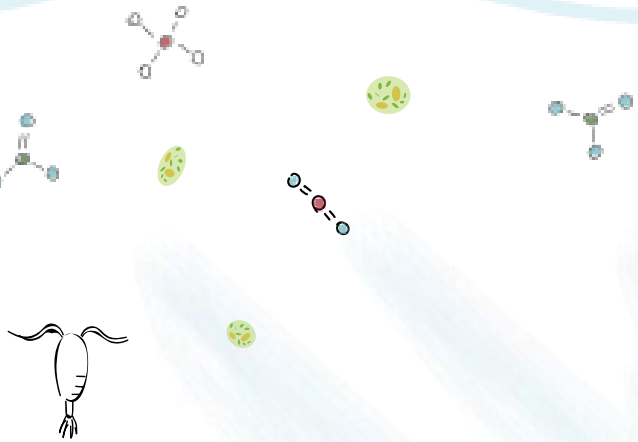

Reactive Transport in the Hydrosphere

Department of Earth Sciences, Faculty of Geosciences, Utrecht University

Lecturers: Lubos Polerecky and Karline Soetaert

Illustrations, narration and video editing: Renee Hageman
Additional contributions: Dries Bonte, University Ghent
Audio effects: mixkit.co

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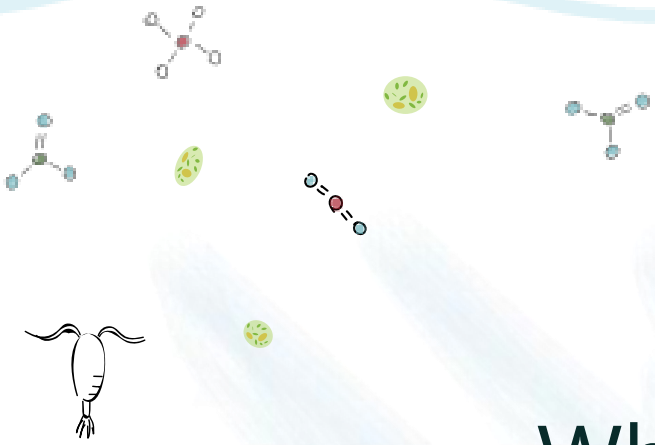

What is a model?

Why do we perform modeling?

Systematic approach to modeling

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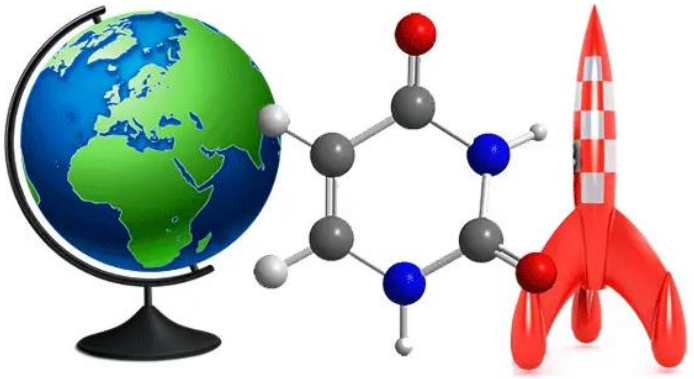
What is a model?

Models are **simplified representations of complex phenomena**

- They are abstraction of reality, so do **not** contain all features of real systems



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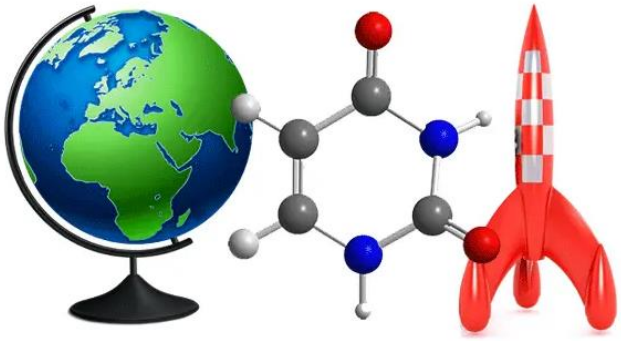
What is a model?



Models are a **simplification of reality**

- serve a **specific purpose**
- contain only **essential** features for what we want to describe
- developed on **temporal and spatial scales of interest**

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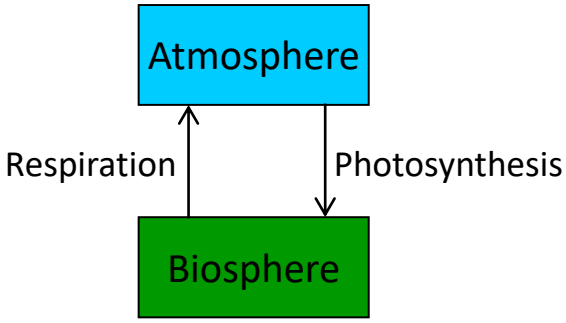
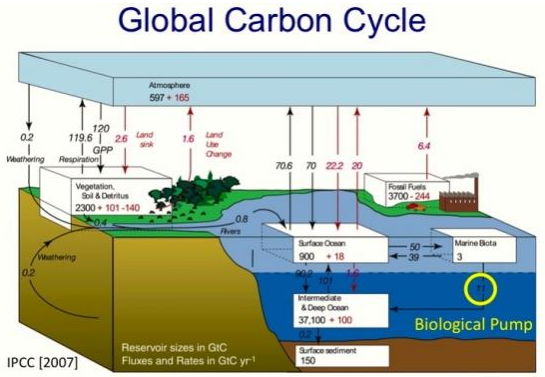
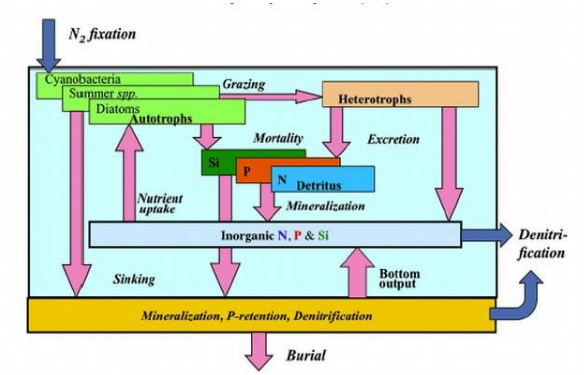
Scientific models

Simplified representation of complex ecological and environmental phenomena







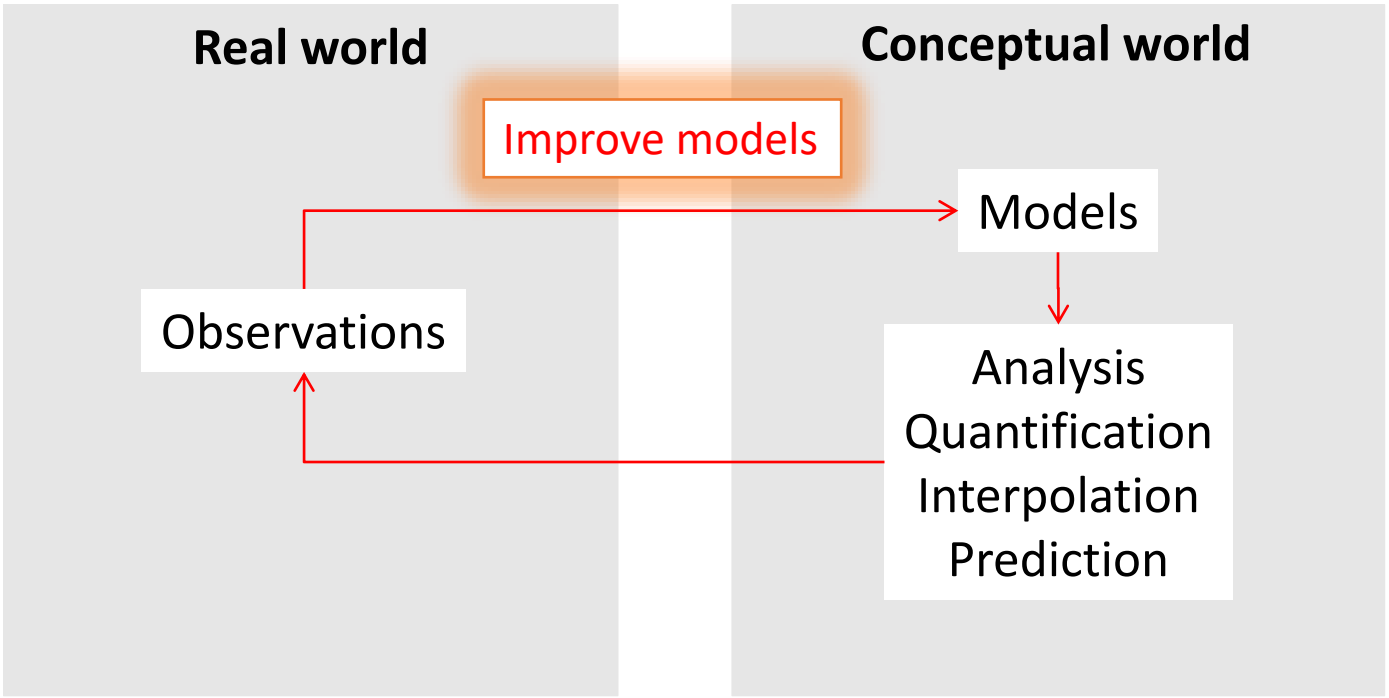
- expressed in the language of **mathematics** and (often) solved by **computers**
- force us to **think logically** and **rigorously**

- allow **testing** of our **understanding** of real systems
- useful to **generate insights**
- allow **generalization**
- can be used for **forecasting** and **management**

Scientific models

Analytical tools

Help us **generate hypotheses** and **guide empirical research**



Scientific models

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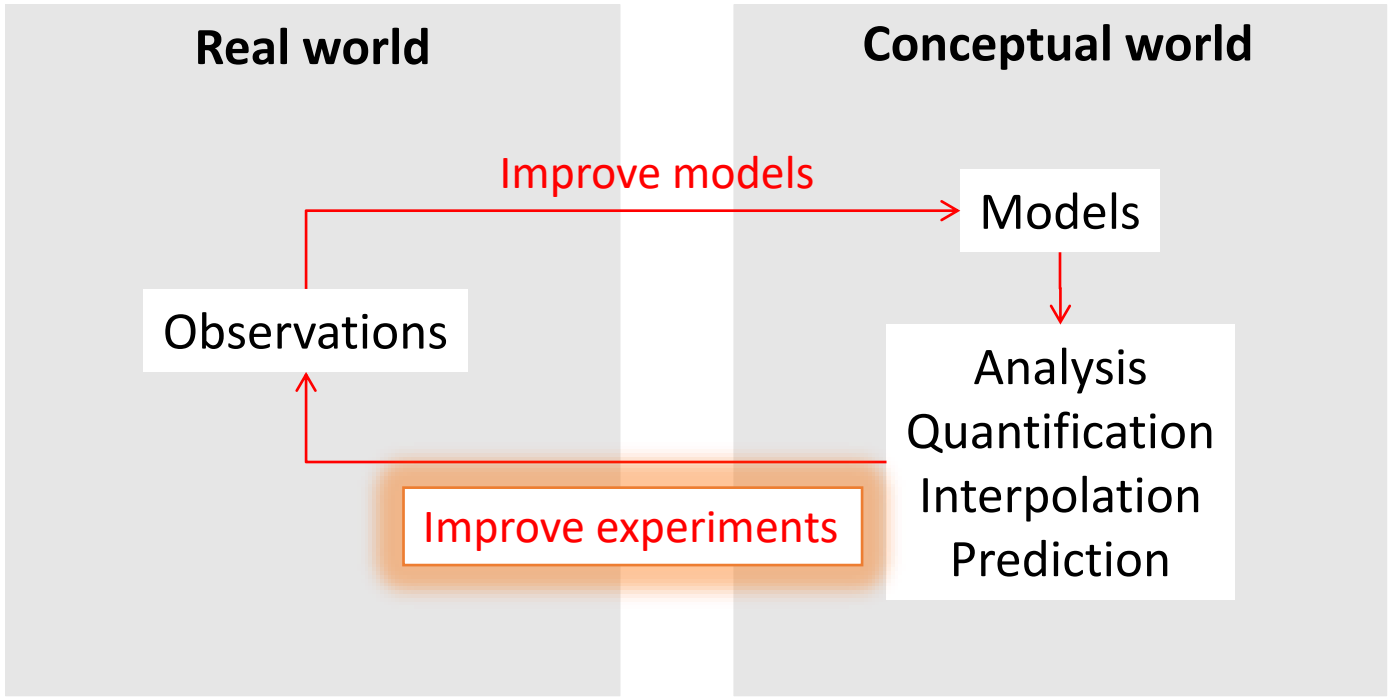
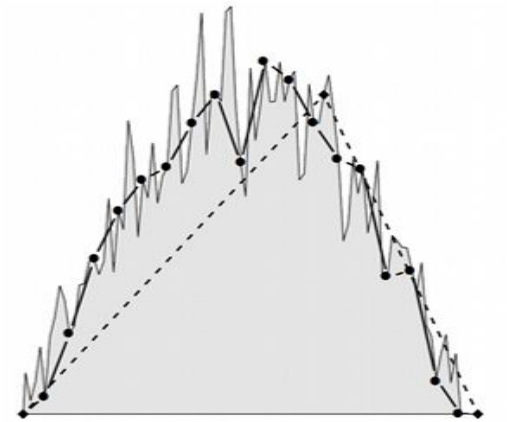
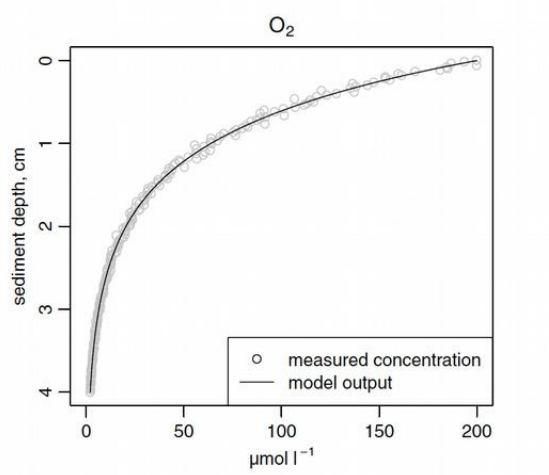


Scientific models

Budgeting & Quantification tools





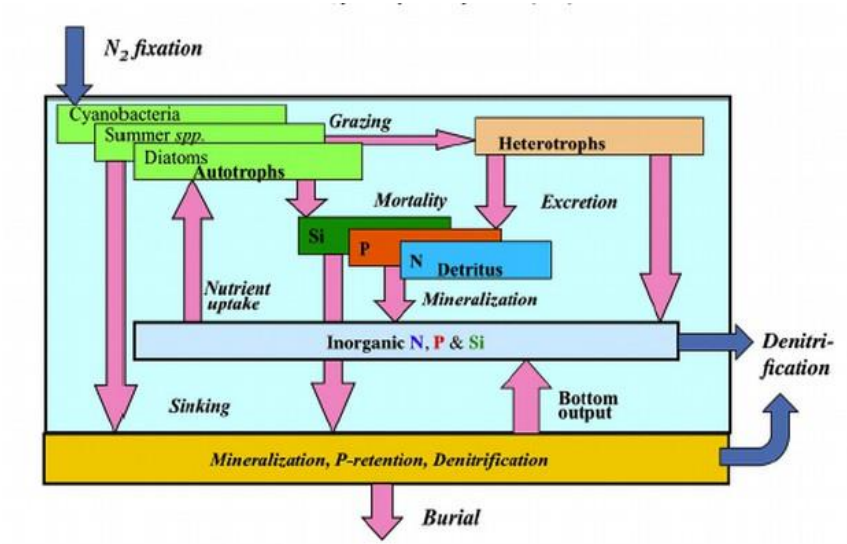
- **Data may contain gaps** due to limited sampling (difficult or too expensive)
- These gaps **can be "filled"** using models that reproduce well the existing data.

- **Process rates**, and their regulation, can be **quantified** by fitting models to experimental data
- **Results** can be used in larger-scale models.

Scientific models

Management tools

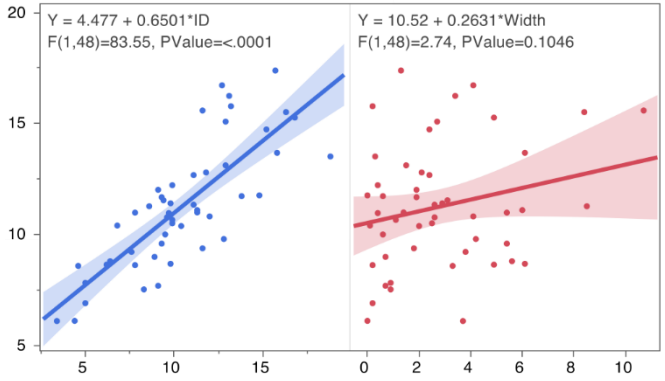
Allow analysis of **consequences** and **costs** of certain **management** actions in advance of effectively **taking** actions.



Develop strategies to mitigate environmental pollution

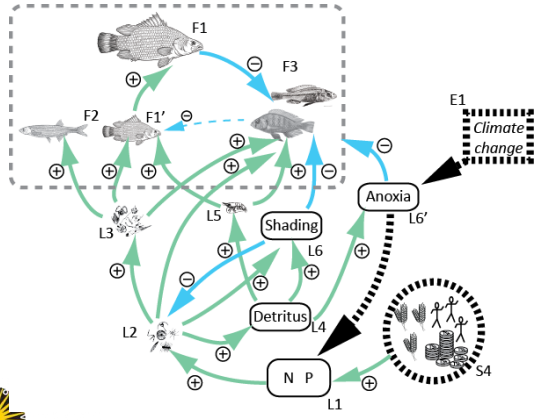
Scientific models

Statistical models



- Important in empirical research
- **descriptive**, **correlative**
- supports prediction and extrapollation, but dangerous to apply to different contexts
- **"black-box"**: understanding of mechanisms and causality is **lacking**

Mechanistic modeling



- **causality explicitly included**: system components are **related** to each other via **processes**
- helps us understand **how** the system **works**, or **what happens** if the system is **altered**

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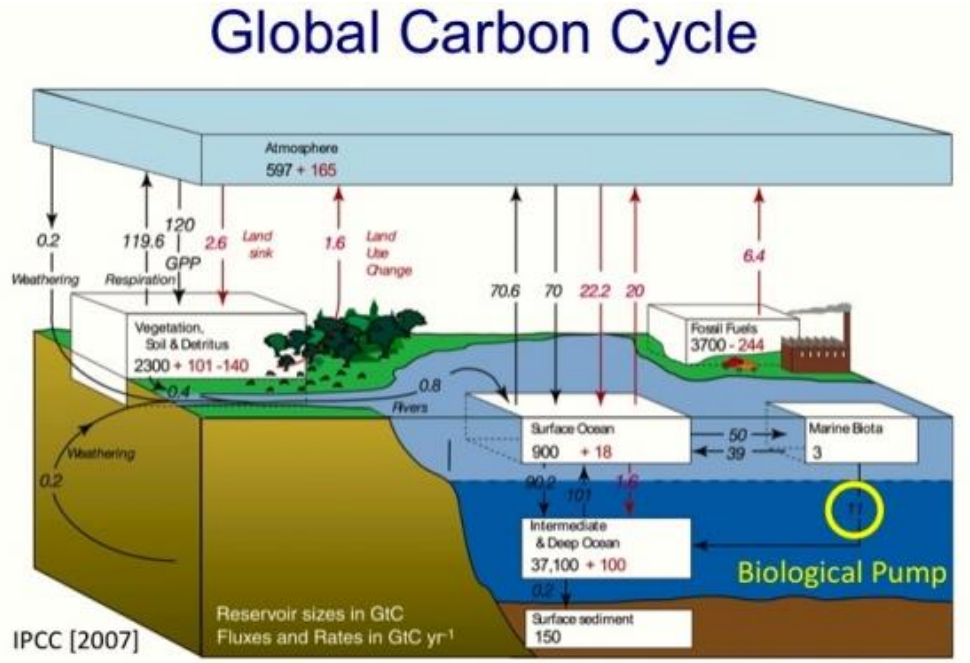
Process-based, mechanistic models

Focus of this course

- **Flux-based** models
- Exchange of **mass** and **energy**
- Study the impact of biogeochemical processes on environment, and vice versa

Example:



Process-based, mechanistic models

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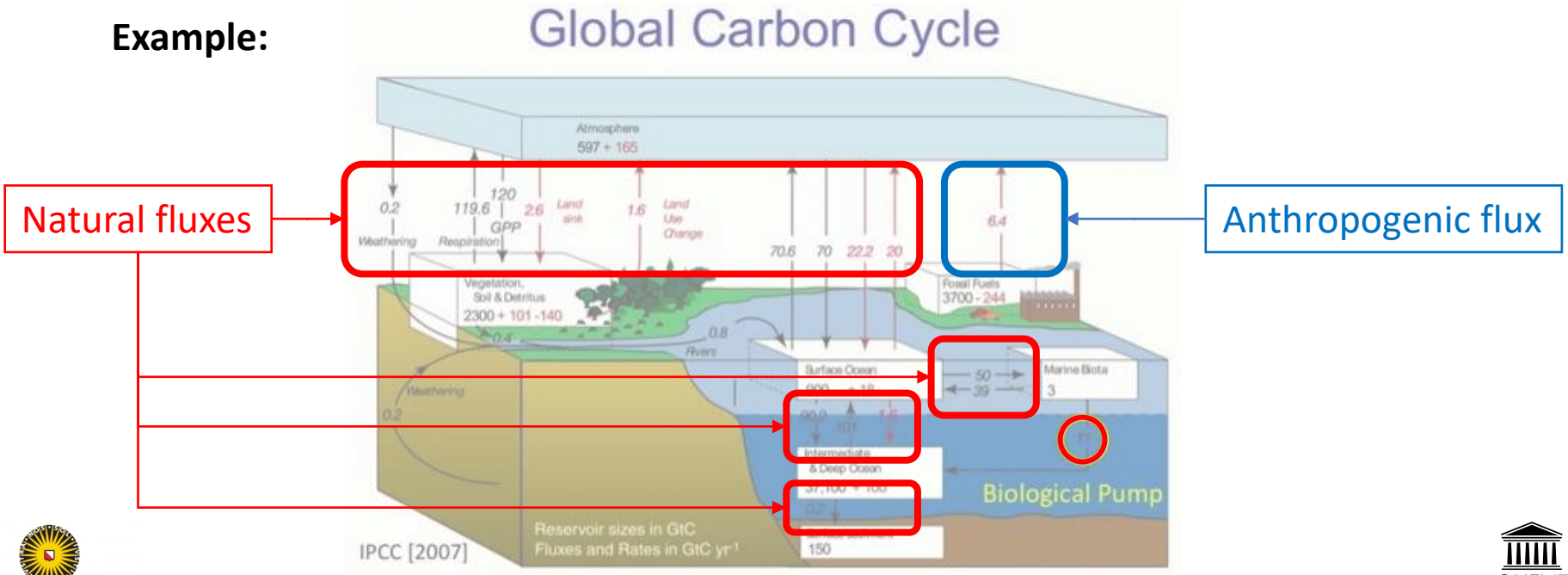
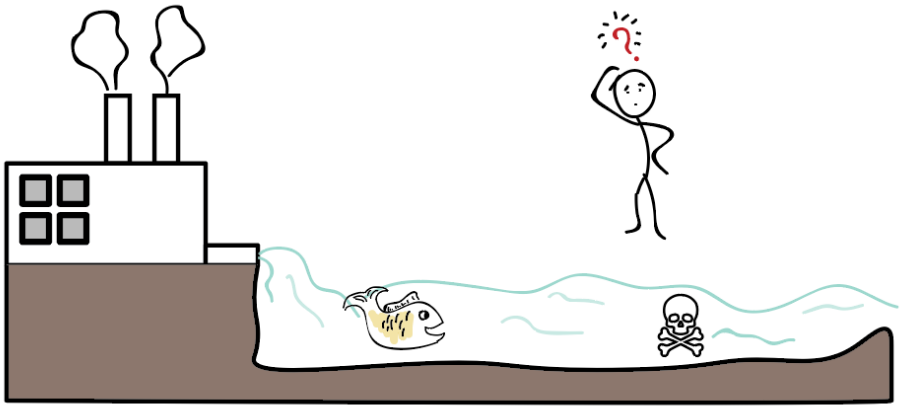
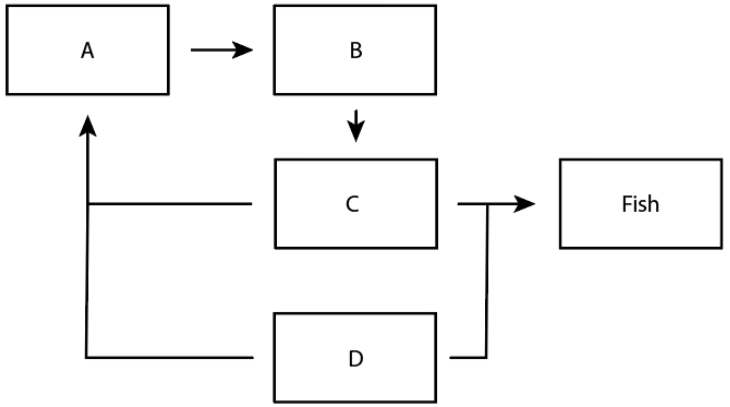


Logical and systematic approach to modeling

1. transfer the problem into a **conceptual diagram**

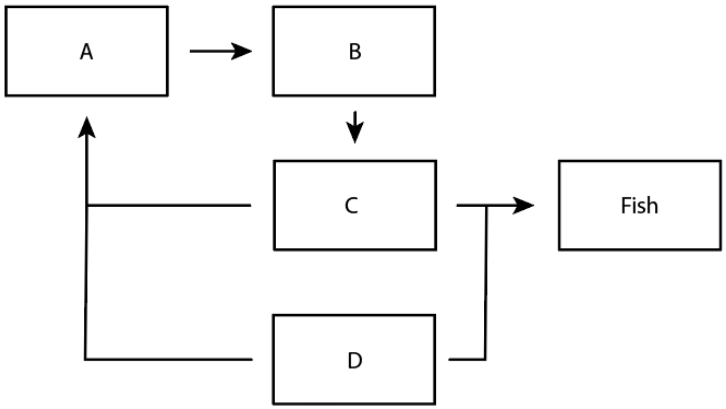




Simplify reality, decide **what matters** and what are irrelevant details.

Logical and systematic approach to modeling

2. **translate** the conceptual diagram **into mathematical equations**



$$\frac{dA}{dt} = F_{CA} + F_{DA} - F_{AB}$$

$$\frac{dB}{dt} = F_{AB} - F_{BC}$$

$$\frac{dC}{dt} = F_{BC} - F_{C\text{-}Fish} - F_{CA}$$

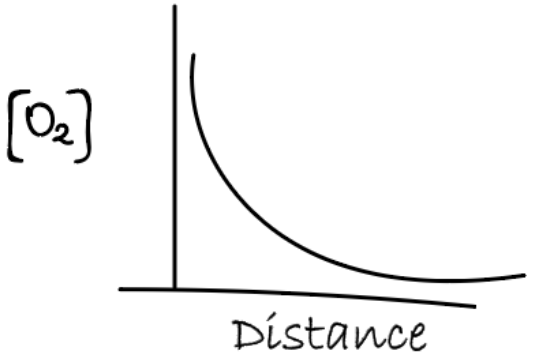
...

Ensure that that the model is **mass balanced** and can therefore be used to make **quantitative predictions**.

Logical and systematic approach to modeling

3. **implement** the equations in a **programming language**
4. use a computer to **generate predictions**

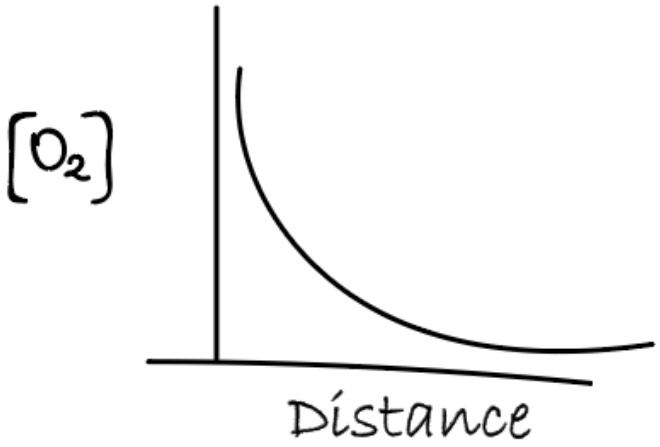
```
NPZ <- function(t, state, parameters)
{
  with(as.list(c(state, parameters)),{

    # Forcing function = Light is a sine function
    # implemented: seasonal variation, light is I,

    I <- Imax*max(0,sin(t*2*pi))


    # Rate expressions - all in units of [mol d-1]
    f1      <- k1*(a+b*I)*NO2 #(Imax and b cancel o
    f2        <- k2*O
    f3        <- k3*NO*O3
    fcomb     <- 1e11         # [mol d-1]


    # Mass balances [mol/day]
    dNO2 <- f3-f1
    dNO  <- f1-f3 + fcomb
    dO   <- f1-f2
    dO3  <- f2-f3


    # the output
    return (list(c(dNO2, dNO, dO, dO3),        # th
                 I = I)  # ordinary output variable
    )
  }) # end of with()=
}  # end of model equations
```

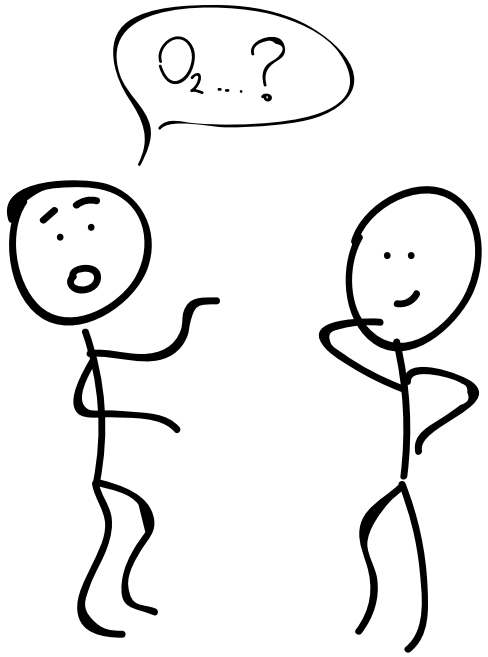


In this course, we will use **R** …
… and do exercises to **practice**, **practice**, **practice**.

Logical and systematic approach to modeling

5. **interpret** and **communicate** the model **results**





Practice communication in a **graphical, oral** and **written** form.

Logical and systematic approach to modeling