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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  - 71% of Earth's surface (335,258,000 km^2)

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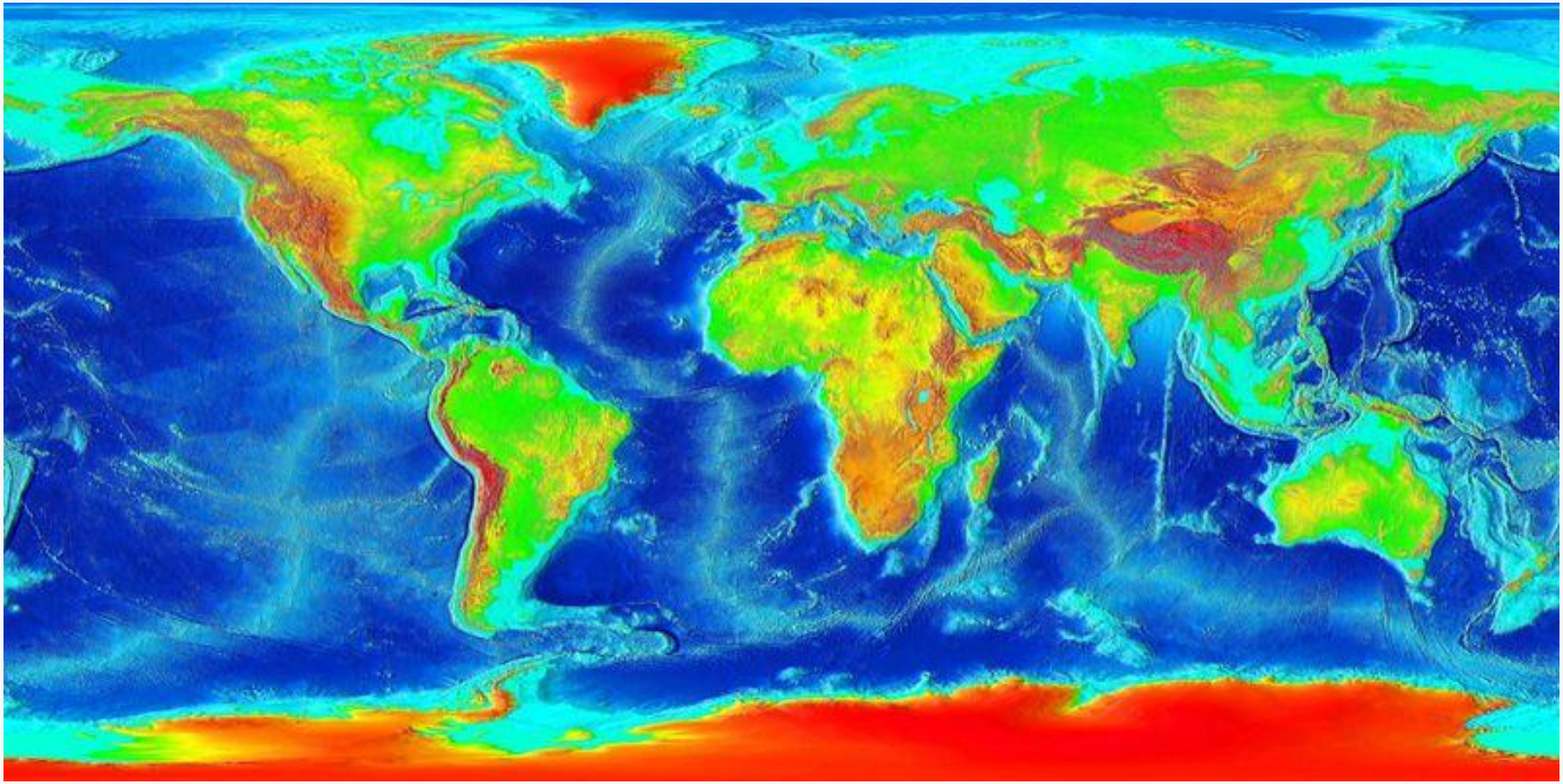

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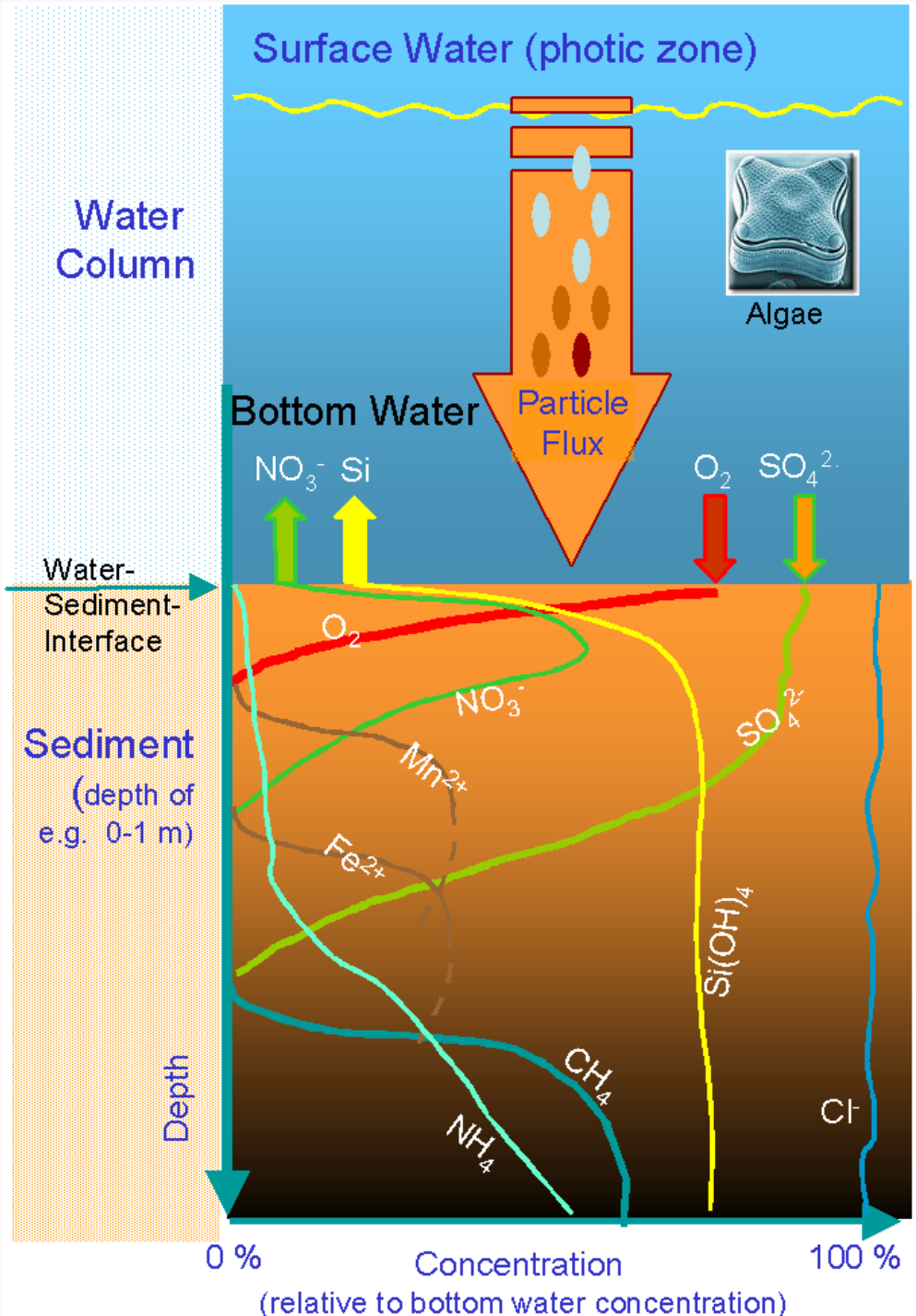
  - Globally important sinks & sources for nutrients
  - High rates of primary productivity


Surface Water (photic zone)
Water Column
Algae
Particle Flux
Bottom Water
NO_3^- Si
O_2 SO_4^{2-}
Water-Sediment-Interface
Sediment
(depth of e.g. 0-1 m)
O_2
NO_3^-
Mn^{2+}
Fe^{2+}
SO_4^{2-}
$Si(OH)_4$
CH_4
NH_4
Cl^-
Depth
0 %
Concentration
(relative to bottom water concentration)
100 %

The maths…

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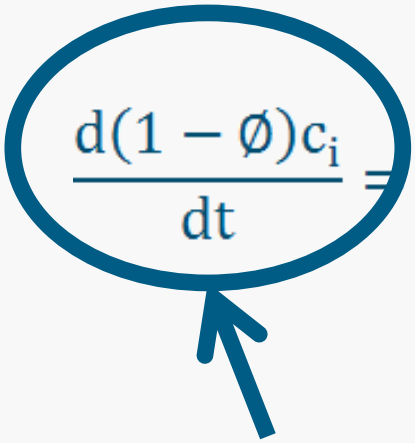

Change in concentration of i

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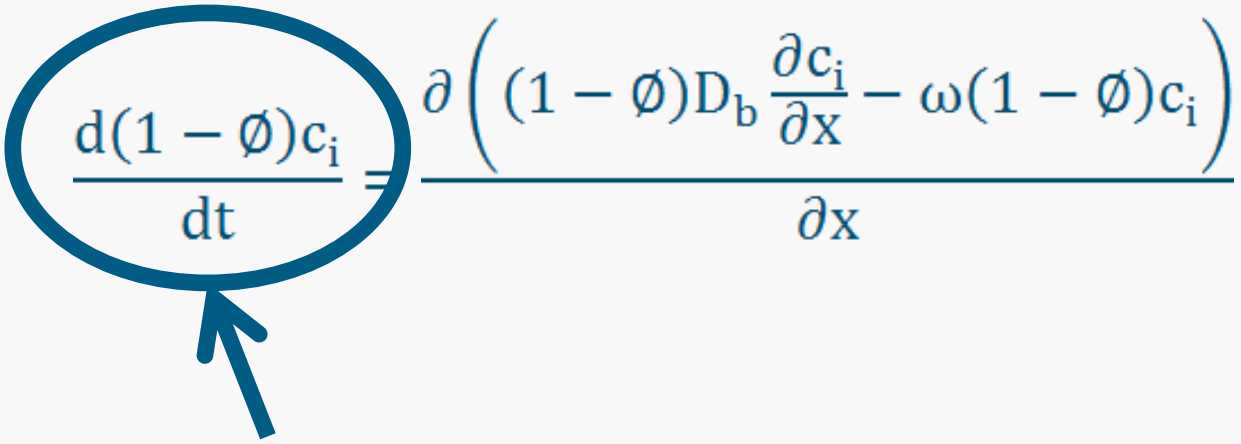

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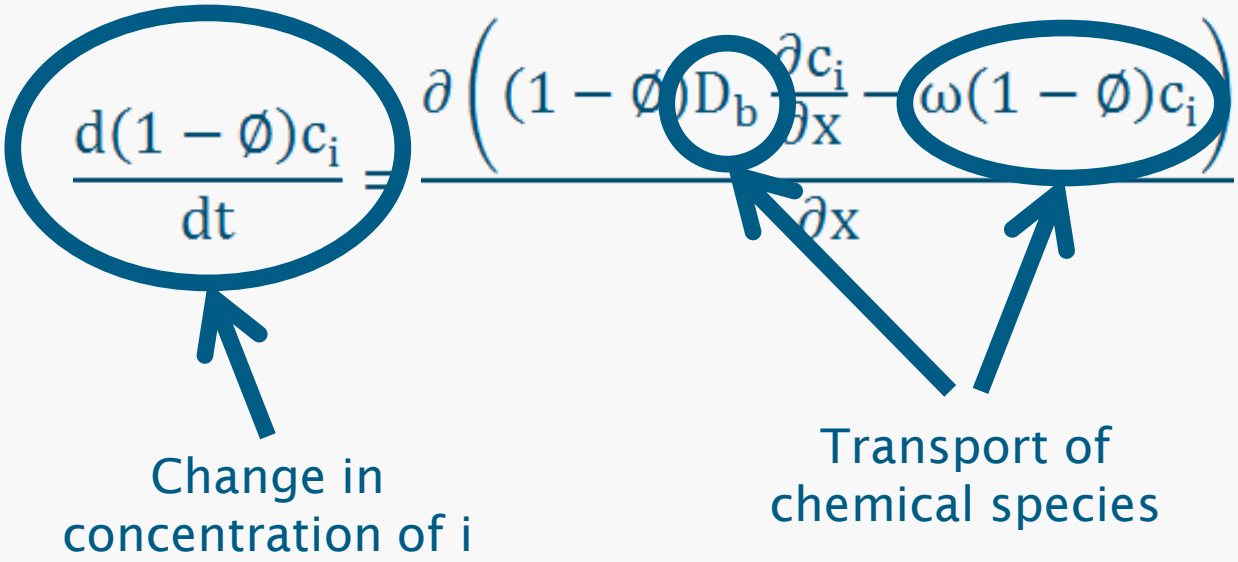

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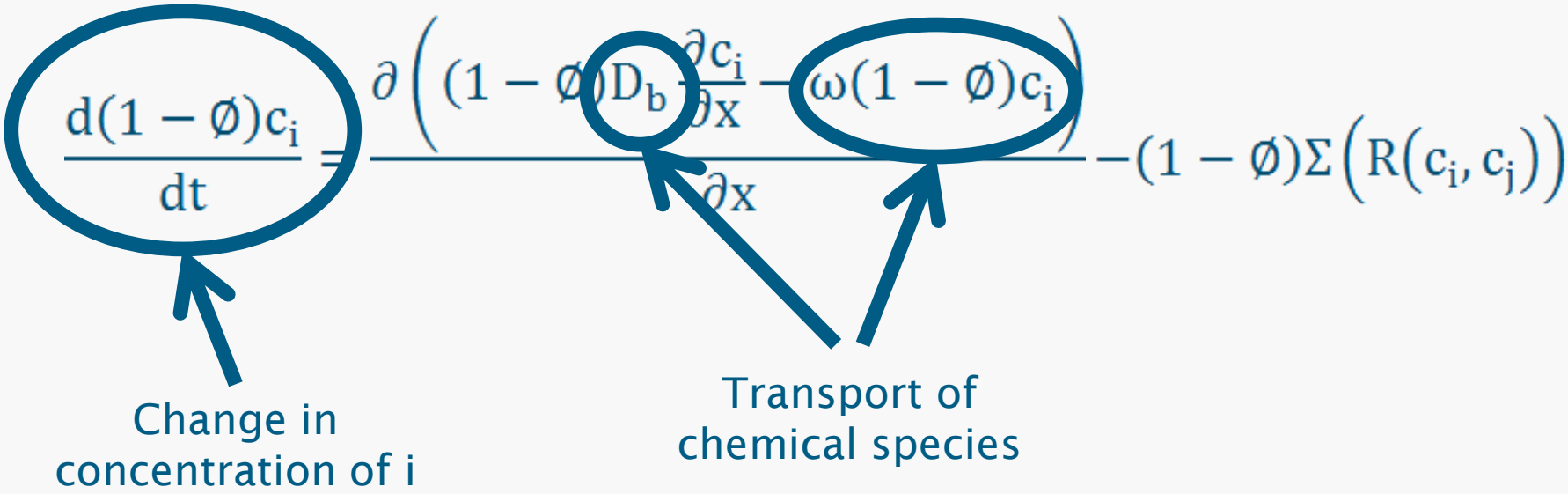

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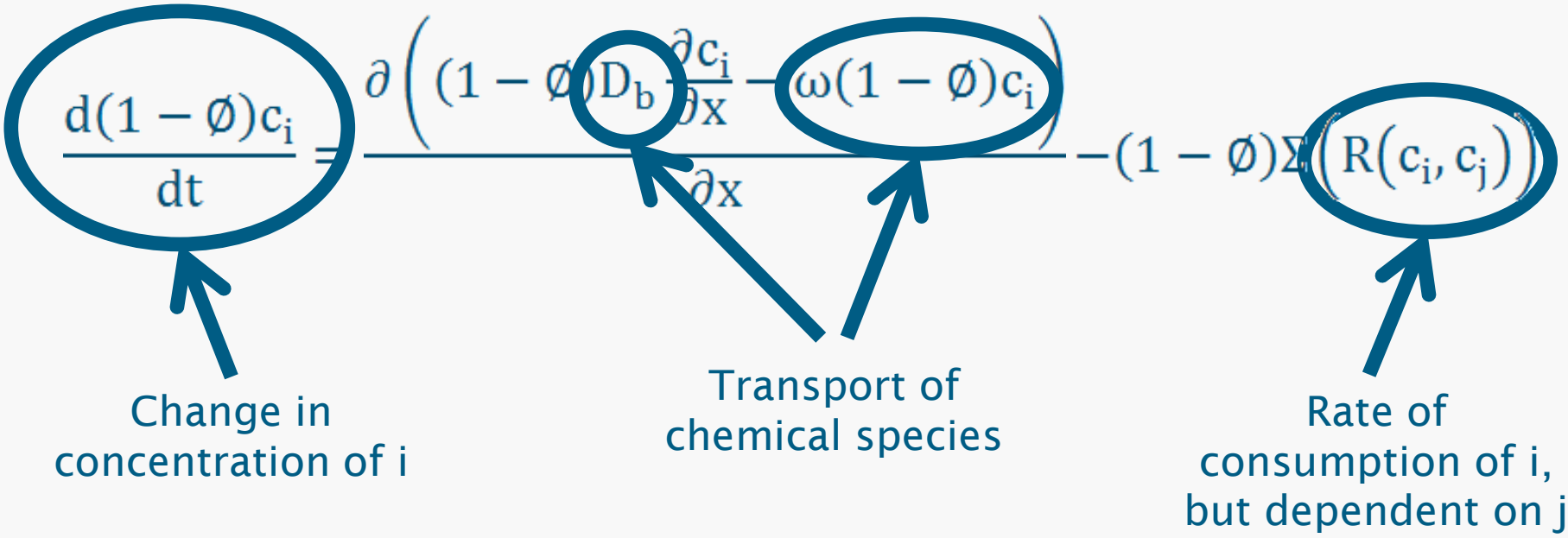

The maths…

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

- Oxic breakdown of organic matter:

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- Oxic breakdown of organic matter:

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

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

Solving the maths

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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).'

Solving the maths (cont…)

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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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modelFunction <- function(t, y, pars){
   #implementation of transport and differential
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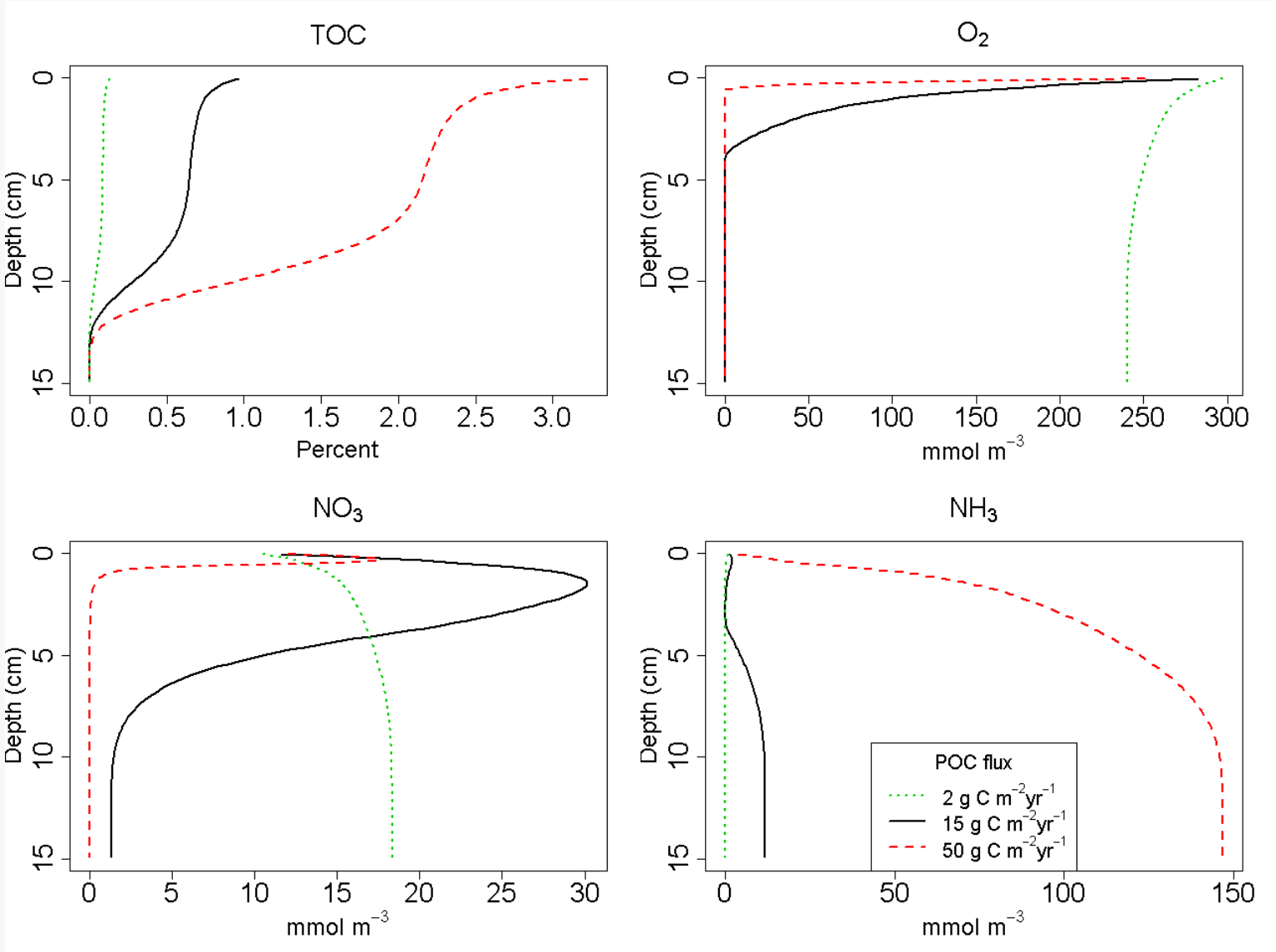
   OC <- y[1:100]; O2 <- y[101:200]
   oxicMin <- r*OC*(O2/(O2+ksO2oxic))
}
ss.output <- steady.1D(y=rep(10,2*100),
   func=modelFunction, parms=c(r=10, ksO2oxic=1))
```

Solving the maths (cont…)

- Simple to implement

```
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))
}
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


TOC
Depth (cm)
0
5
10
15
0.0
0.5
1.0
1.5
2.0
2.5
3.0
Percent
O_2
0
50
100
150
200
250
300
mmol m^{-3}
NO_3
0
5
10
15
20
25
30
mmol m^{-3}
NH_3
0
50
100
150
mmol m^{-3}
POC flux
2 g C $m^{-2}yr^{-1}$
15 g C $m^{-2}yr^{-1}$
50 g C $m^{-2}yr^{-1}$


CEFAS ENDEAVOUR
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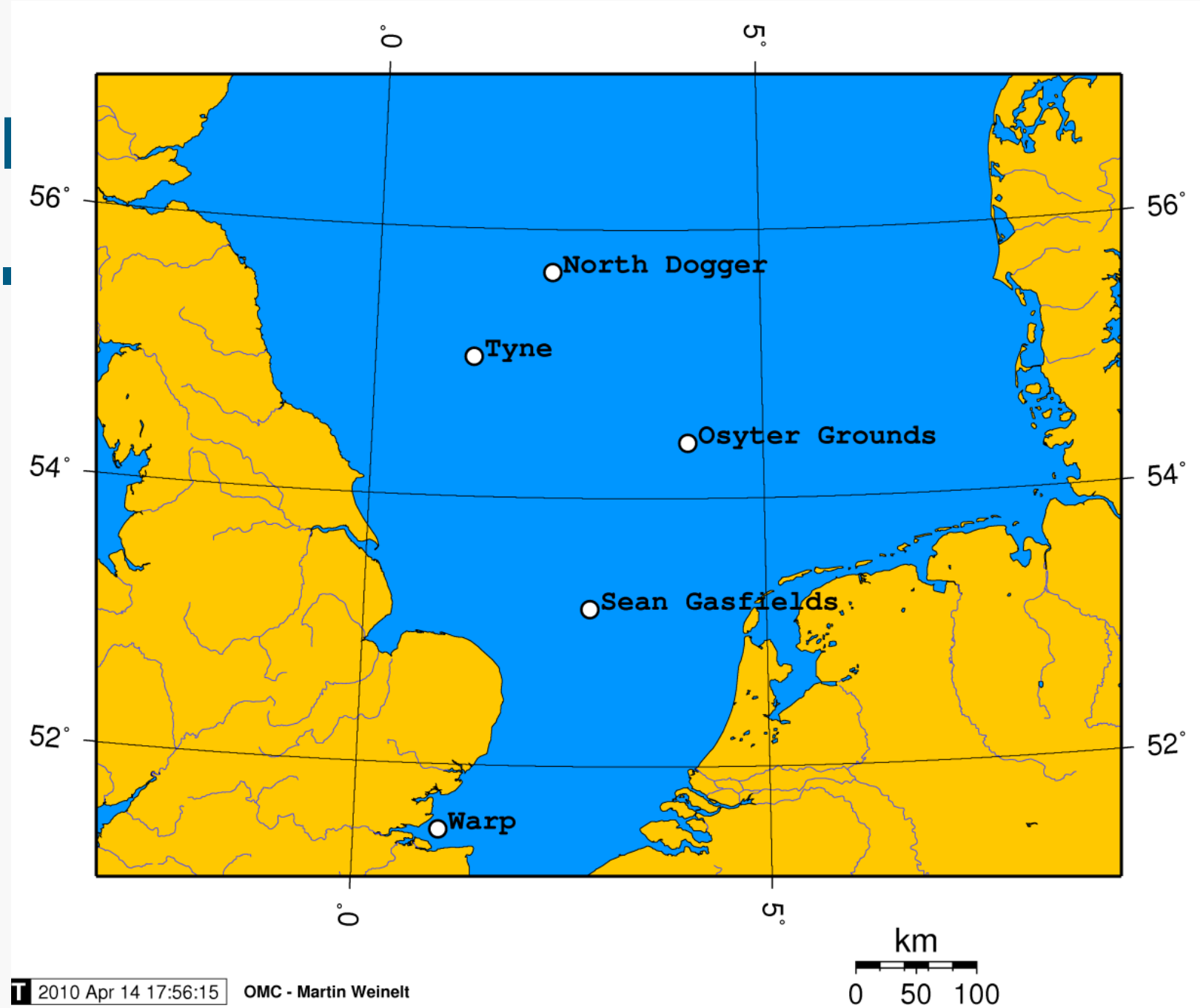
Data management

- Data
  - Multiple sites, cruises, repeat measurements & parameters


0°
5°
56°
54°
52°
North Dogger
Tyne
Osyter Grounds
Sean Gasfields
Warp
km
0 50 100
2010 Apr 14 17:56:15
OMC - Martin Weinelt

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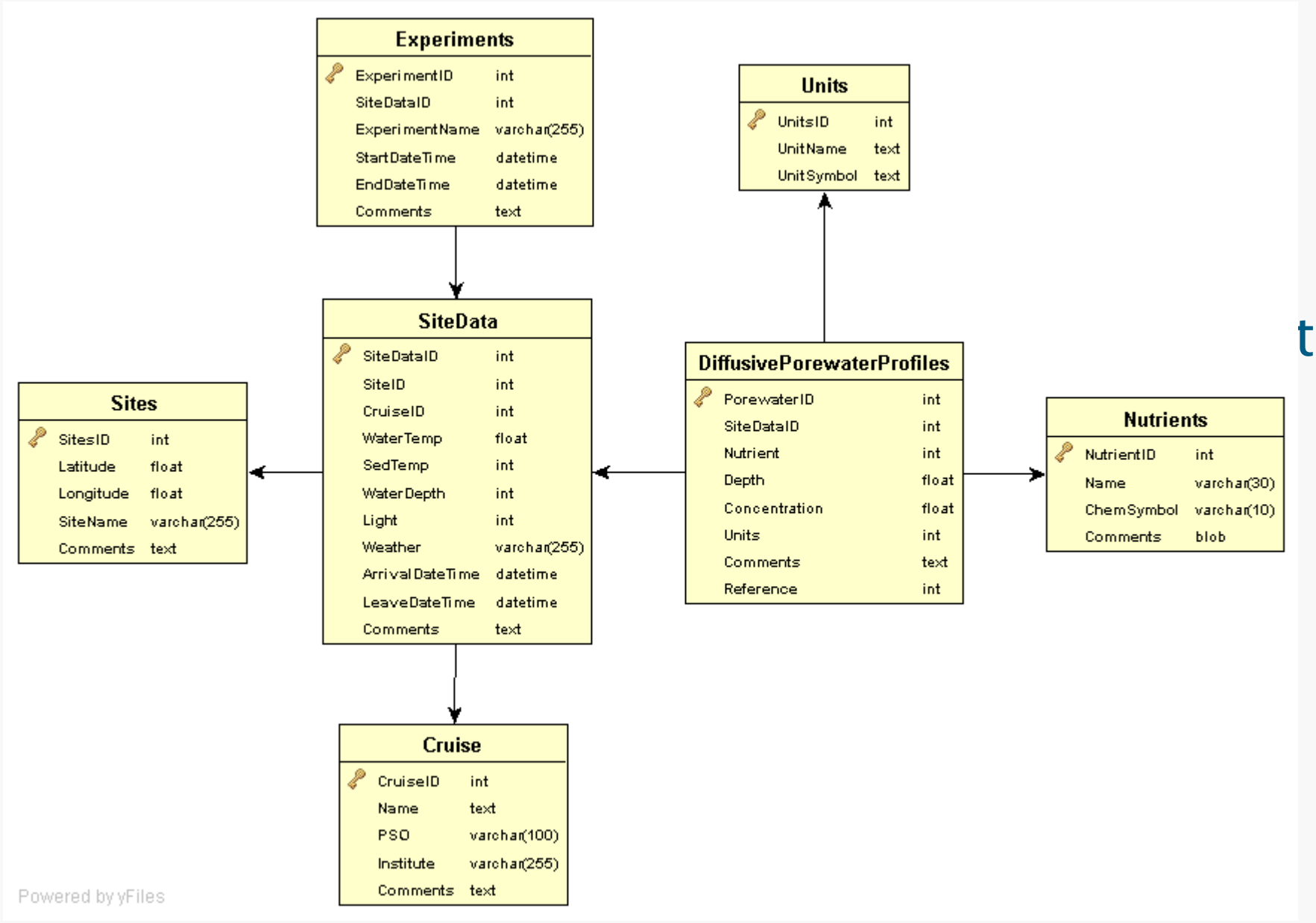
- R + MySQL (+ RJDBC/rJava)


Experiments
ExperimentID int
SiteDataID int
ExperimentName varchar(255)
StartDateTime datetime
EndDateTime datetime
Comments text
Units
UnitsID int
UnitName text
UnitSymbol text
SiteData
SiteDataID int
SiteID int
CruiseID int
WaterTemp float
SedTemp int
WaterDepth int
Light int
Weather varchar(255)
ArrivalDateTime datetime
LeaveDateTime datetime
Comments text
DiffusivePorewaterProfiles
PorewaterID int
SiteDataID int
Nutrient int
Depth float
Concentration float
Units int
Comments text
Reference int
Sites
SitesID int
Latitude float
Longitude float
SiteName varchar(255)
Comments text
Nutrients
NutrientID int
Name varchar(30)
ChemSymbol varchar(10)
Comments blob
Cruise
CruiseID int
Name text
PSO varchar(100)
Institute varchar(255)
Comments text
Powered by yFiles

ts

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- Post-processing / data consistency checking carried out in R

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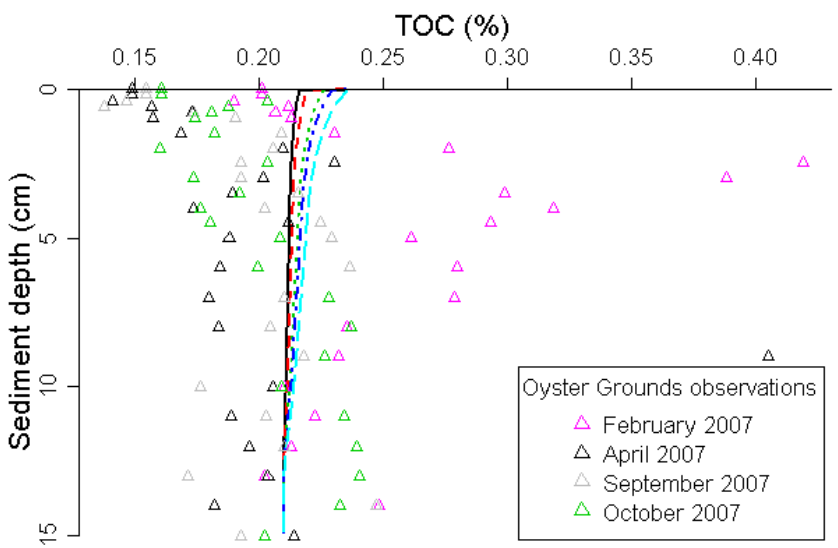
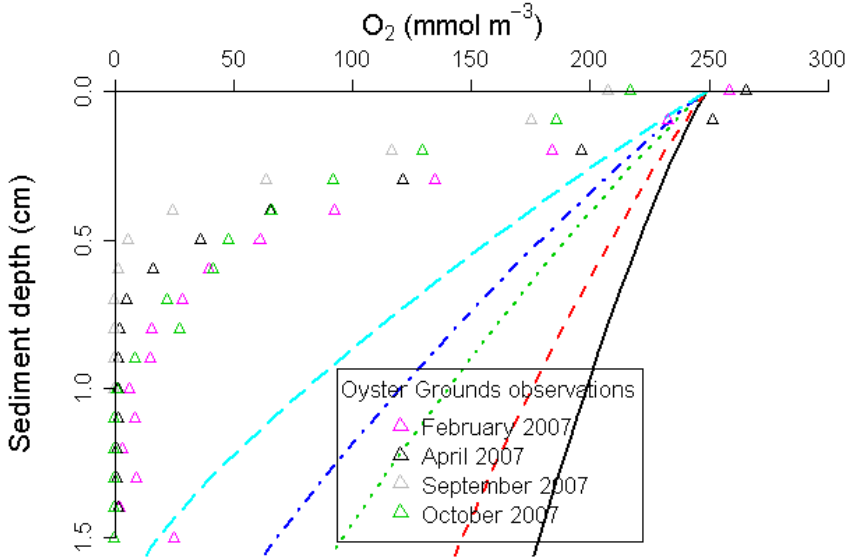
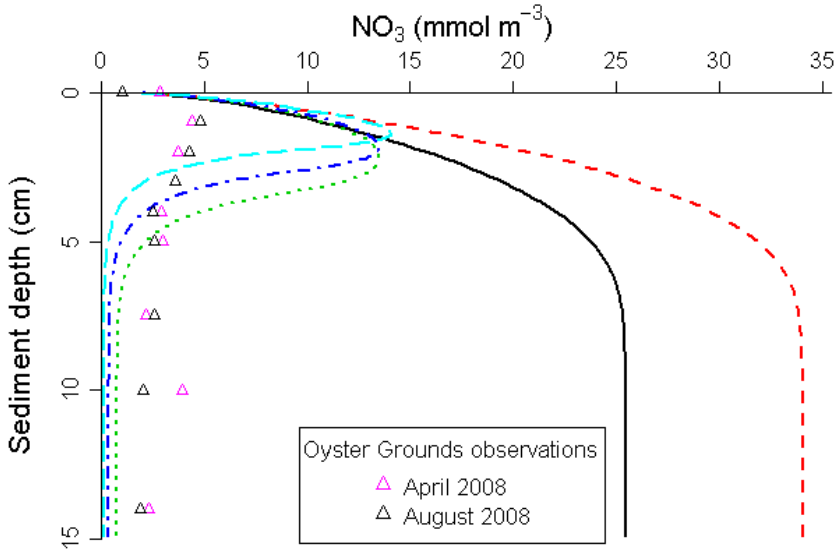
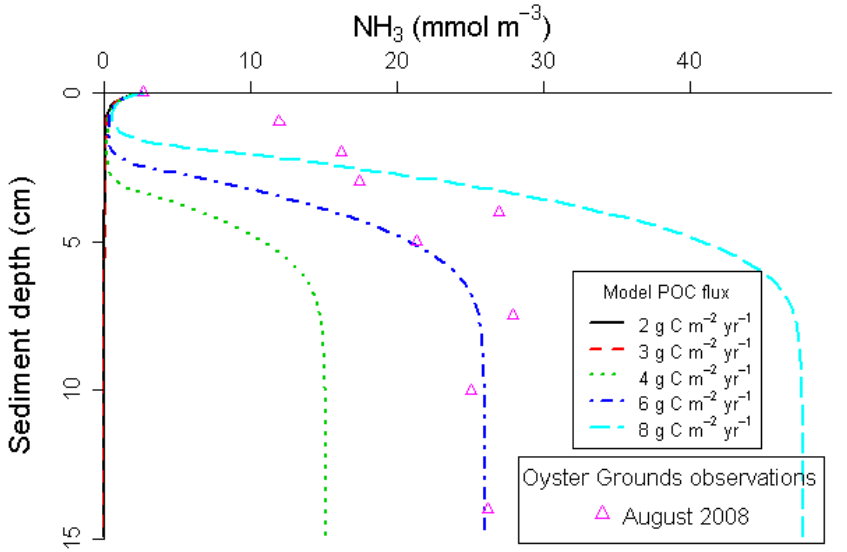
- Post-processing / data consistency checking carried out in R
- Allows model calibration to be carried out


TOC (%)
0.15
0.20
0.25
0.30
0.35
0.40
Sediment depth (cm)
0
5
10
15
Oyster Grounds observations
February 2007
April 2007
September 2007
October 2007


O2 (mmol m−3)
0
50
100
150
200
250
300
Sediment depth (cm)
0.0
0.5
1.0
1.5
Oyster Grounds observations
February 2007
April 2007
September 2007
October 2007


NO3 (mmol m−3)
0
5
10
15
20
25
30
35
Sediment depth (cm)
0
5
10
15
Oyster Grounds observations
April 2008
August 2008


NH3 (mmol m−3)
0
10
20
30
40
Sediment depth (cm)
0
5
10
15
Model POC flux
2 g C m−2 yr−1
3 g C m−2 yr−1
4 g C m−2 yr−1
6 g C m−2 yr−1
8 g C m−2 yr−1
Oyster Grounds observations
August 2008

Model testing & model calibration

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- Sensitivity analysis
  - Allows us to discover the most sensitive model parameters

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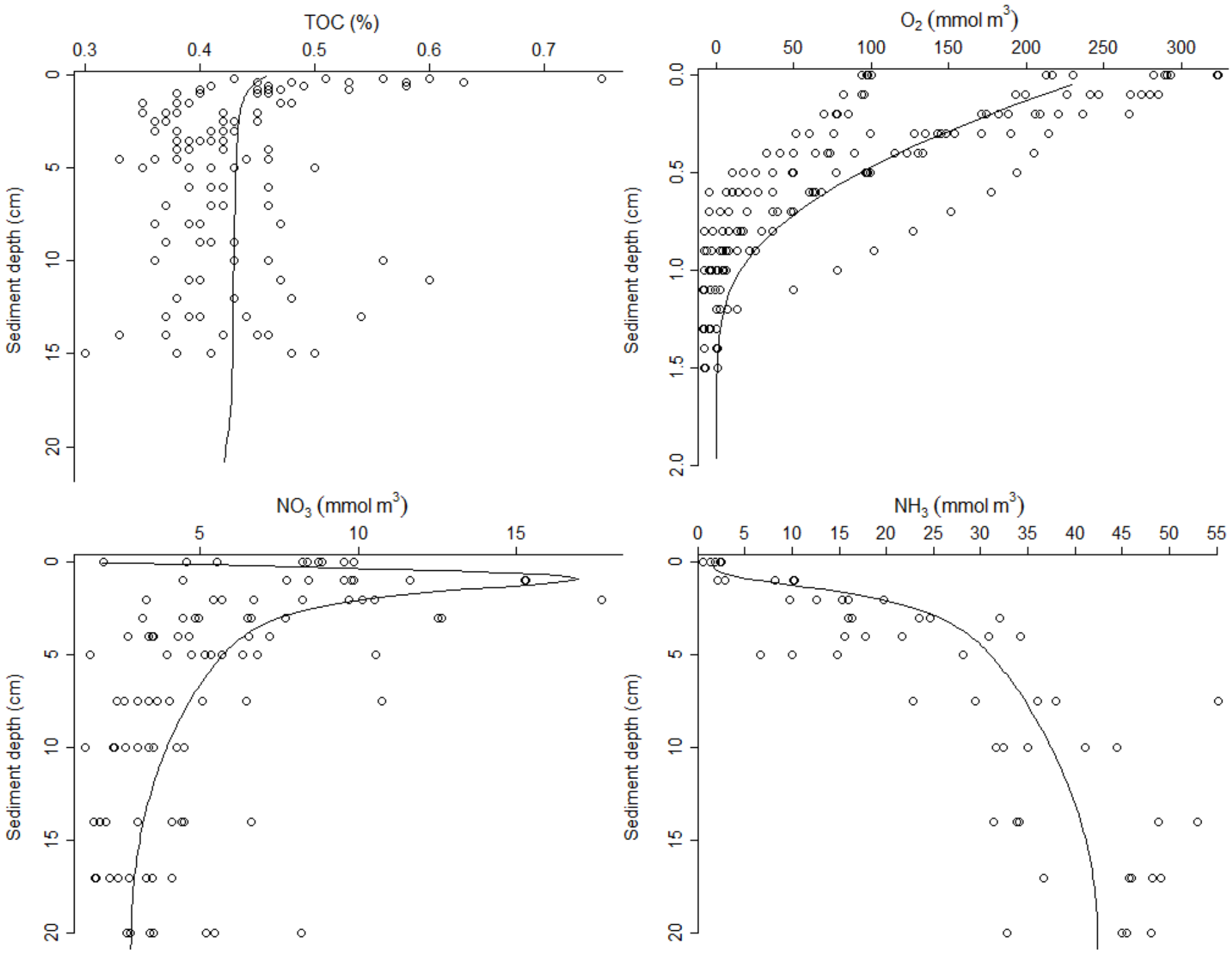
  - Allows us to discover the most sensitive model parameters
- Genetic algorithm
  - (Relatively) efficient method of making model output fit real data


TOC (%)
0.3
0.4
0.5
0.6
0.7
Sediment depth (cm)
0
5
10
15
20
O_2 (mmol m^3)
0
50
100
150
200
250
300
Sediment depth (cm)
0.0
0.5
1.0
1.5
2.0
NO_3 (mmol m^3)
5
10
15
Sediment depth (cm)
0
5
10
15
20
NH_3 (mmol m^3)
0
5
10
15
20
25
30
35
40
45
50
55
Sediment depth (cm)
0
5
10
15
20

Future ideas / personal interests

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  - Public engagement of science

Any questions?

- Acknowledgements:
  - Funding: **NERC** & **Defra**
  - University of Southampton
    - Boris Kelly-Gerreyn, Peter Statham, Adrian Martin, Andy Yool, John Hemmings, Charlie Thompson, Carl Amos
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  - University of Portsmouth
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  - Cefas
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  - UEA
    - Keith Weston
  - Partrac Ltd
    - Kevin Black, Rachel Helsby
  - Crew of *Cefas Endeavour*