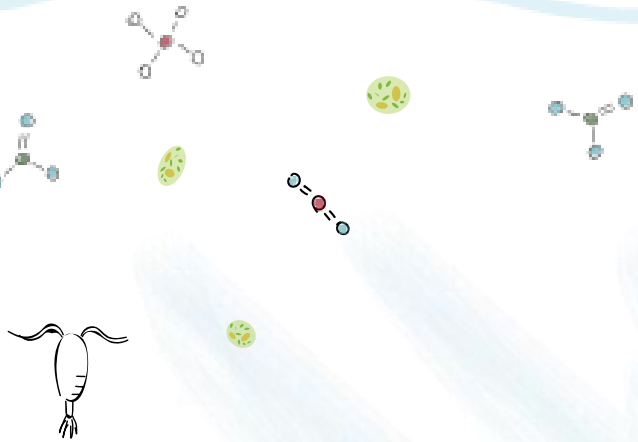

Reactive Transport in the Hydrosphere

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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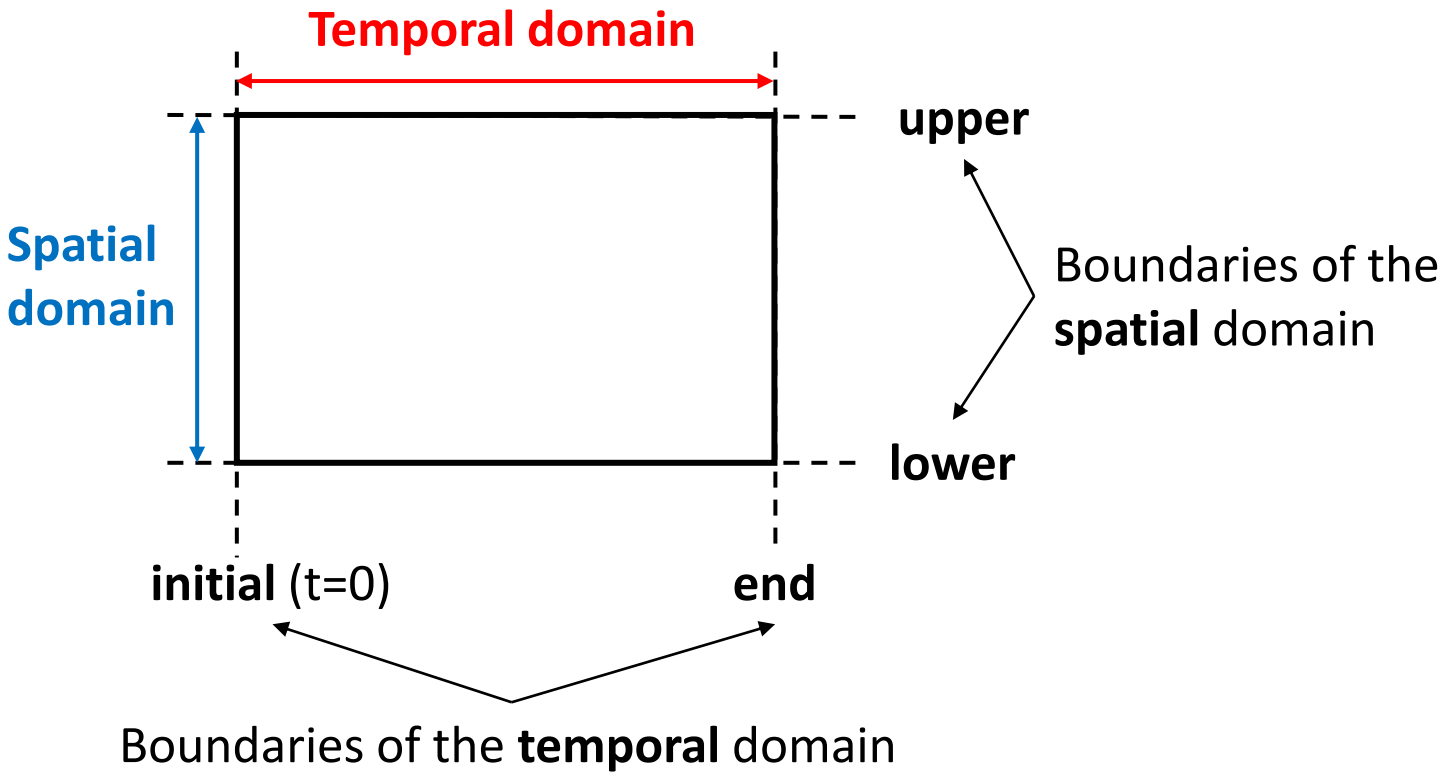
Solving reaction-transport equation

$$\frac{\partial C_f}{\partial t} = \frac{1}{f} \cdot \frac{\partial}{\partial x}\left(f \cdot D_f \cdot \frac{\partial C_f}{\partial x} \right) - \frac{1}{f} \cdot \frac{\partial}{\partial x}\left(f \cdot v_f \cdot C_f \right) + R_f$$

f = volume fraction



We need to specify **conditions** at **some** of these **boundaries**!

Boundary conditions

Steady state:

$$\mathbf{0} = \frac{\partial C_f}{\partial t} = \frac{1}{\boldsymbol{f}} \cdot \frac{\partial}{\partial x}\left(\boldsymbol{f} \cdot D_f \cdot \frac{\partial C_f}{\partial x}\right) - \frac{1}{\boldsymbol{f}} \cdot \frac{\partial}{\partial x}\left(\boldsymbol{f} \cdot v_f \cdot C_f\right) + R_f$$

Only conditions at **spatial boundaries** are required

For every component!

If diffusion is negligible:

Transport in **1** direction!

upper

v_f = advective transport

→ **1 boundary condition required**

If diffusion is important:

Transport in **2** directions!

upper

diffusive transport

lower

→ **2 boundary conditions required**

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Boundary conditions

Typically:

Upper boundary (e.g., sediment-water interface, start of a river stretch)

- Imposed **flux** for **solid** substances (e.g., particulate organic carbon, mineral particles)
- Imposed **concentration** in the liquid phase for **solutes** (e.g., O_2, nutrients)

Lower boundary (**if** needed, i.e., if diffusive transport cannot be neglected)

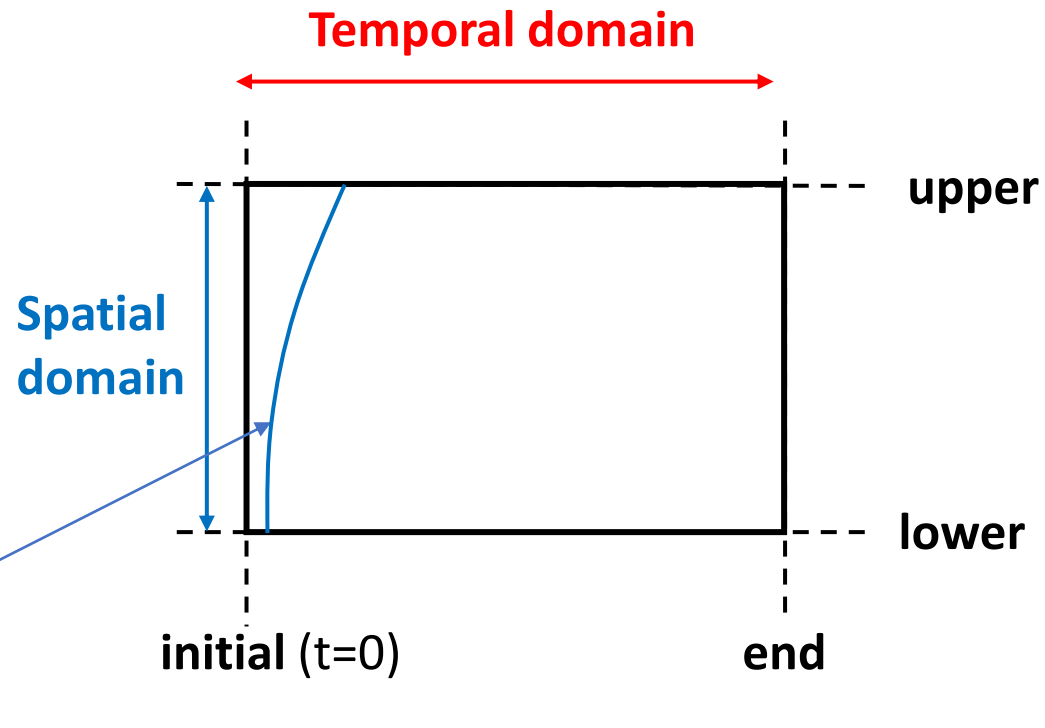
- **Zero gradient** for both solids/solutes

  (Based on the idea that resources that drive reactions are depleted at the lower boundary -> ***"nothing happens any more"*** -> no spatial variation)

In general, boundary conditions must reflect **realistic** assumptions about the modeled system!

Boundary conditions

Transient state:

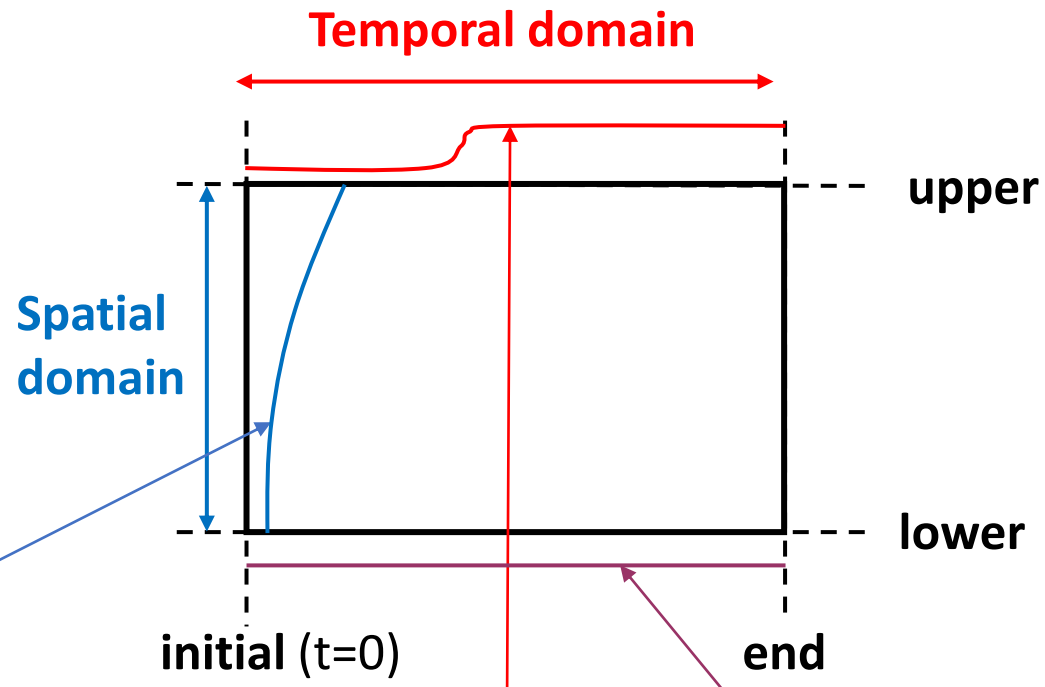


1. $C(0, x) = C_{ini}(x)$ **Initial** distribution for the **entire spatial** domain.

Boundary conditions

Transient state:

For every component!



1. $C(0, x) = C_{ini}(x)$ **Initial** distribution for the **entire spatial** domain.

2. **Imposed over** the **entire temporal** domain.

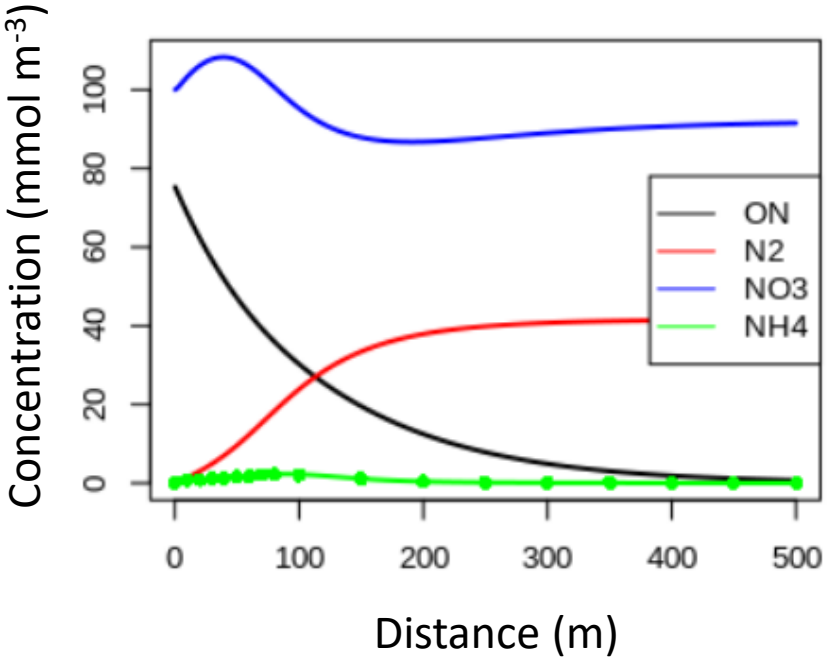
   If diffusion **is** negligible: $C_{upper}(t)$ or $J_{upper}(t)$

   If diffusion **cannot** be neglected: $C_{upper}(t)$ or $J_{upper}(t)$ & $C_{lower}(t)$ or $J_{lower}(t)$

Examples of solutions

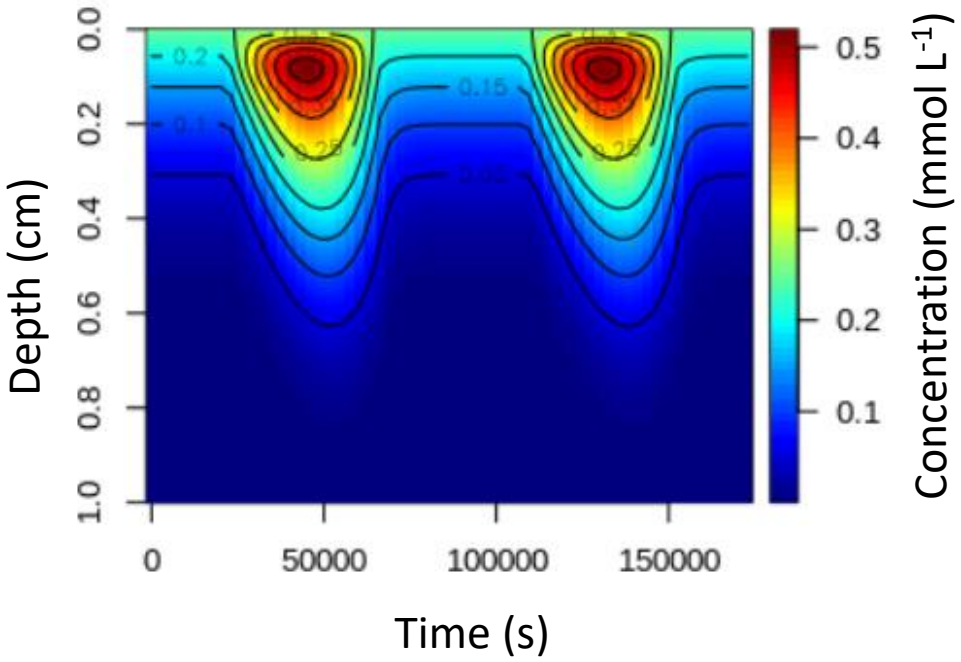
Steady state

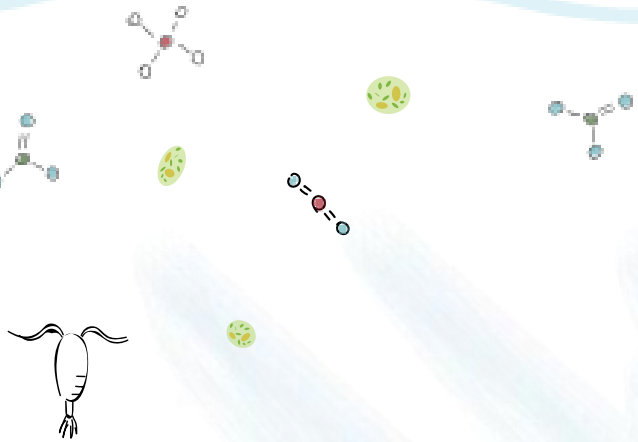
Dissolved N species along an aquifer



Transient

O2 in a microphytobenthic biofilm





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