



# Reactive Transport in the Hydrosphere

Department of Earth Sciences, Faculty of Geosciences, Utrecht University

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Additional contributions: Dries Bonte, University Ghent

Audio effects: mixkit.co

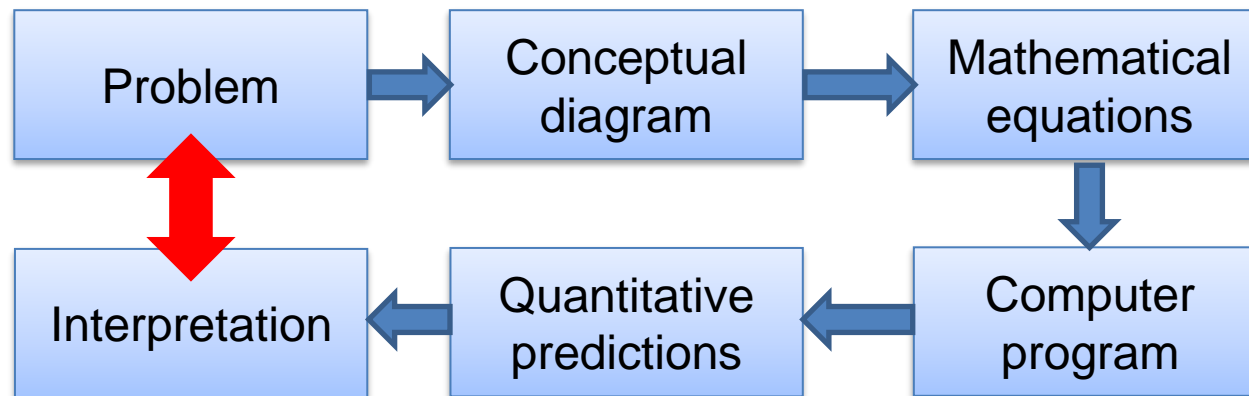


Universiteit Utrecht



# Course philosophy and focus

- develop an **appreciation** for the importance of **mathematics** and **computational** approaches to answer fundamental and applied questions in **biogeochemistry**
- teach you how to make models “from scratch” by following a **systematic and logical approach**



We will use **R** as our coding platform





Prof. Dr. Karline Soetaert ([k.e.r.soetaert@uu.nl](mailto:k.e.r.soetaert@uu.nl))  
**Ghent University / Utrecht University / NIOZ Yerseke**

- **Biologist** and **computer** scientist
- Modeling of **ecological** and **biogeochemical** processes in marine environments

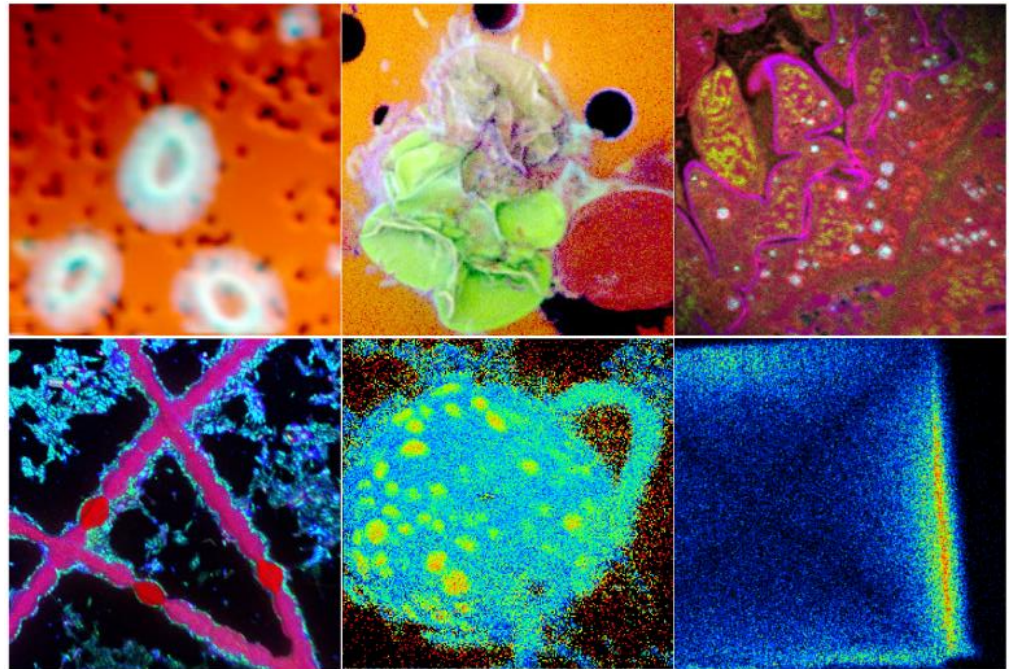




Dr. Lubos Polerecky ([l.polerecky@uu.nl](mailto:l.polerecky@uu.nl))

**Utrecht University / Head of the UU nanoSIMS facility**

- **Physicist & Engineer**, multidisciplinary research (Earth Sciences, a bit of Life & Material sciences)
- Models to **interpret** nanoSIMS data and **embed** them in a wider biogeochemical context





# Course format

## FLIPPED CLASSROOM

AT HOME



TRADITIONAL  
LECTURE MATERIAL

DURING CLASS



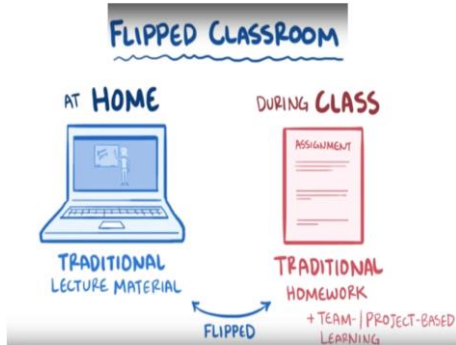
TRADITIONAL  
HOMEWORK

+ TEAM- / PROJECT-BASED  
LEARNING

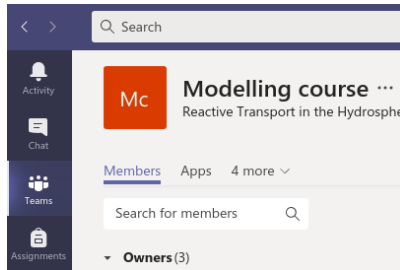
FLIPPED



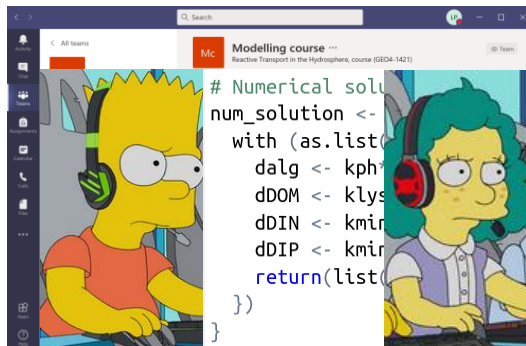
# Course format



- **Learn basic concepts and theory** by watching videos
- take **notes**
- **think** about what you have learned
- note **questions**



- **Class discussions** (~30 min)
- **prepare yourself** well ahead

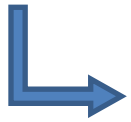


- **Work in groups** (3-4 students) to **solve problems**
- Put theory into practice, hands-on experience
- we will visit your group to answer questions and provide hints

This year: contact via **Teams**

# To pass the course

- Final grade at least 5.5, and mid-term exam grade at least 5.5 (one resit).
- **Homework** assignment (after 4 weeks: 1x written report, 15%)
- **Mid-term exam** (after 5 weeks: 3 hrs, 40%)
- **Final project** (end: written report, 25%; oral presentation + discussion, 20%)



Evaluated as a **group effort**:

- one report + one presentation per group
- each group member will receive the same grade

## Work ethics:

- This is **not a competition**
- **Collaborate** within groups
- **Reach out** to other groups
- **Best learning if you try to explain your ideas to someone else.**

# Get the textbook as an e-book

Available from **Springer** using your Solid-ID

<https://link.springer.com/book/10.1007/978-1-4020-8624-3>

Online toegang naar <https://link.springer.com/book/10.1007/978-1-4020-8624-3>

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Universiteit Utrecht



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 Springer Link



**A Practical Guide to Ecological Modelling**  
Using R as a Simulation Platform

Editors ([view affiliations](#))  
Karline Soetaert, Peter M.J. Herman

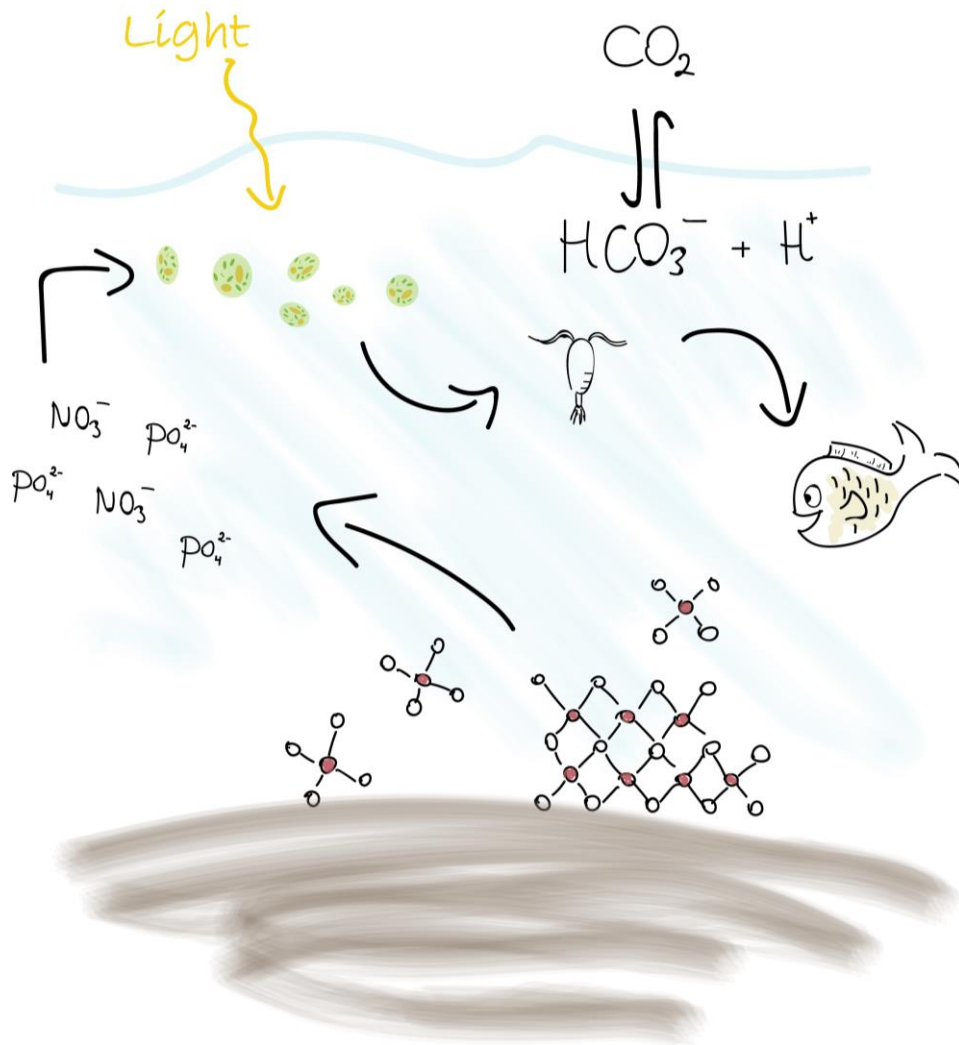
Textbook

77	2	44k
Citations	Mentions	Downloads

Additional material as **handouts** – via Blackboard



# What kind of models are we going to study in this course?



## Biogeochemical models

- Ecological **interactions** (predator - prey)
- Organic matter **production**
- Organic matter **mineralization**
- Mineral **dissolution/formation**
- Cycling of **C coupled to N, Fe, S, P**, etc.

# What kind of models are we going to study in this course?

## Biogeochemical models

### **Mechanistic mathematical models:**

- Processes (mechanisms) described mathematically
- Formally and numerically precise (describing mass balance)
- Model predictions can be directly compared with experimental data

### **Subject of inquiry:**

- Exchange of mass and energy
- Variation in time and space

### **Studied systems:**

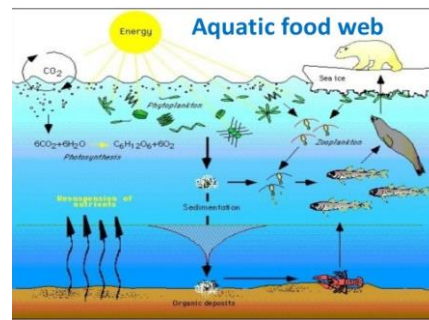
1. Rivers
2. Sediments
3. Aquifers
4. Lakes & Oceans
5. Earth



# What kind of models are we going to study in this course?

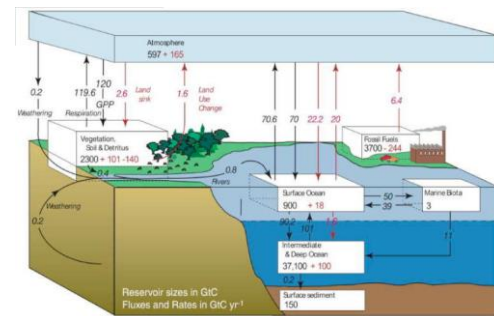
Start of the course: **box-models**

Ecological interactions

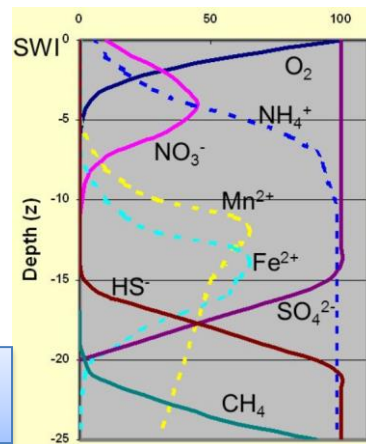


0D

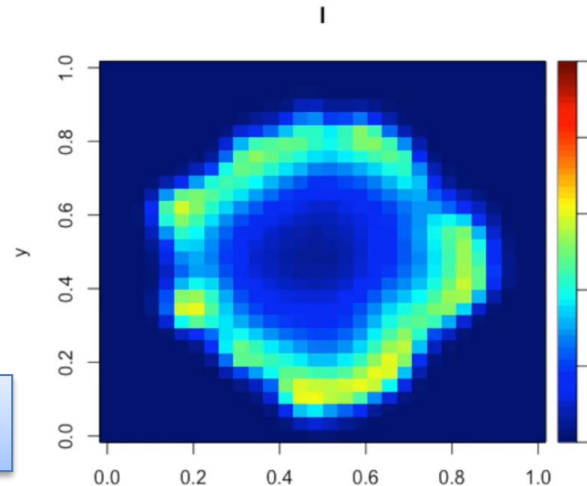
Global element cycles



Subsequently: **include spatial context**



1D



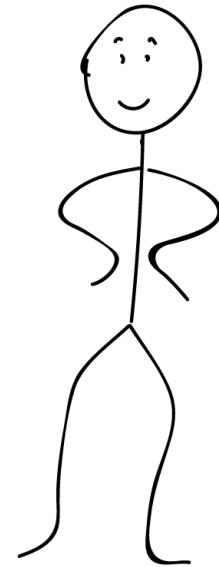
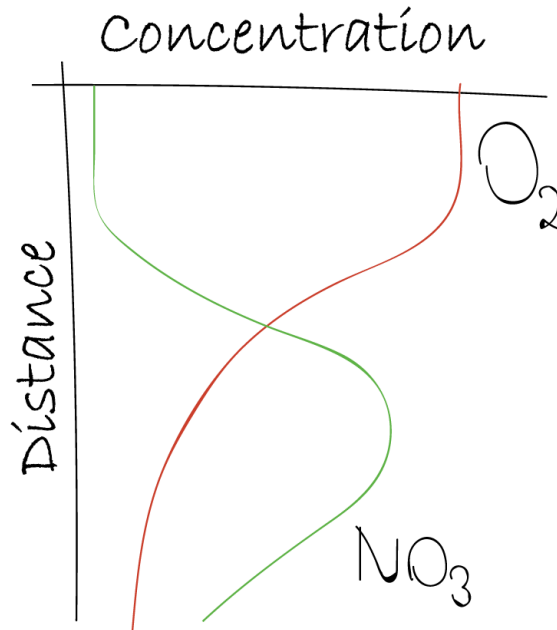
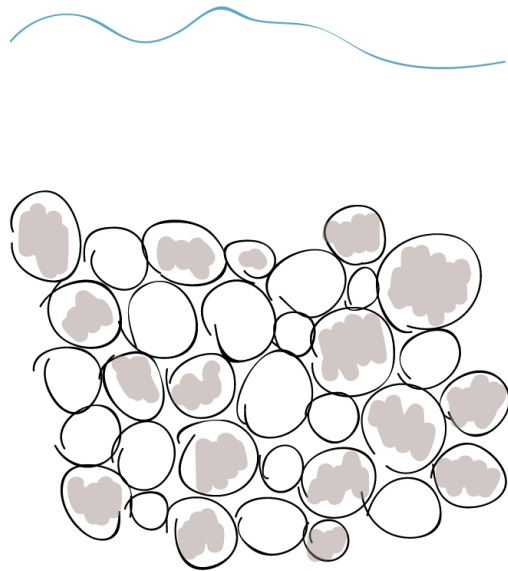
2D



# What kind of models are we going to study in this course?

## Sedimentologist's view

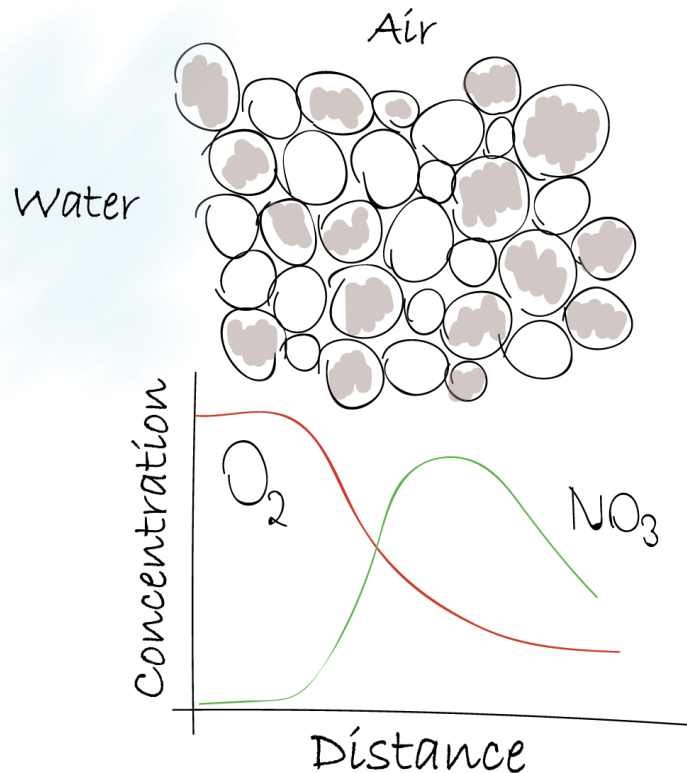
"Sediment setting"



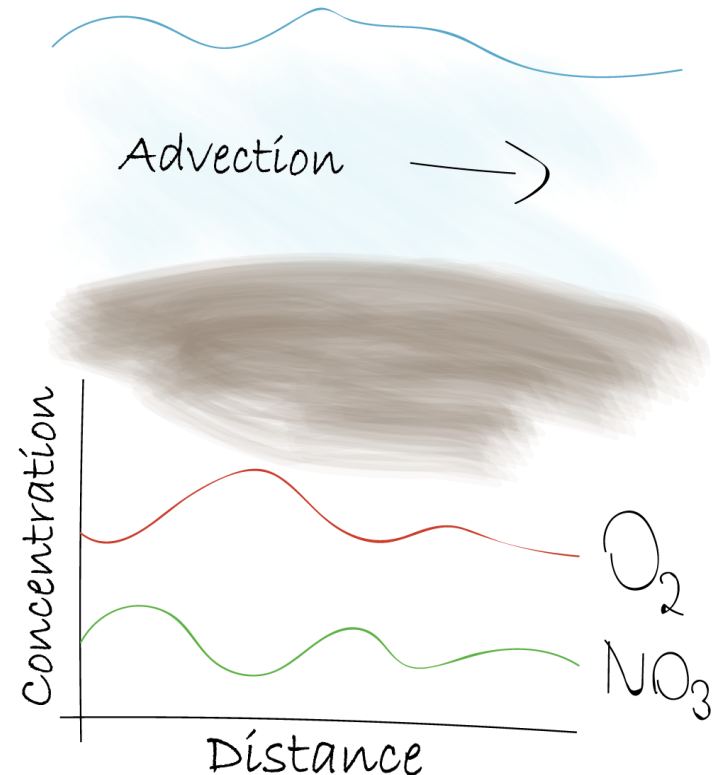
# What kind of models are we going to study in this course?

## Hydrologist's view

"Aquifer setting"



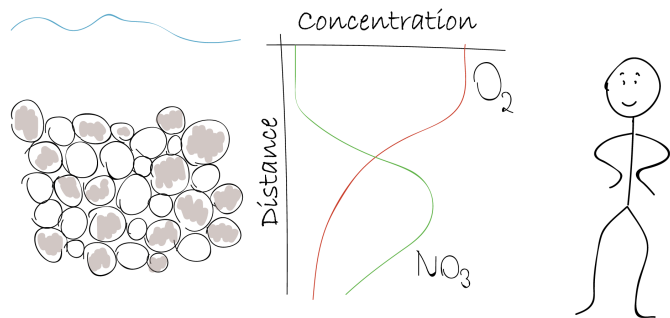
"River setting"



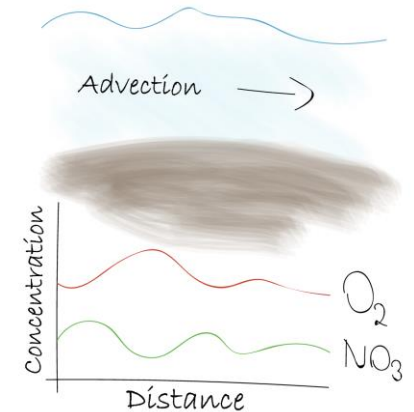
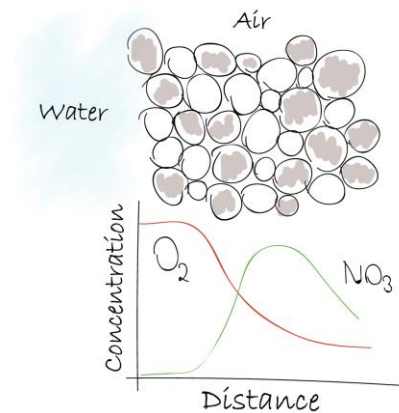


# What kind of models are we going to study in this course?

## Sedimentologist's view



## Hydrologist's view



**Equations will be the same!**



# Final projects:

develop a model (from scratch) for one of the following topics

Formation of  $\text{CH}_4$  bubbles  
in marine sediments



C+S cycling

Algal blooms due to  
eutrophication



C+N+P cycling

Role of iron reduction  
in C-org mineralization



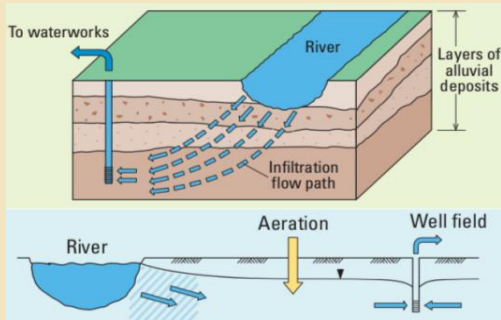
C+Fe cycling

Light vs. chemical energy  
utilization



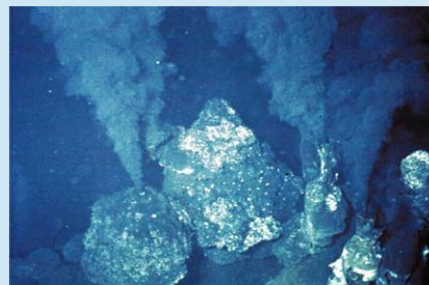
C+S cycling

River bank filtration



C+N cycling

Sub-seafloor  $\text{CaCO}_3$  precipitation  
driven by AOM



C+S cycling

Main tasks given

You can expand further  
as you wish.