Building a process-based model, from scratch

Camille Minaudo

Sistemes Dinàmics en Ecologia

UNIVERSITAT DE BARCELONA

Outline

- PART 1
  - What is a process-based model?
  - Why do we want process-based models?
  - Building a model from scratch
  - Modelling lake metabolism rates
- PART 2
  - Step-by-step model implementation using R, GitHub and Binder

What is a process-based model?

- A representation of the way the world works
- Reproduces a level of realism
- However, models are necessary simplifications and do not explain all the variance in observational data
- A process-based model is a model that takes an object-oriented perspective, identifying:
  - the relevant entities (included properties)
  - their state
  - and their behaviours.

Why process-based models?

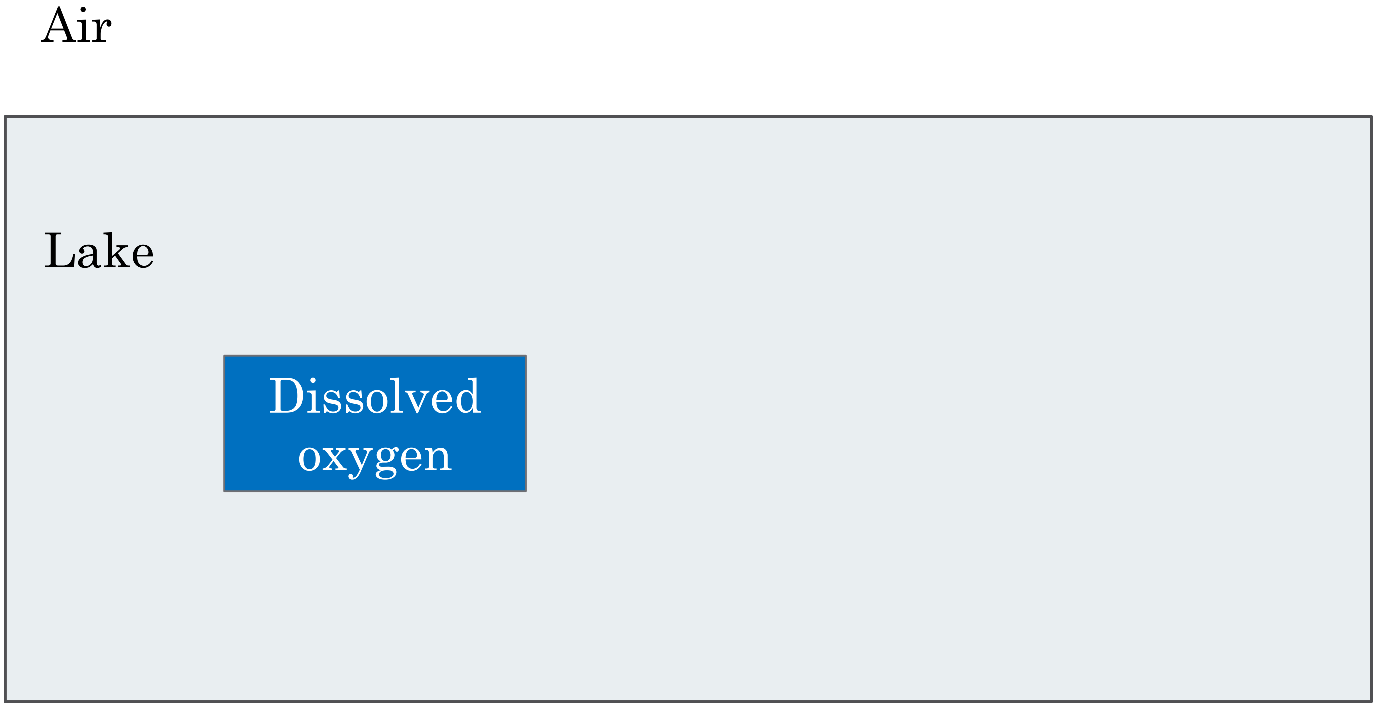
- Can be used for scenarios that are out of sample
- To challenge our level of understanding of the way our world works
  - From system A to system B
- Accommodates a variety of data, even if sampled irregularly
- Used to infill missing data

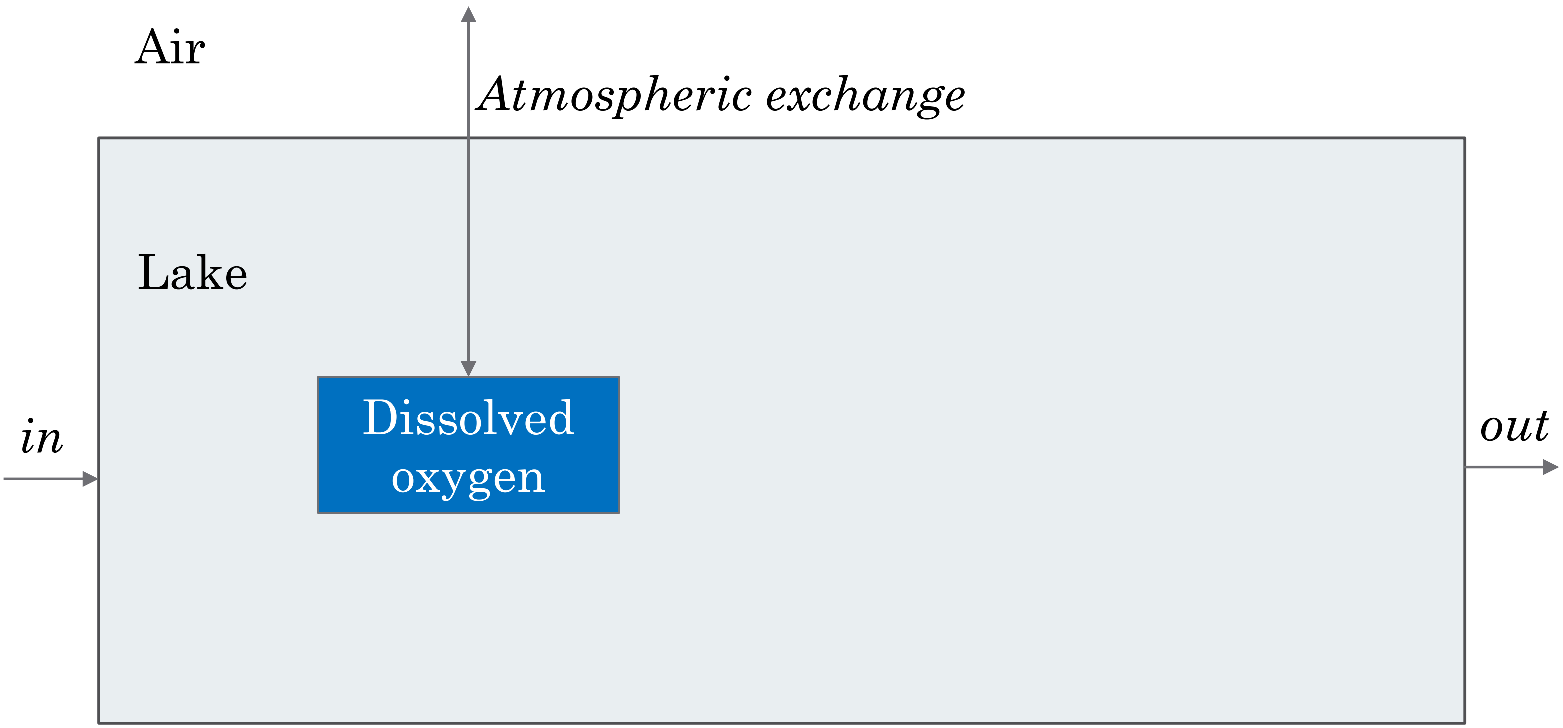
Building a model from scratch

- What do I want to model?
  - State variables
- What do I know about my state variables?
  - State
  - Behaviour = processes (= equations)
  - Boundary conditions
- What data (observations) do I need?
- How do I want to build my model?
  - Numerical scheme
  - Programming language
  - Numerical platform
- Let's go!

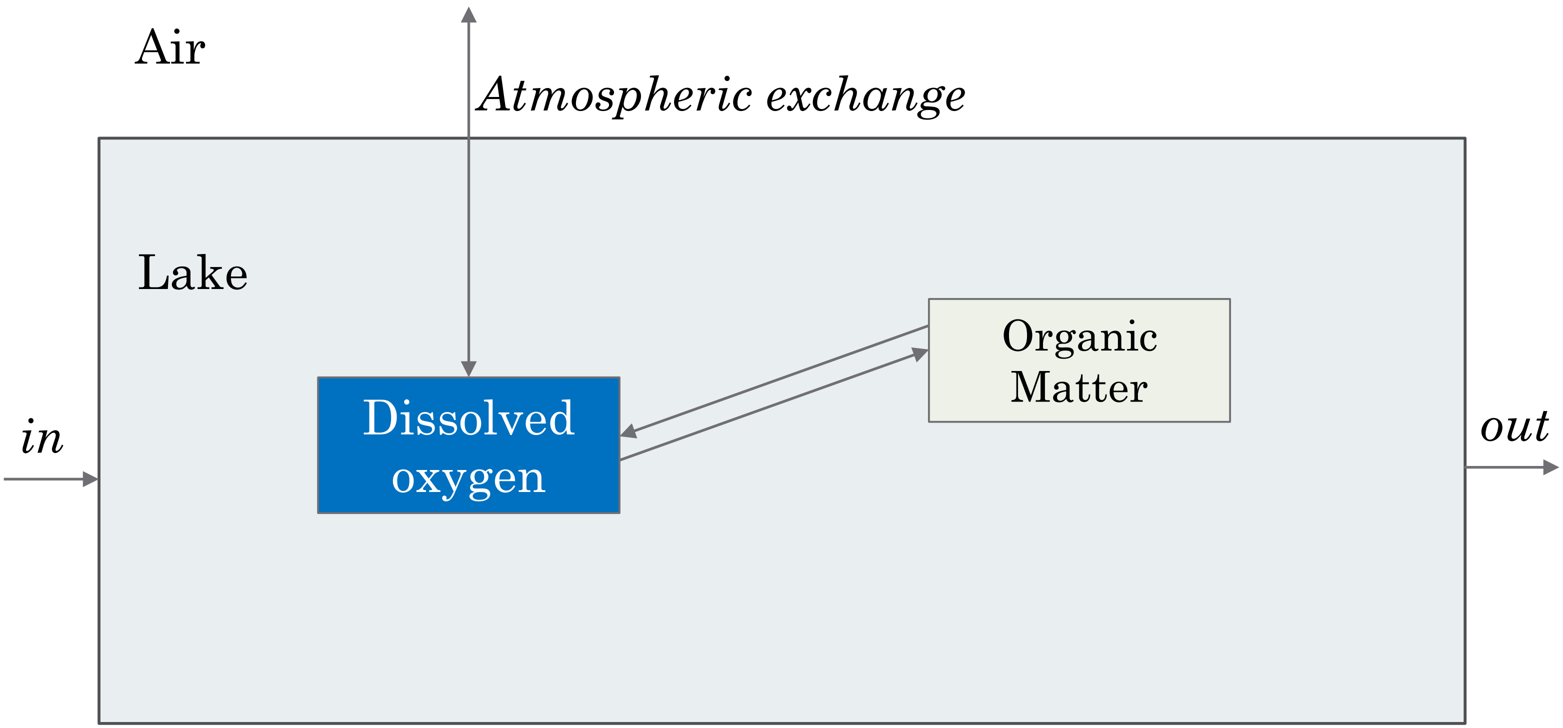
Application

Modelling lake metabolism rates

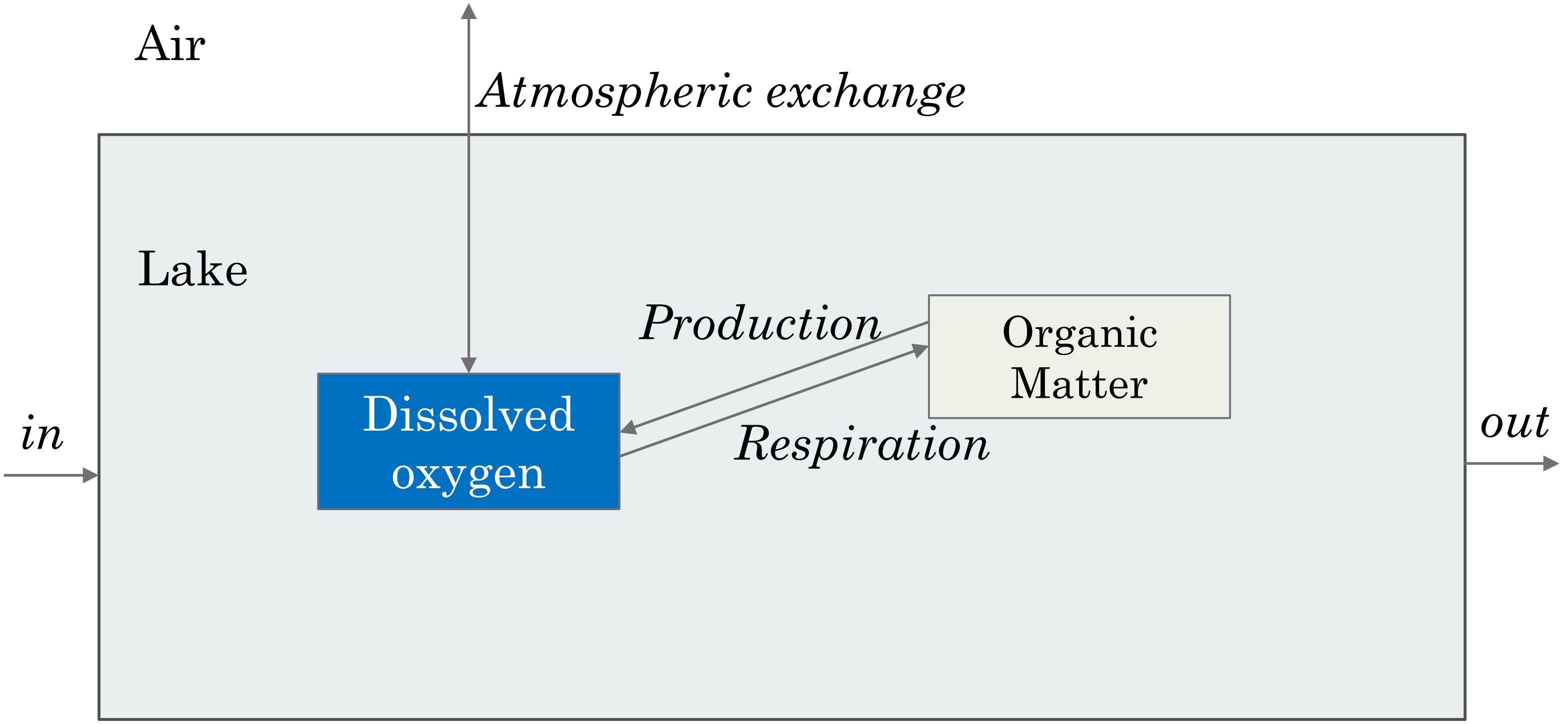

Air
Lake
Dissolved oxygen



$$\frac{dDO(t)}{dt} = f(Physical_{fluxes}(t))$$

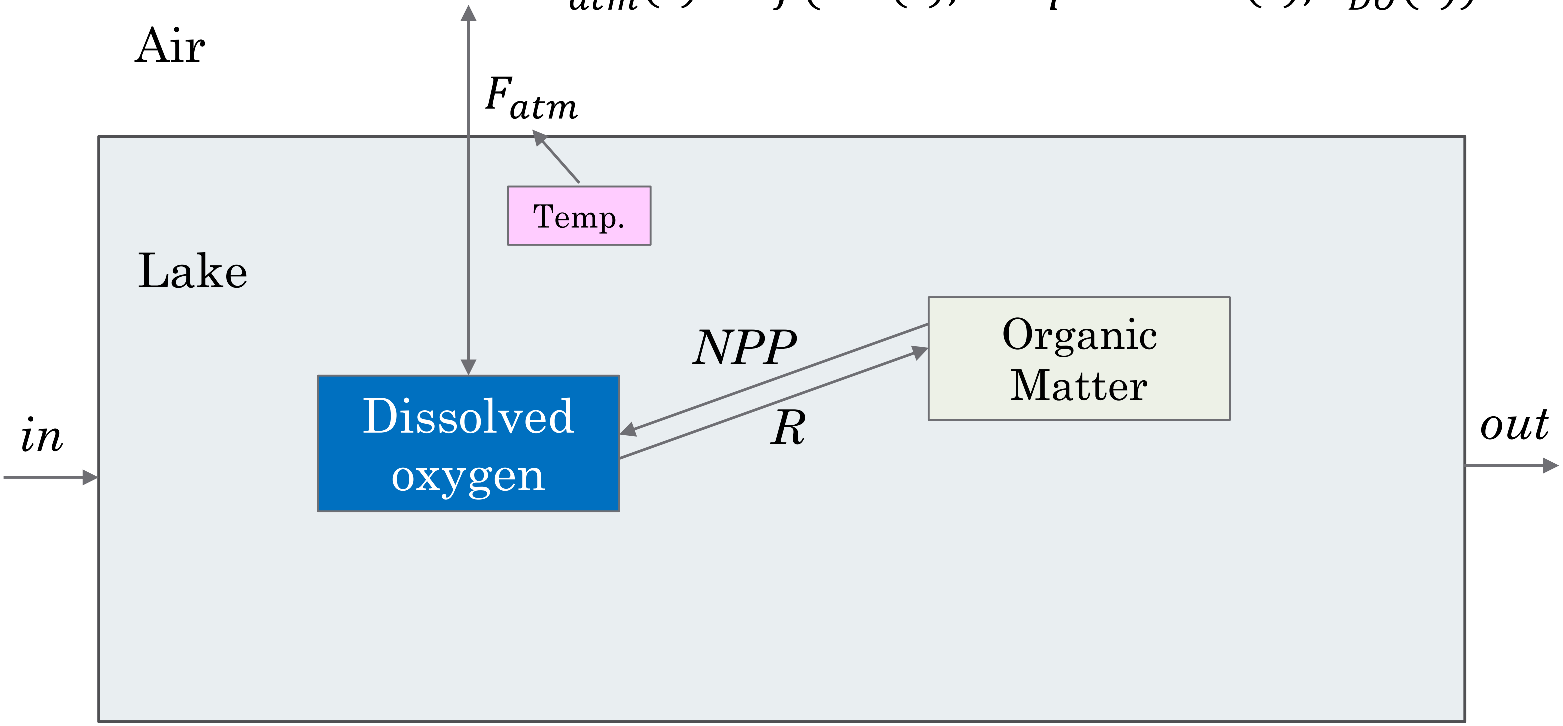


$$\frac{dDO(t)}{dt} = f(Organic\ Matter, Physical_{fluxes}(t))$$



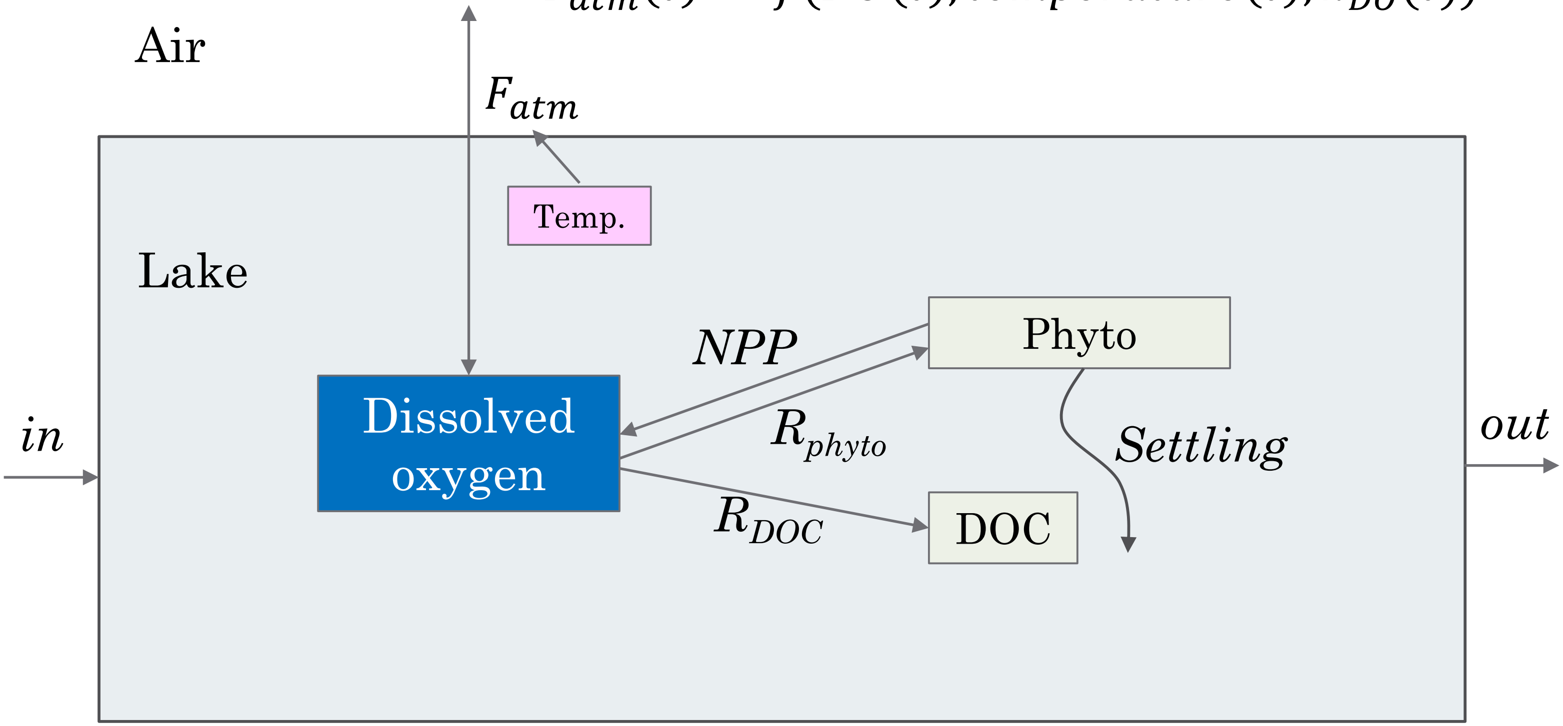
$$\frac{dDO(t)}{dt} = Production(t) - Respiration(t) + Physical_{fluxes}(t)$$

$$F_{atm}(t) = f(DO(t), temperature(t), k_{DO}(t))$$



$$\frac{dDO(t)}{dt} = NPP(t) - R(t) + F_{atm}(t) + \varphi\,(t)$$

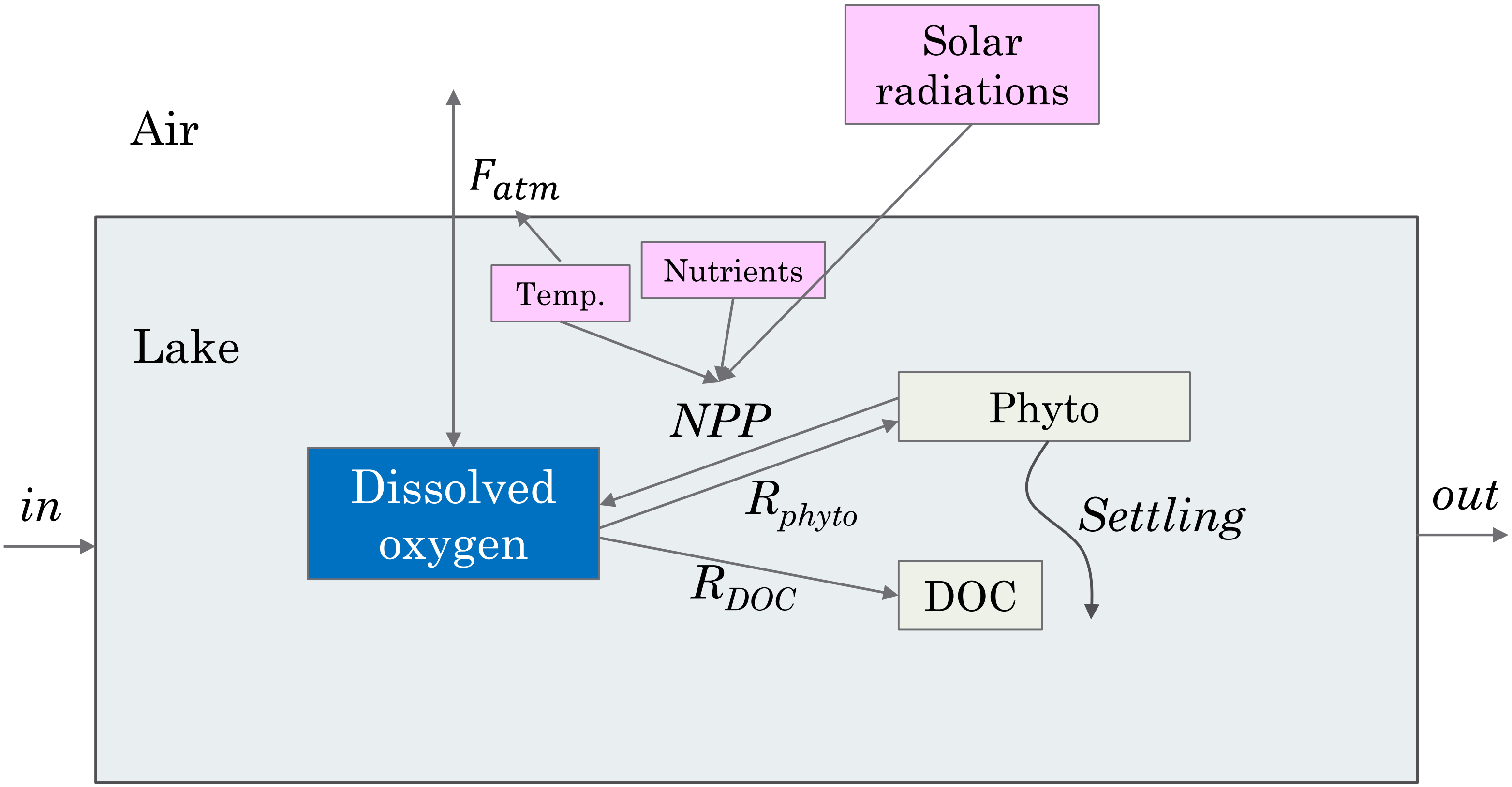
$$F_{atm}(t) = f(DO(t), temperature(t), k_{DO}(t))$$



$$\frac{dDO(t)}{dt} = NPP(t) - R(t) + F_{atm}(t) + \varphi\,(t)$$

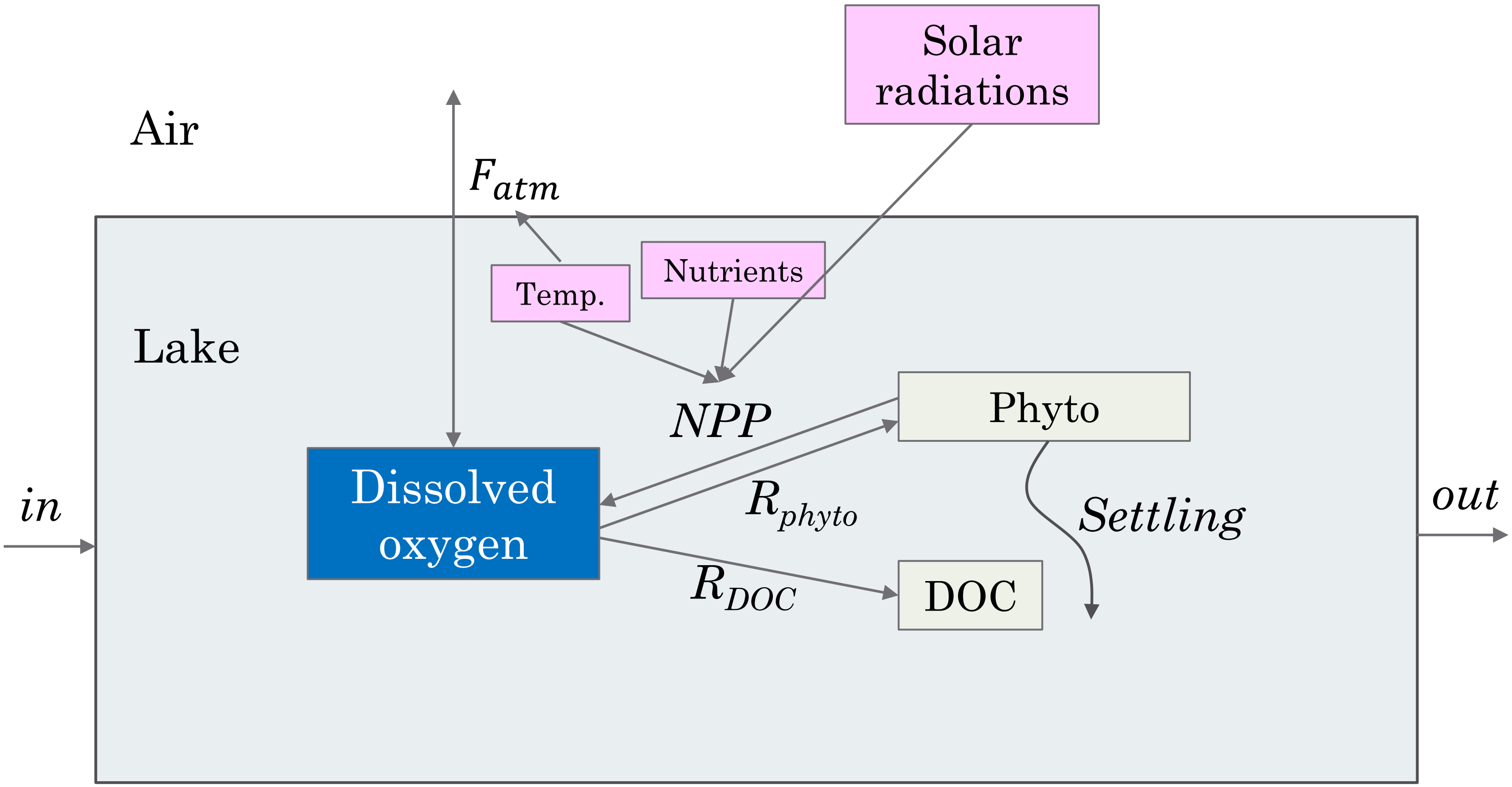
$$R(t) = R_{phyto}(t) + R_{DOC}(t)$$

$$\frac{dPhyto(t)}{dt} = NPP(t) - R_{phyto}(t) - Settling(t)$$



$$\frac{dDO(t)}{dt} = NPP(t) - (R_{phyto}(t) + R_{DOC}(t)) + F_{atm}(t) + \varphi\ (t)$$

$$NPP(t)\ = f(Radiations(t), [Nutrients](t), temperature(t))$$

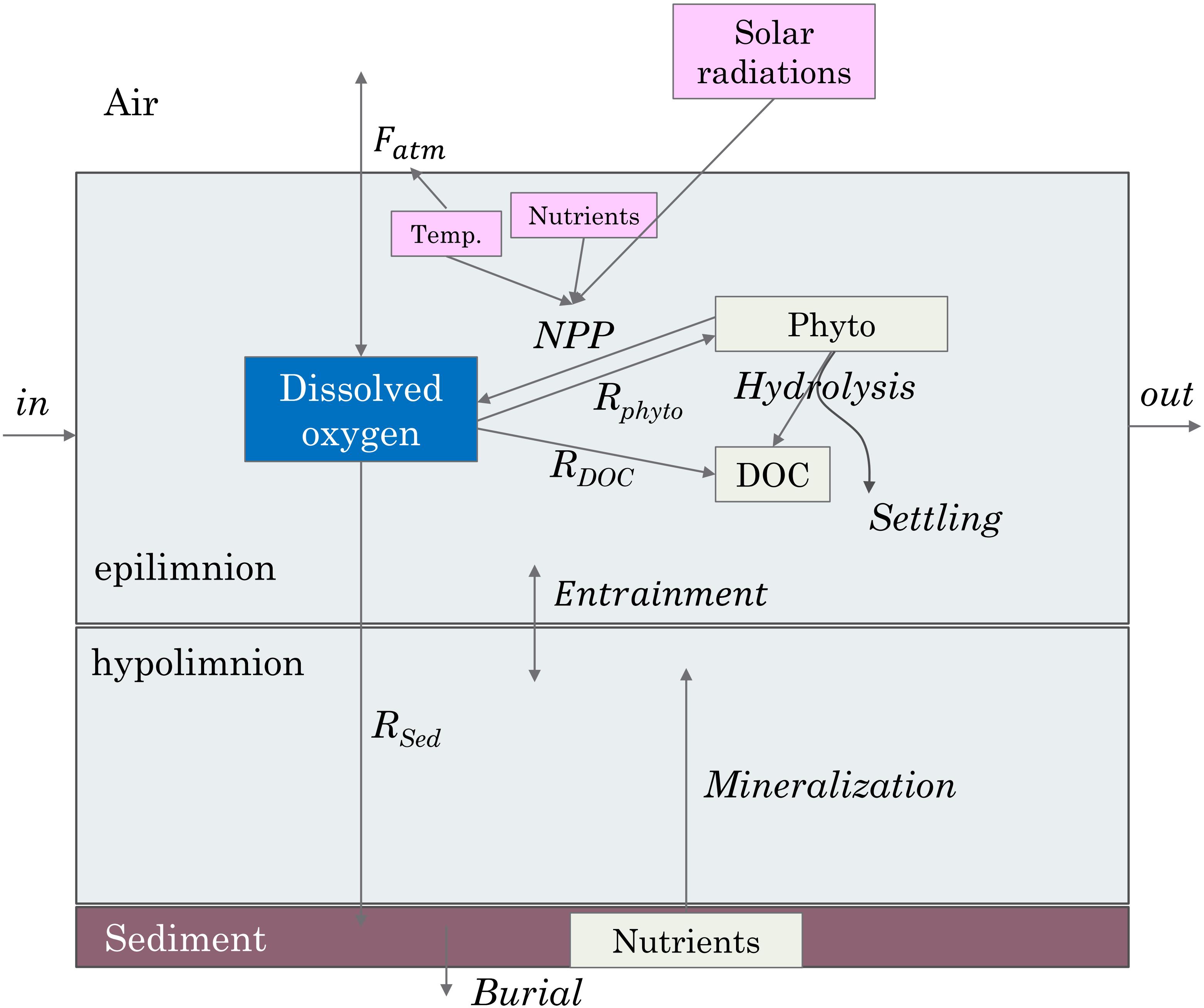


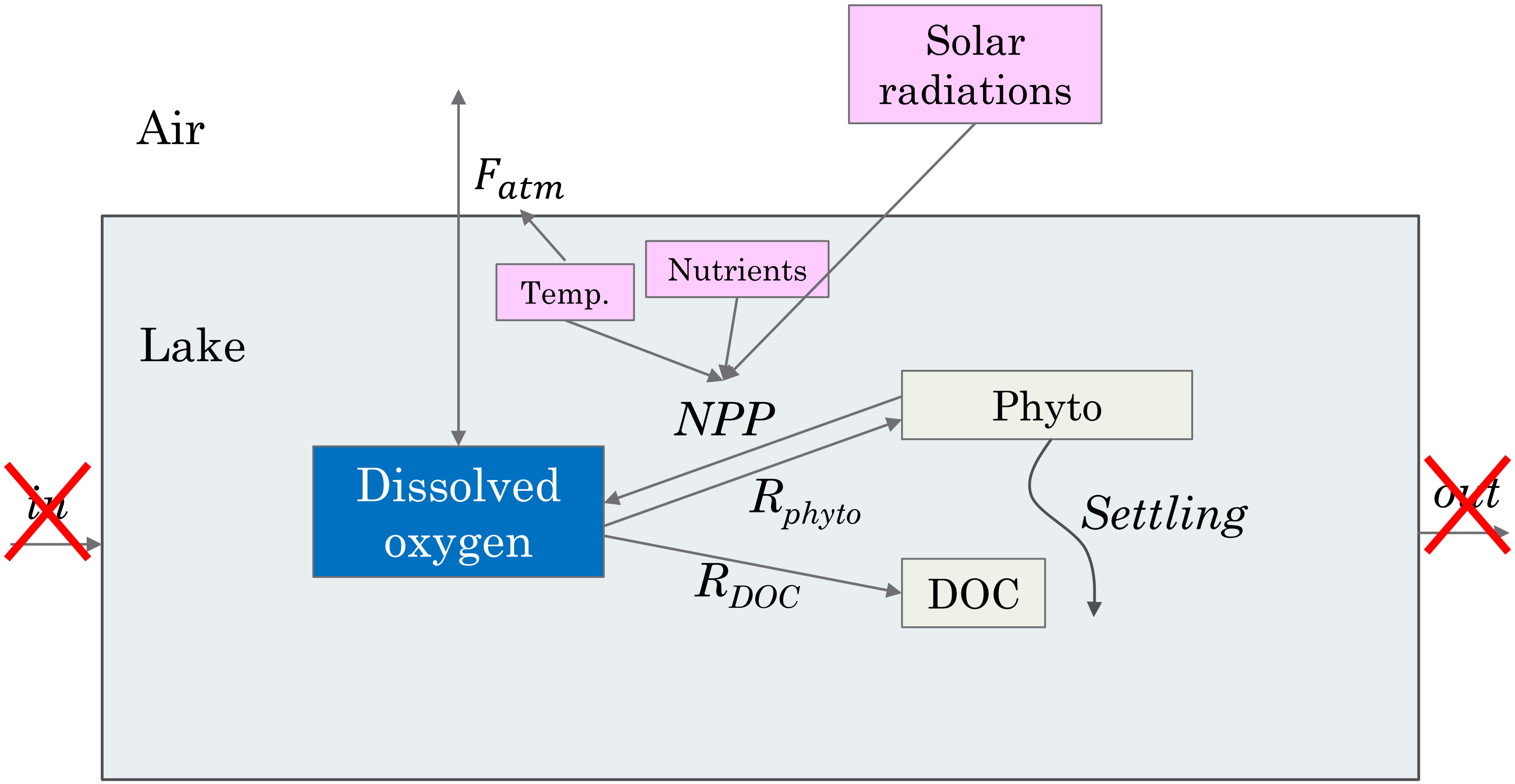
$$\frac{dDO(t)}{dt} = NPP(t) - (R_{phyto}(t) + R_{DOC}(t)) + F_{atm}(t) + \varphi\ (t)$$

$$NPP(t) \ = f(Radiations(t), [Nutrients](t), temperature(t))$$

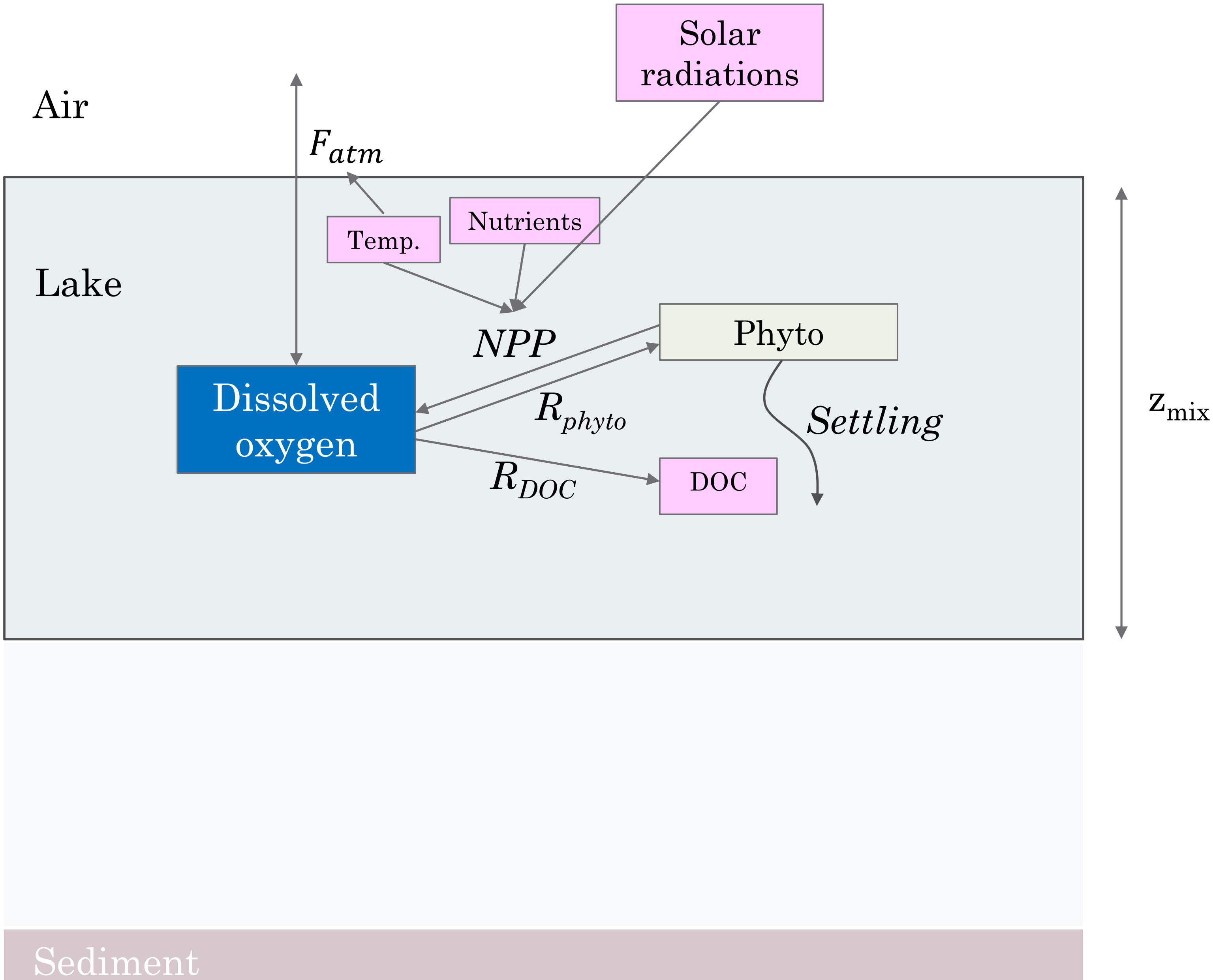
$$R_{DOC}(t) = f([DOC](t))$$

$$Settling(t) = f(z_{mix}\ (t), Phyto(t))$$


Solar radiations
Air
F_{atm}
Nutrients
Temp.
NPP
Phyto
Hydrolysis
in
Dissolved oxygen
R_{phyto}
out
R_{DOC}
DOC
Settling
epilimnion
Entrainment
hypolimnion
R_{Sed}
Mineralization
Sediment
Nutrients
Burial



$$\frac{dDO(t)}{dt} = NPP(t) - (R_{phyto}(t) + R_{DOC}(t)) + F_{atm}(t) + \cancel{\varphi(t)}$$


Solar radiations
Air
F_{atm}
Temp.
Nutrients
Lake
NPP
Phyto
Dissolved oxygen
R_{phyto}
Settling
z_{mix}
R_{DOC}
DOC
Sediment

In discrete time form

$$\frac{dDO(t)}{dt} = NPP(t) - (R_{phyto}(t) + R_{DOC}(t)) + F_{atm}(t)$$

$$DO(t) = DO(t-1) + NPP(t) \cdot k_{C \to O2} - (R_{phyto}(t) + R_{DOC}(t)) \cdot k_{C \to O2} + F_{atm}(t)$$

Oxygen at the current time step *(t)*, is equal to what it was at the previous time step (*t-1*), plus the mass movement of oxygen through a set of processes : gross primary production, respiration, atmospheric exchange and physics.

In a R code:

```
doPredic[i] = doPredic[i-1] + npp[i]*CtoO2 - Rtot[i]*CtoO2 + fatm[i]
```

In discrete time form

$$\frac{dPhyto(t)}{dt} = NPP(t) - R_{phyto}(t) - Settling(t)$$

$$phyto(t) = \ phyto(t-1) + \ NPP(t) - R_{phyto}(t) - Settling(i)$$

Phytoplankton biomass at the current time step (*t)*, is equal to what it was at the previous time step (*t-1*), plus what is being produced through photosynthesis, minus what is lost by respiration and settling

In a R code:

```
phyto[i] = phyto[i-1] + npp[i] - Rphyto[i] – Settling[i]
```

Additional equations

$$F_{atm}(t) = dt \cdot k_{DO}\big(DO_{sat}(t) - DO(t-1)\big)/z_{mix}$$

$$DO_{sat}(t) = -6 \cdot 10^{-5} \cdot wTemp(t)^3 + 69 \cdot 10^{-4} \cdot wTemp(t)^2 \\ -0.3906 \cdot wTemp(t) + 14.578$$

$$Settling(t) = dt \cdot phyto(t-1)\,\frac{settling_{phyto}}{z_{mix}}$$

$$NPP(t) = dt \cdot PAR(t) \cdot phosphorus \cdot pNPP \cdot \theta_{NPP}^{(wTemp(t)-20)}$$

$$R_{DOC}(t) = dt \cdot DOC \cdot docR$$

$$R_{phyto}(t) = dt \cdot phyto(t-1) \cdot phytoR \cdot \theta_{R}^{(wTemp(t)-20)}$$

$$R(t) = R_{DOC}(t) + R_{phyto}(t)$$

These equations (in a R code)

```
fatm[i] = dt * kDO * (dosat[i] - doPredic[i-1]) / zMix

dosat[i] = -0.00006 * wTemp[i]^3 + 0.0069 * wTemp[i]^2
         - 0.3906 * wTemp[i] + 14.578

Settling[i] = dt * phyto[i-1] * settlingPhyto/zMix

npp[i] = dt * PAR[i] * phosphorus * pNPP *
            thetaNPP^(wTemp[i] - 20)

RDOC[i] = dt * DOC * docR

Rphyto[i] = dt * phyto[i-1] * phytoR * thetaR^(wTemp[i] - 20)

Rtot[i] = RDOC[i] + Rphyto[i]
```

Constants

Constant name	value	units	Definition
$k_{C\rightarrow O2}$	32/12	d.l.	Molar ratio between C and O2
k_{DO}	1	m/d	Gas exchange coefficient, usually computed from wind speed
z_{mix}	10	m	Depth of mixed layer (or epilimnion)
$settling_{phyto}$	1	m/d	Settling velocity of phytoplankton cells
$phosphorus$	0.050	µgP/L	Phosphorus concentration
$pNPP$	0.08	mgC/unitP/unitLight	Conversion factor
θ_{NPP}	1.2	d.l.	Arrhenius coefficient for temperature adjustment for NPP
DOC	5	mg/L	Dissolved organic C concentration
$docR$	0.02	d.l.	1^{st} order decay of DOC
$phytoR$	0.8	d.l.	1^{st} order decay of phytoplankton
θ_R	1.08	d.l.	Arrhenius coefficient for temperature adjustment for R

Demo

https://github.com/camilleminaudo/oxygen-model-student

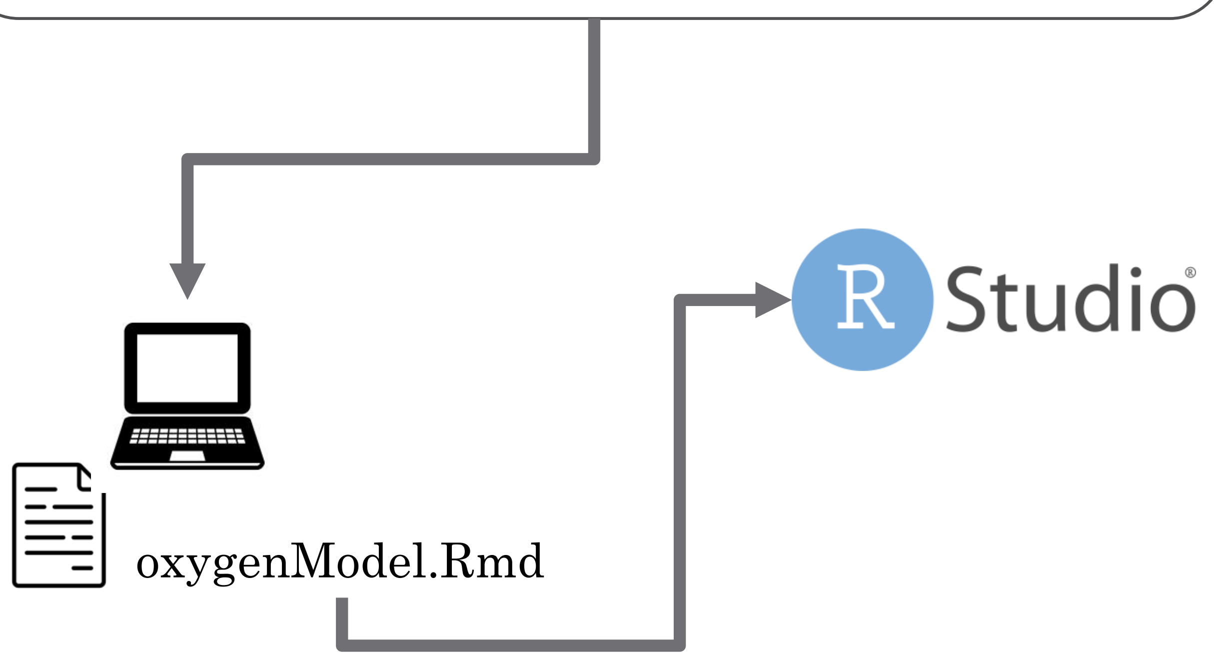
Part 2

Model implementation

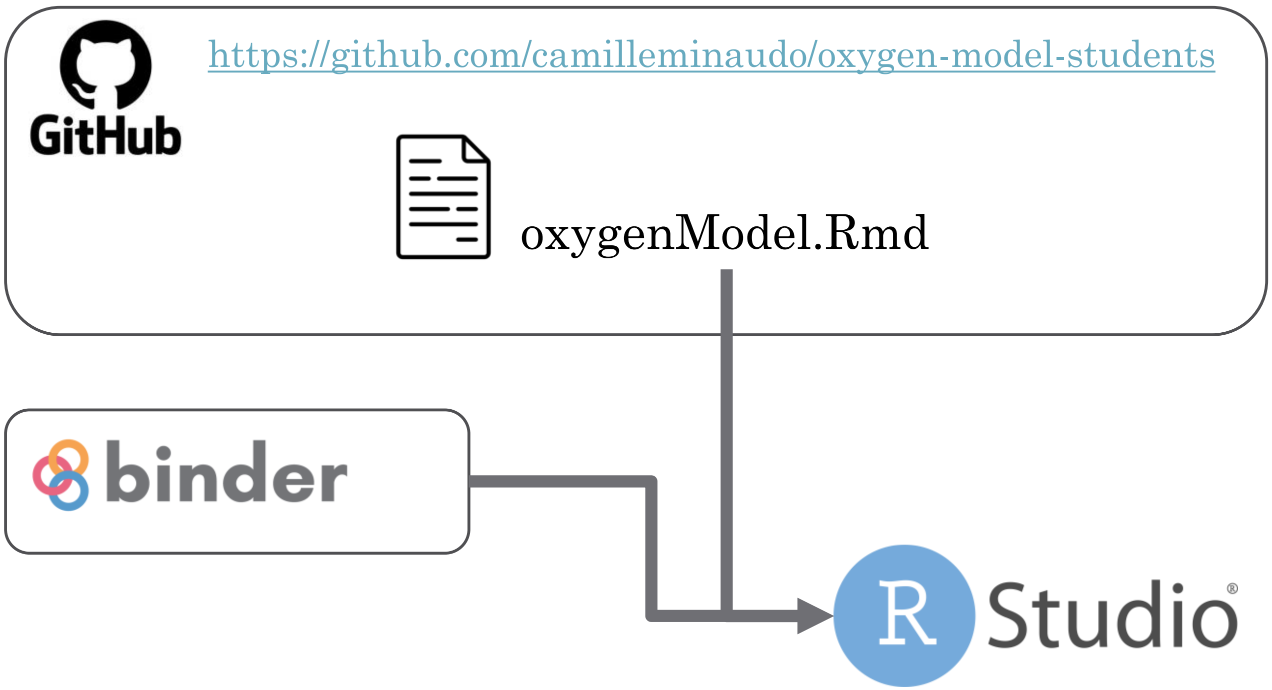
You have RStudio installed

https://github.com/camilleminaudo/oxygen-model-students

- Option A: download the entire repository
- Option B: clone to this repository



You don’t have RStudio installed



The model, step by step

- (Create a GitHub account)
- Go to https://github.com/camilleminaudo/oxygen-model-students
- Click on “lauch binder” in the README.md file
- Wait for installation and Jupyter install
- Open a Rstudio notebook
- Open the file oxygenModel.Rmd
- Follow instructions and run the model