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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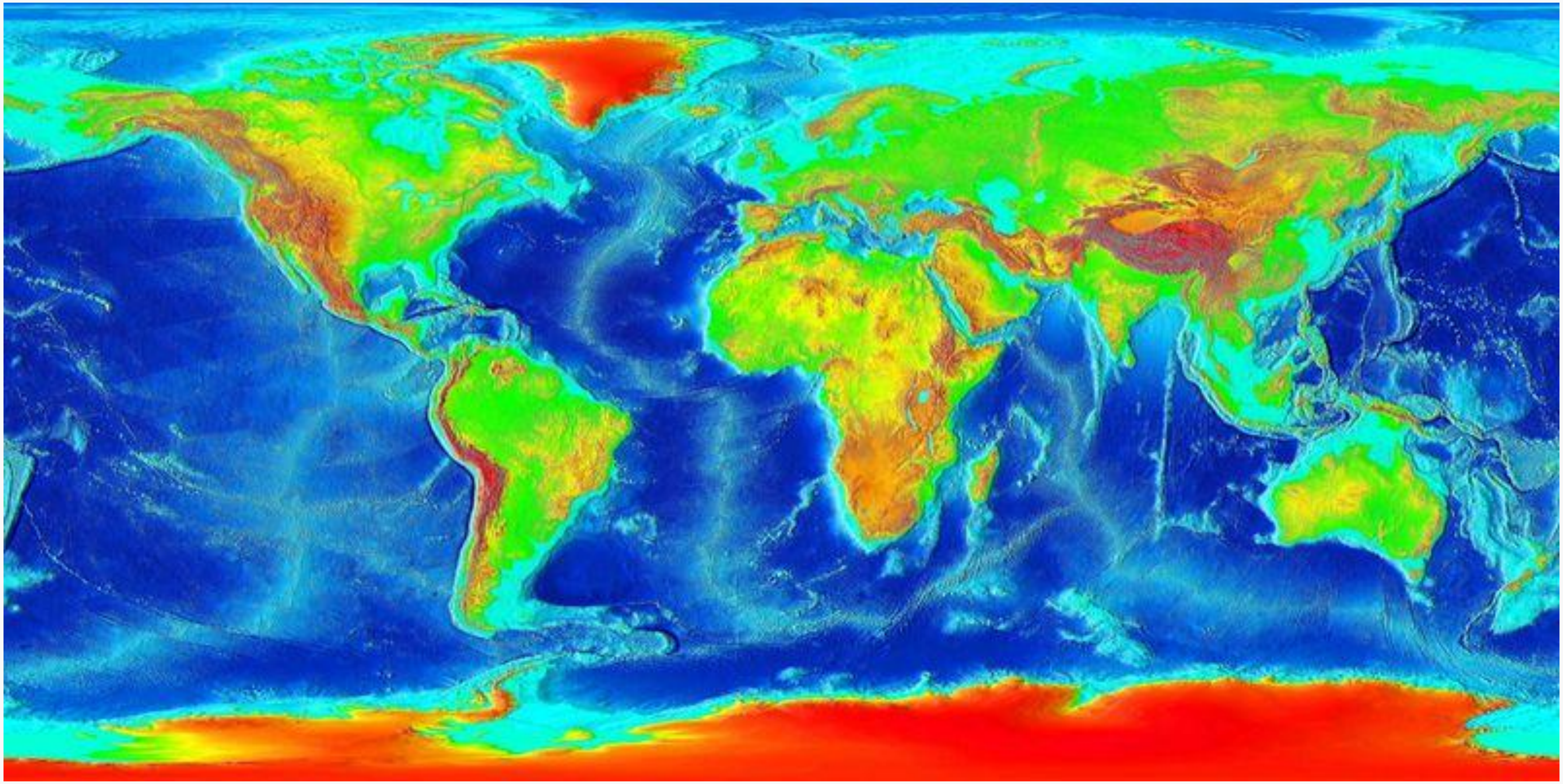

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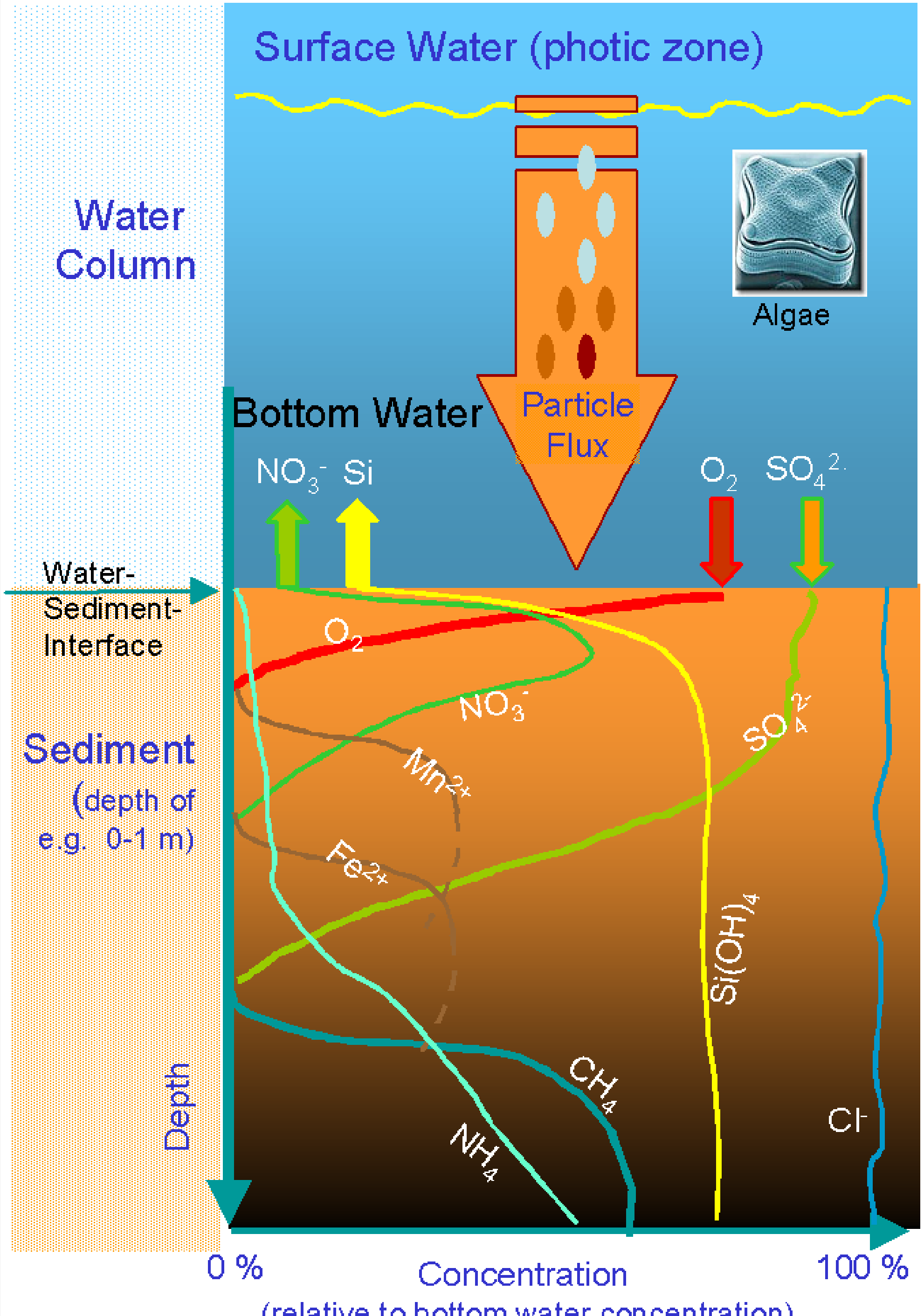
  - Globally important sinks & sources for nutrients
  - High rates of primary productivity



Surface Water (photic zone)
Water Column
Algae
Bottom Water
Particle Flux
NO3- Si
O2 SO4 2-
Water-Sediment-Interface
Sediment
(depth of e.g. 0-1 m)
Depth
O2
NO3-
Mn2+
Fe2+
SO4 2-
Si(OH)4
CH4
NH4
Cl-
0 %
100 %
Concentration
(relative to bottom water concentration)

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Change in concentration of i

Transport of chemical species

Rate of consumption of i, but dependent on j

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

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

Solving the maths (cont…)

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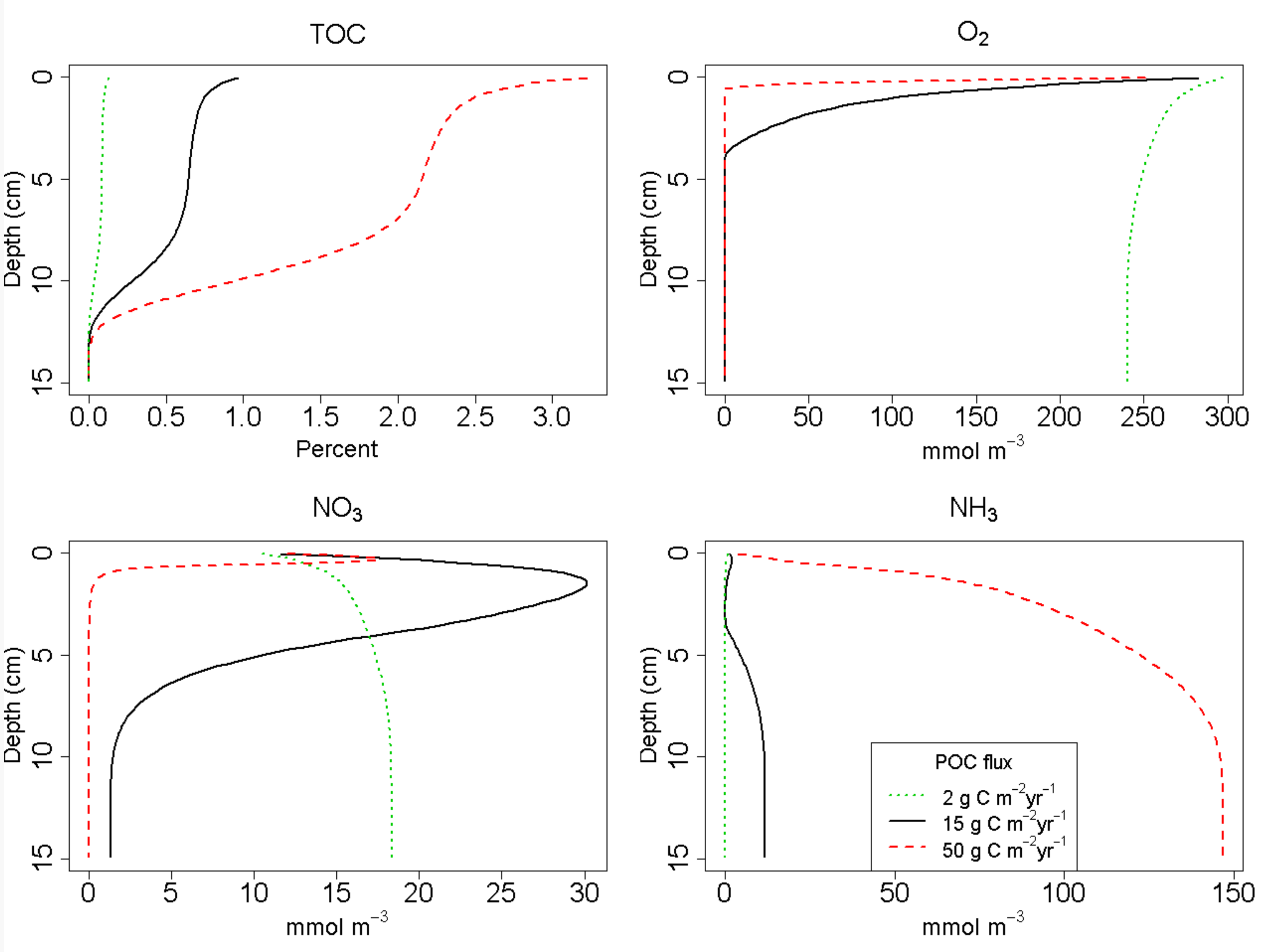
}
ss.output <- steady.1D(y=rep(10,2*100),
   func=modelFunction, parms=c(r=10, ksO2oxic=1))
dyn.output <- ode.1D(y=ss.output$y, times=0:364,
   func=modelFunction, parms=pars)
```

Output



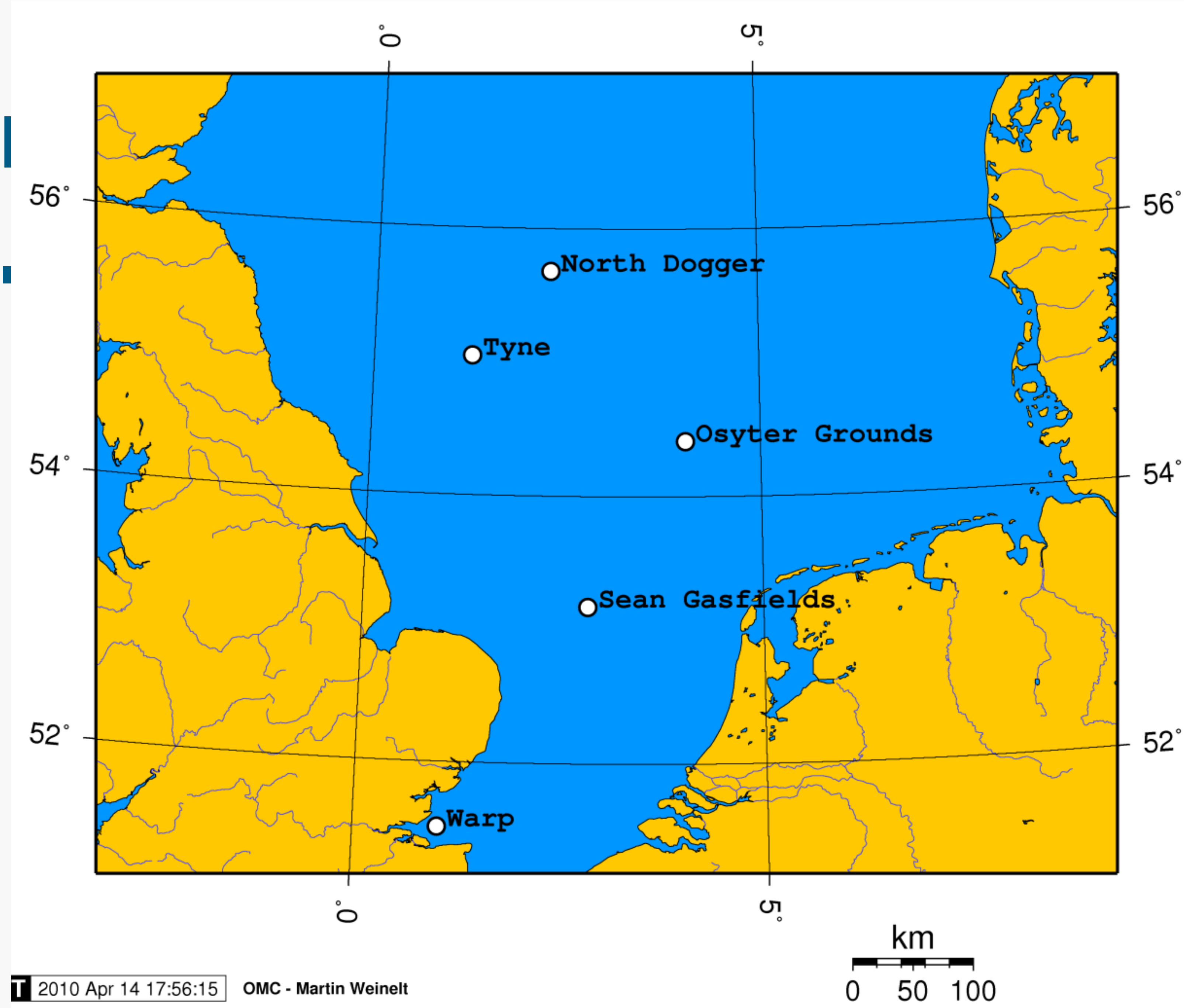
TOC
Depth (cm)
Percent
0.0
0.5
1.0
1.5
2.0
2.5
3.0
O_2
mmol m^{-3}
0
50
100
150
200
250
300
NO_3
0
5
10
15
20
25
30
NH_3
0
50
100
150
POC flux
2 g C $m^{-2}yr^{-1}$
15 g C $m^{-2}yr^{-1}$
50 g C $m^{-2}yr^{-1}$


CEFAS ENDEAVOUR
Copyright (c) - Ashley Hunn

Data management

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

ents



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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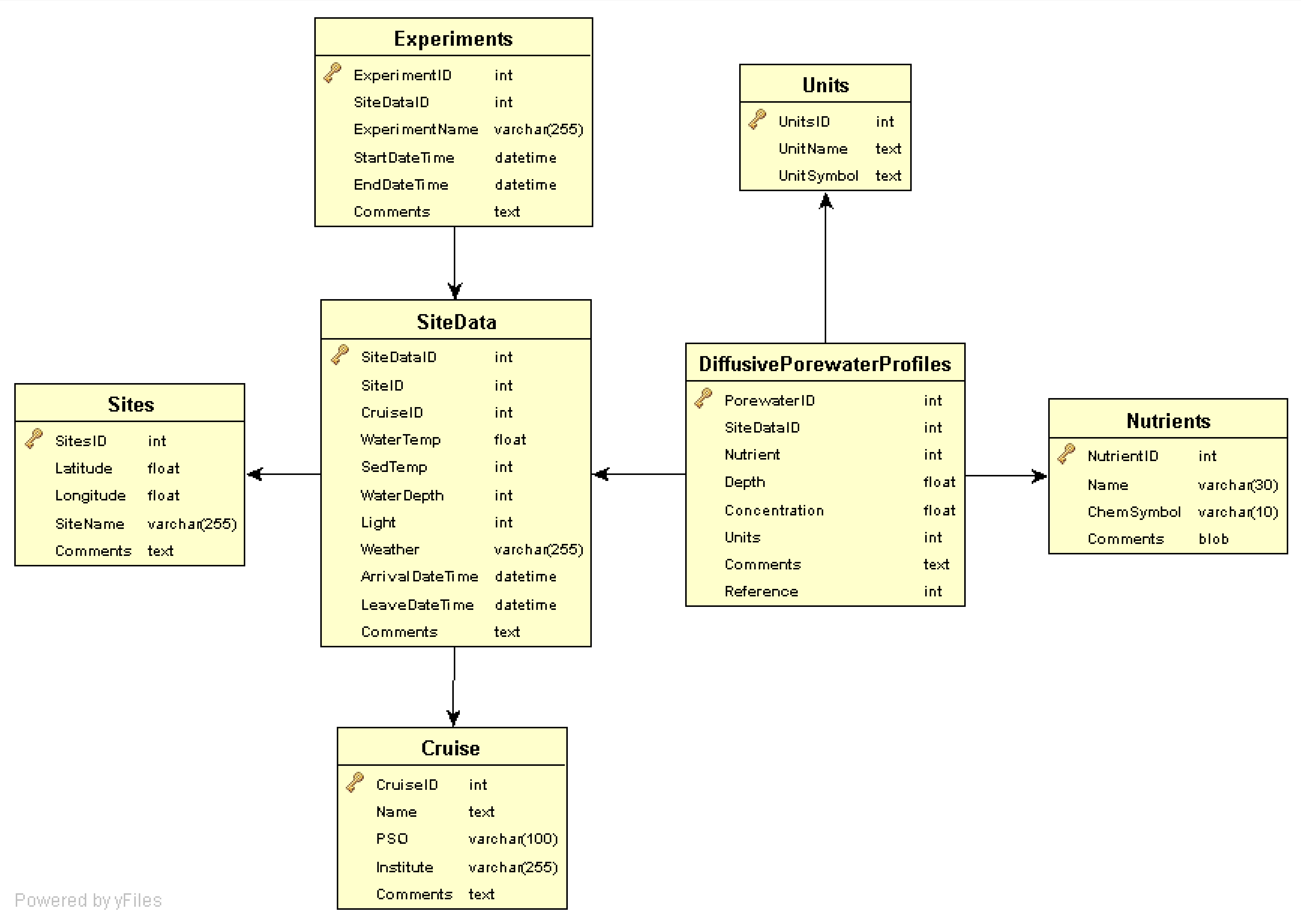

Experiments
ExperimentID int
SiteDataID int
ExperimentName varchar(255)
StartDateTime datetime
EndDateTime datetime
Comments text
Units
UnitsID int
UnitName text
UnitSymbol text
SiteData
SiteDataID int
SiteID int
CruiseID int
WaterTemp float
SedTemp int
WaterDepth int
Light int
Weather varchar(255)
ArrivalDateTime datetime
LeaveDateTime datetime
Comments text
Sites
SitesID int
Latitude float
Longitude float
SiteName varchar(255)
Comments text
DiffusivePorewaterProfiles
PorewaterID int
SiteDataID int
Nutrient int
Depth float
Concentration float
Units int
Comments text
Reference int
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

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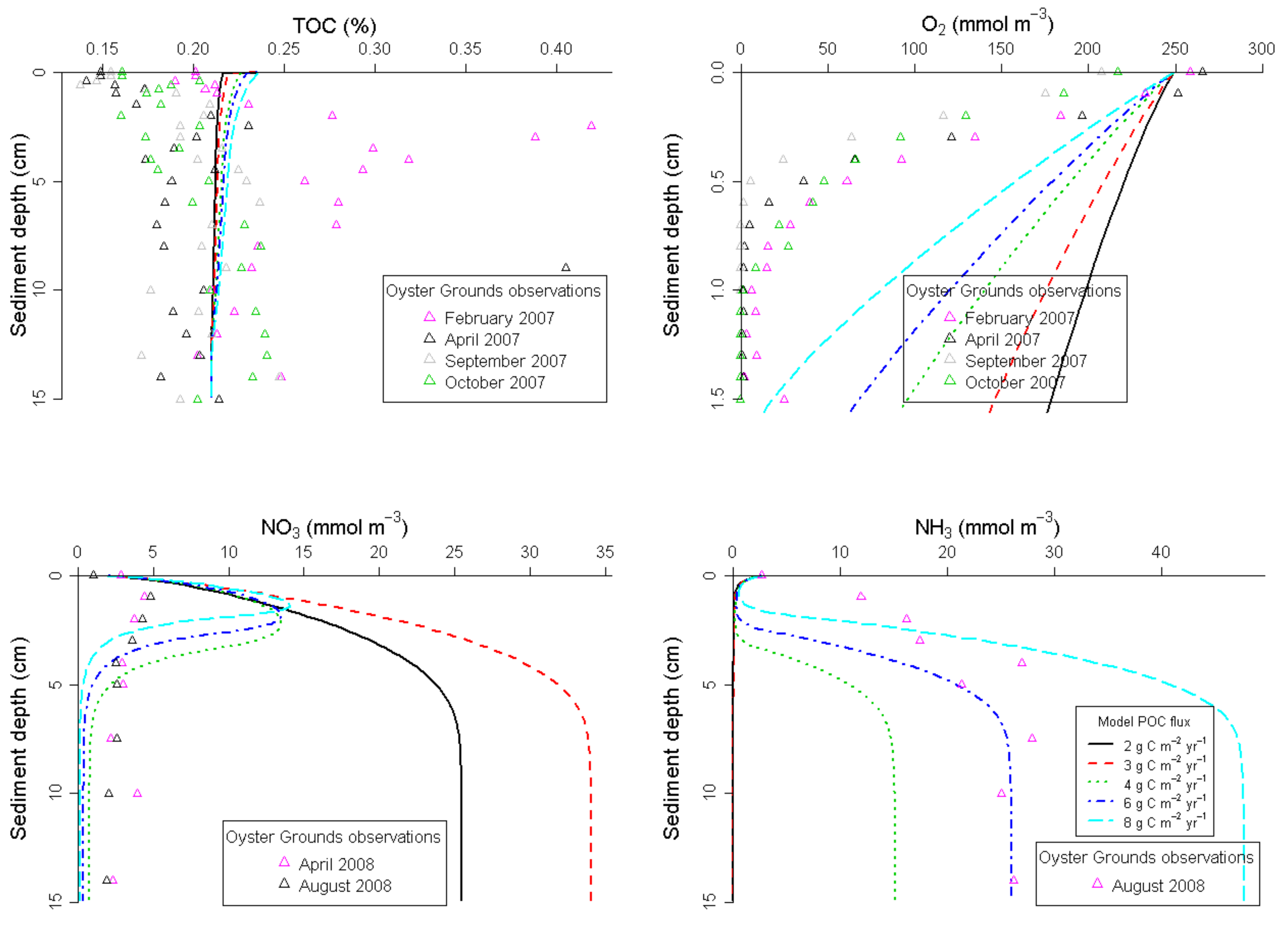
- Allows model calibration to be carried out



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
0.0 0.5 1.0 1.5
NO3 (mmol m-3)
0 5 10 15 20 25 30 35
Oyster Grounds observations
April 2008
August 2008
NH3 (mmol m-3)
0 10 20 30 40
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
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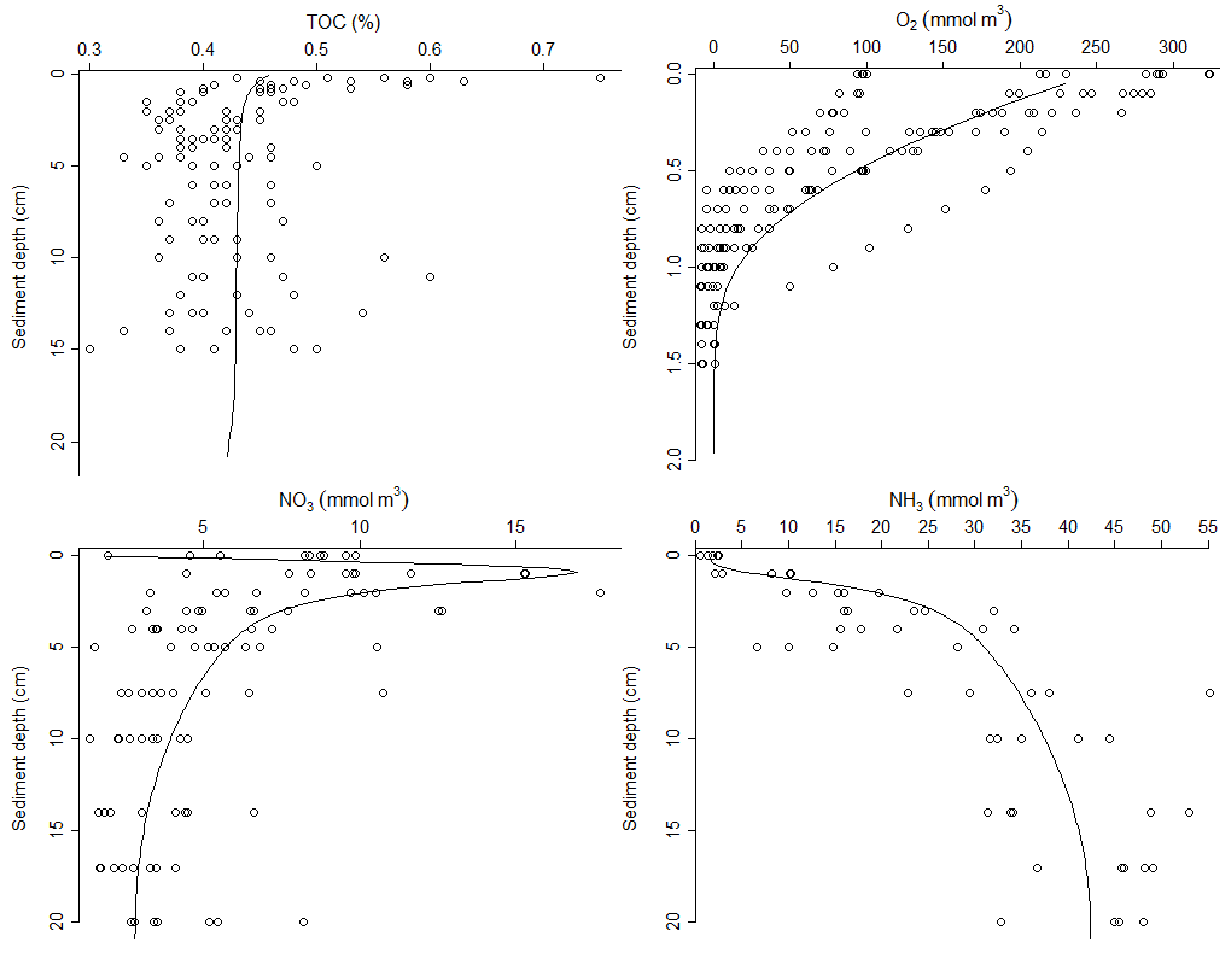
  - Allows us to discover the most sensitive model parameters
- Genetic algorithm
  - (Relatively) efficient method of making model output fit real data


TOC (%)
Sediment depth (cm)
O_2 (mmol m^3)
Sediment depth (cm)
NO_3 (mmol m^3)
Sediment depth (cm)
NH_3 (mmol m^3)
Sediment depth (cm)

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  - Public engagement of science

Any questions?

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