numerator of the right-hand side, with an arrow pointing to the text "Transport of chemical species".

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$$\frac{d(1 - \phi)c_i}{dt} = \frac{\partial}{\partial x} \left((1 - \phi)D_b \frac{\partial c_i}{\partial x} - \omega(1 - \phi)c_i \right) - (1 - \phi)\Sigma(R(c_i, c_j))$$

Change in concentration of i

Transport of chemical species

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Annotations with arrows pointing to specific parts of the equation:

- Change in concentration of i** : Points to the left-hand side term $\frac{d(1 - \phi)c_i}{dt}$.
- Transport of chemical species**: Points to the divergence term $\frac{\partial}{\partial x} \left((1 - \phi)D_b \frac{\partial c_i}{\partial x} - \omega(1 - \phi)c_i \right)$.
- Rate of consumption of i , but dependent on j** : Points to the reaction term $(1 - \phi)\sum_j R(c_i, c_j)$.

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- Oxidic breakdown of organic matter:

$$R_{O_2} = \kappa[OM] \left(\frac{[O_2]}{[O_2] + \kappa S_{oxic}} \right)$$

Transport

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- `Grid <- setup.grid.1D(N=100,dx.1=0.1,L=15)`
 - `Grid$x.mid, Grid$x.int, Grid$dx`
- `O2tran <- tran.1D (C=O2, C.up=bwO2, dx=Grid)`
 - **Other arguments allow specific transport terms to be used**

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 - rootSolve: ‘Nonlinear root finding, equilibrium and steady-state analysis of ordinary differential equations’
 - deSolve: ‘General solvers for initial value problems of ordinary differential equations (ODE), partial differential equations (PDE), differential algebraic equations (DAE), and delay differential equations (DDE).’

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```
modelFunction <- function(t, y, pars){  
  #implementation of transport and differential  
  #equations; e.g:  
  OC <- y[1:100]; O2 <- y[101:200]  
  oxicMin <- r*OC*(O2/(O2+ksO2oxic))  
}
```


Solving the maths (cont...)

– Simple to implement

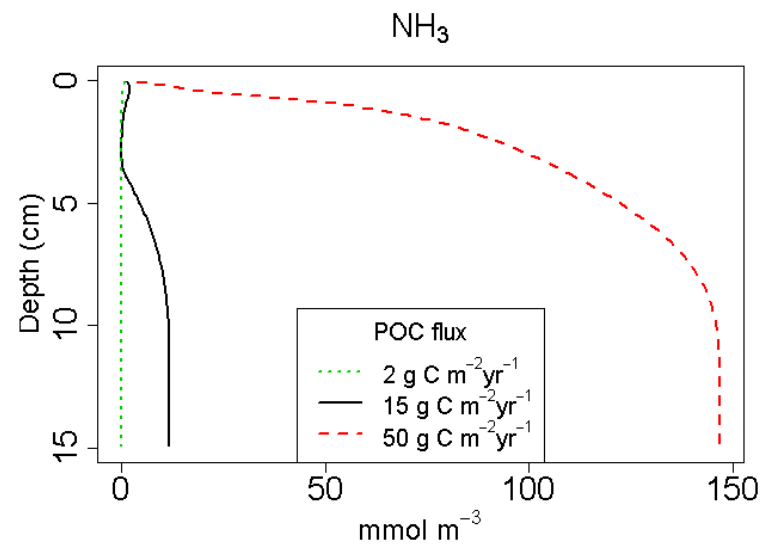
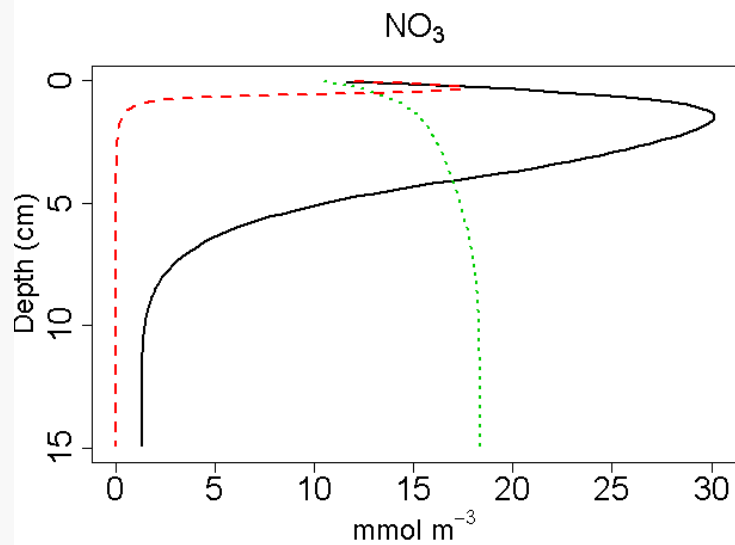
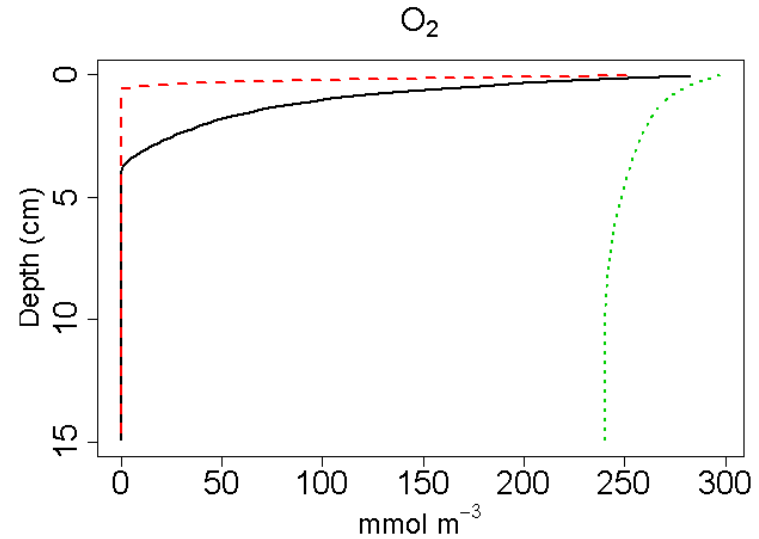
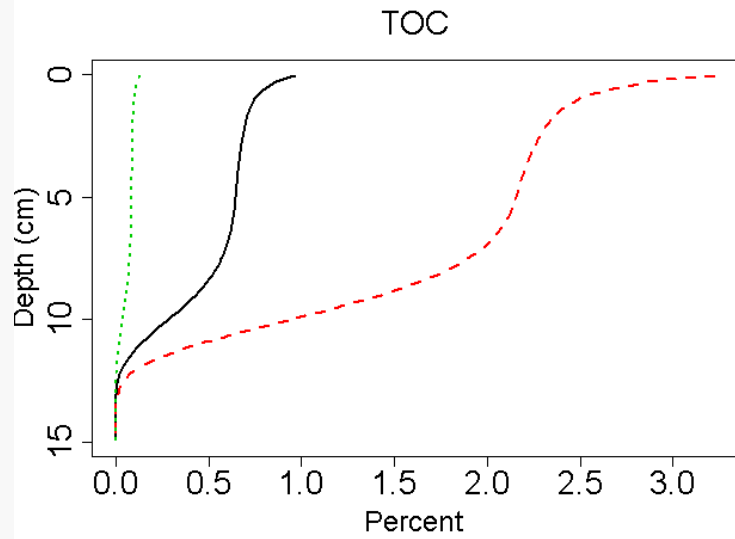
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}  
  
ss.output <- steady.1D(y=rep(10,2*100),  
  func=modelFunction, parms=c(r=10, ksO2oxic=1))
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Solving the maths (cont...)

– Simple to implement

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modelFunction <- function(t, y, pars){  
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  oxicMin <- r*OC*(O2/(O2+ksO2oxic))  
}  
  
ss.output <- steady.1D(y=rep(10,2*100),  
  func=modelFunction, parms=c(r=10, ksO2oxic=1))  
  
dyn.output <- ode.1D(y=ss.output$y, times=0:364,  
  func=modelFunction, parms=pars)
```

Output

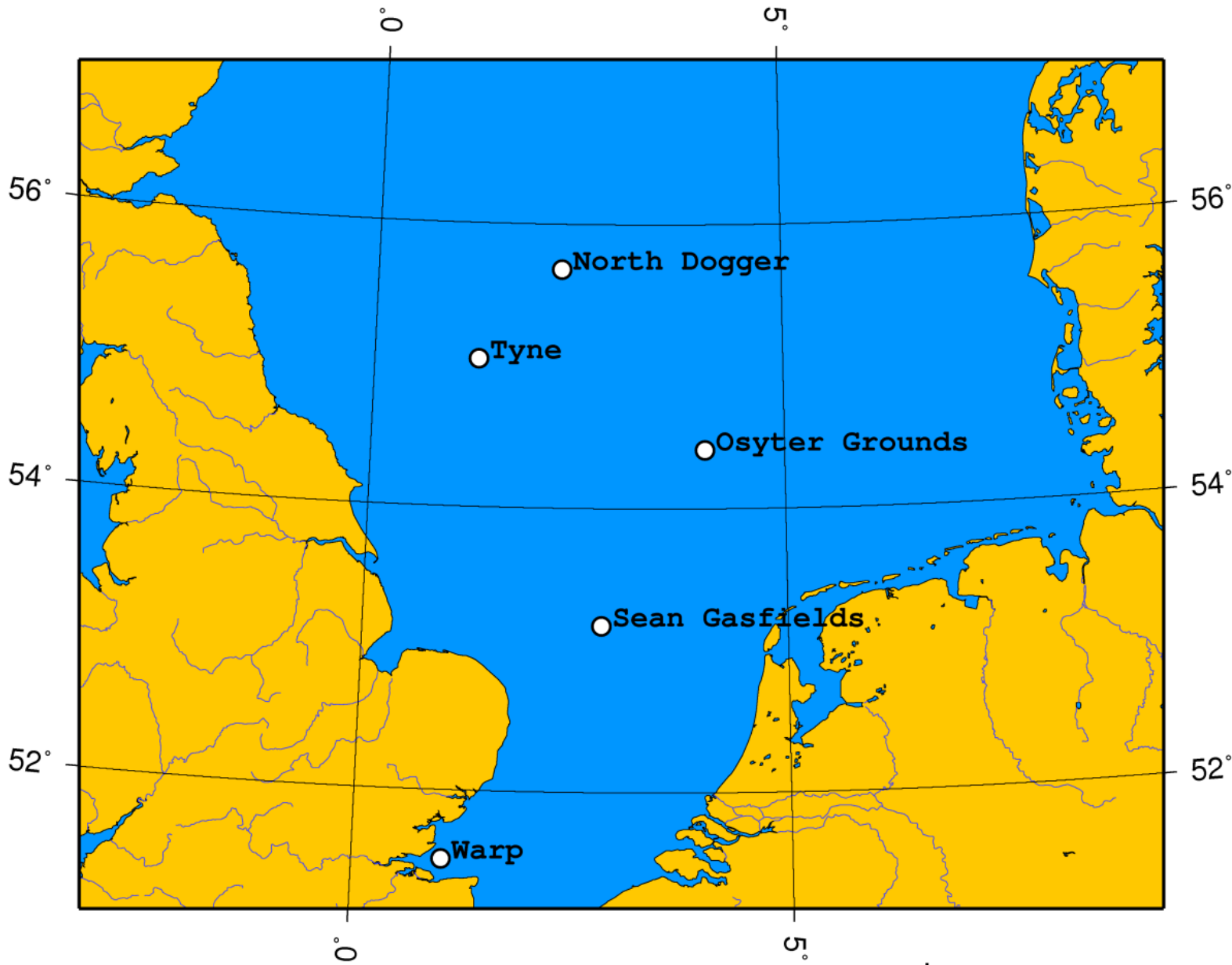




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Data management

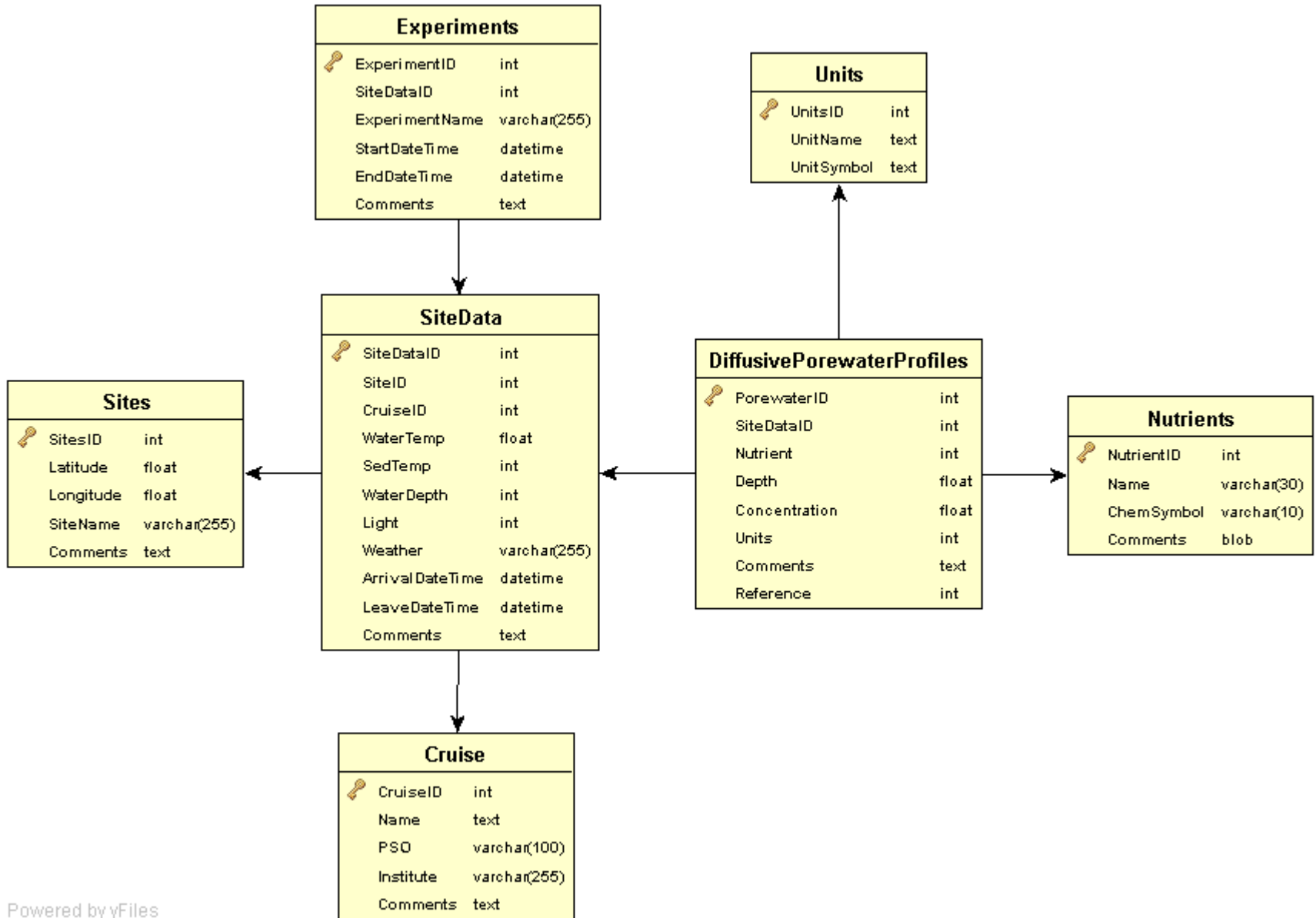
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 - Multiple sites, cruises, repeat measurements & parameters



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Data management

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- R + MySQL (+ RJDBC/rJava)

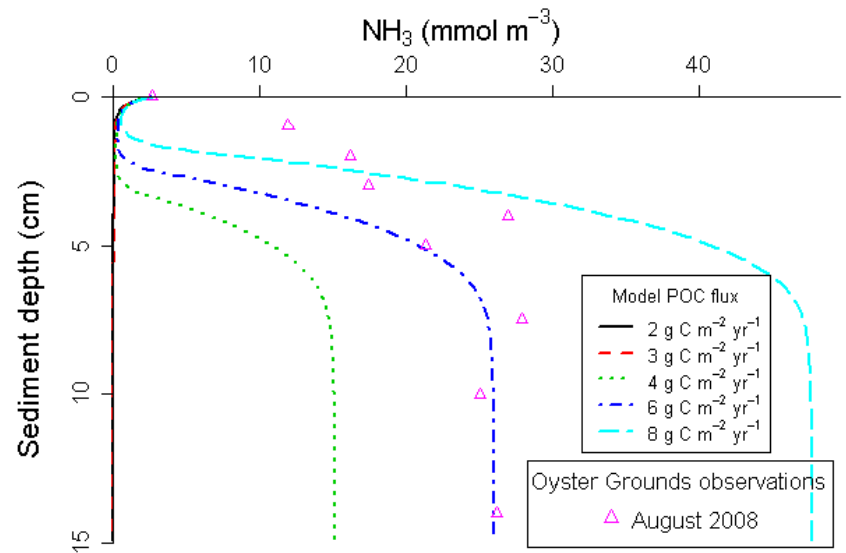
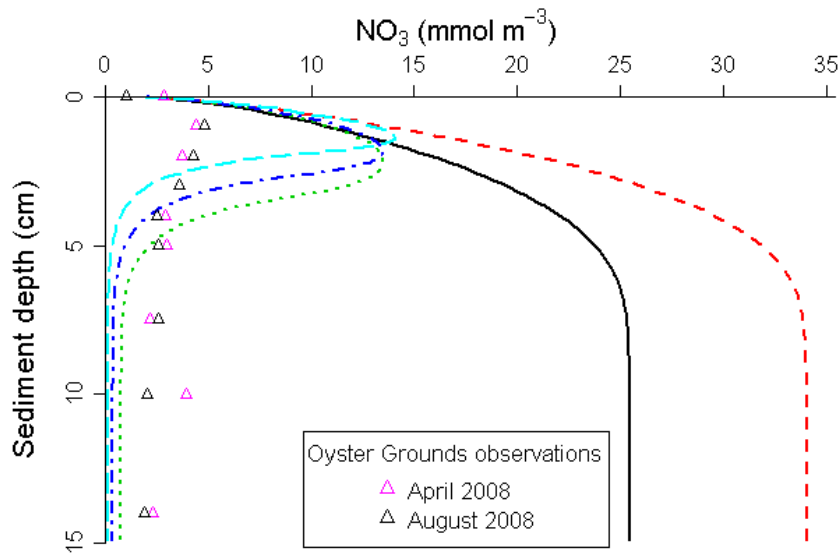
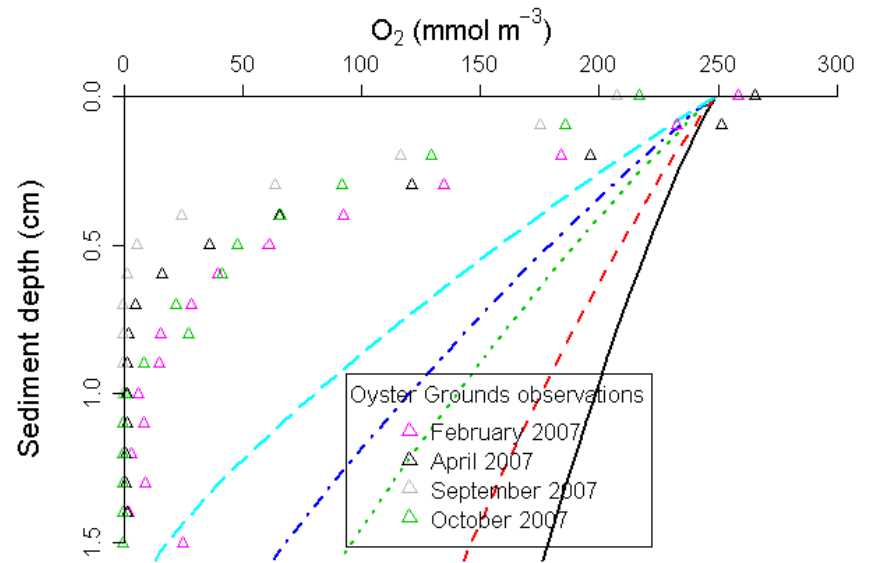
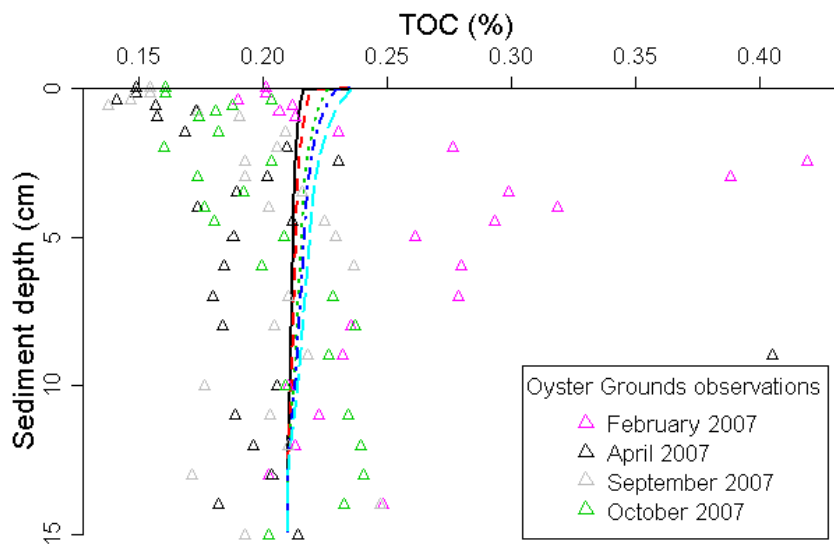


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- Post-processing / data consistency checking carried out in R
- Allows model calibration to be carried out



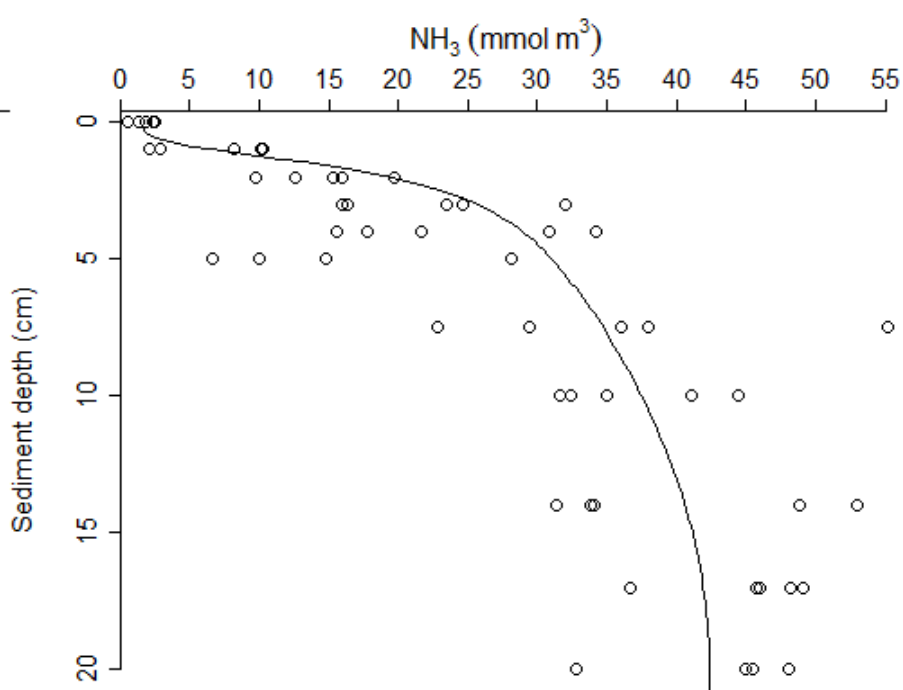
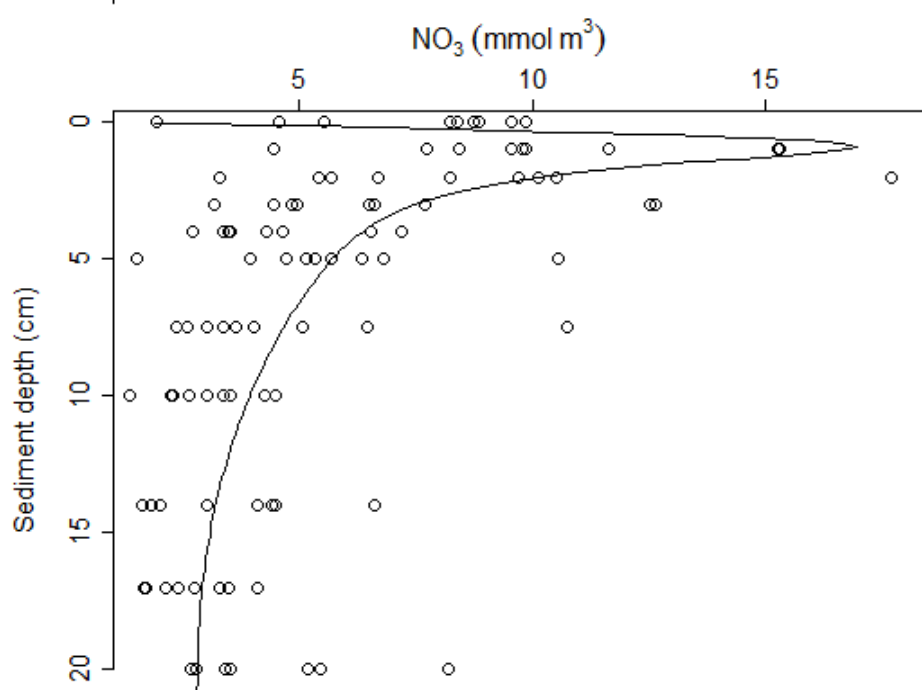
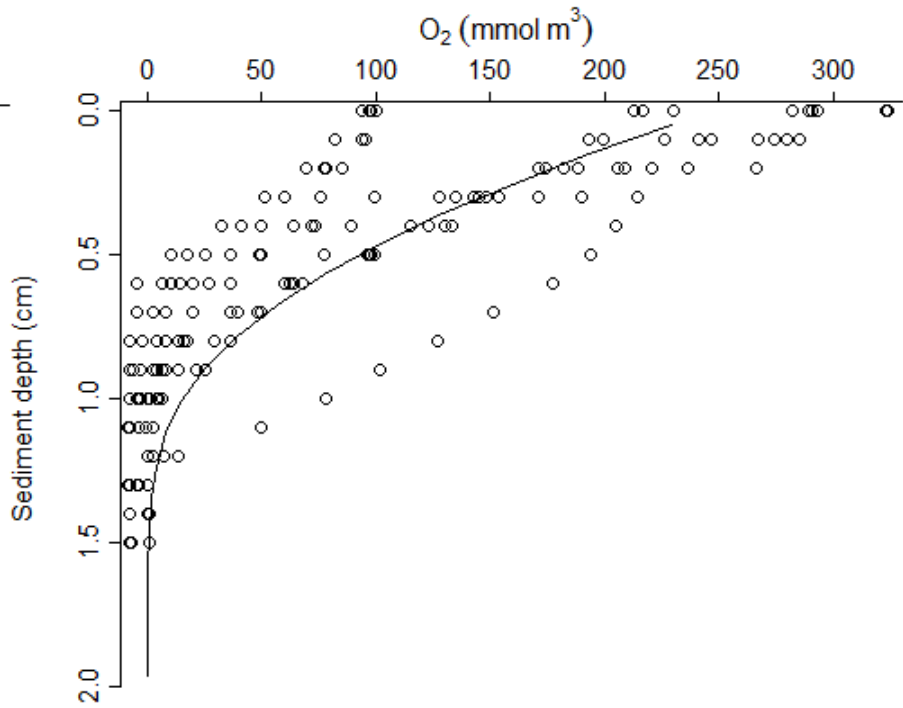
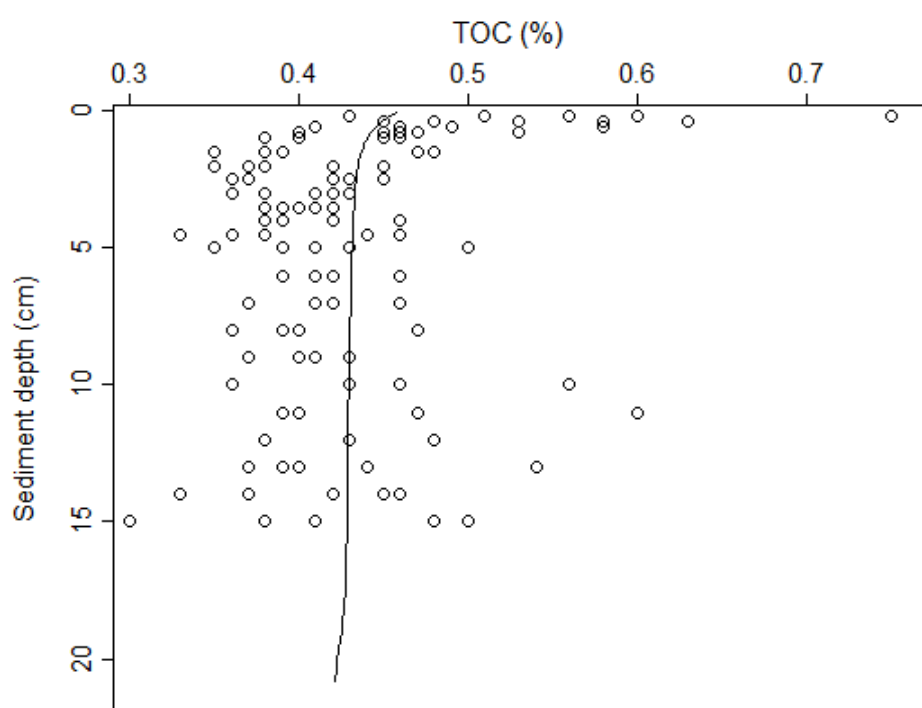
Model testing & model calibration

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 - Allows us to discover the most sensitive model parameters

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- Sensitivity analysis
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- Genetic algorithm
 - (Relatively) efficient method of making model output fit real data



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 - Public engagement of science

Any questions?

▪ Acknowledgements:

- Funding: **NERC & Defra**
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 - Keith Weston
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