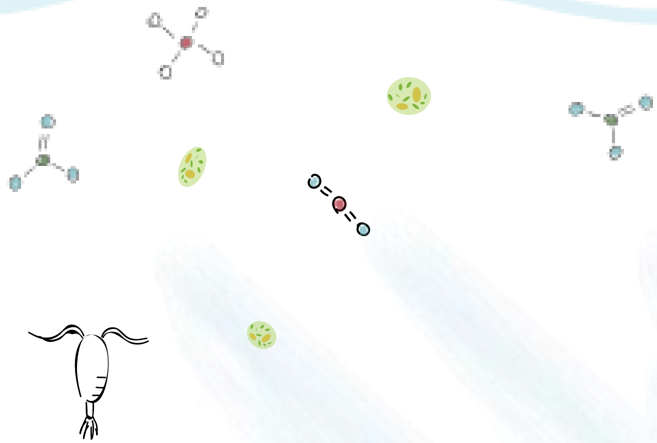

Reactive Transport in the Hydrosphere

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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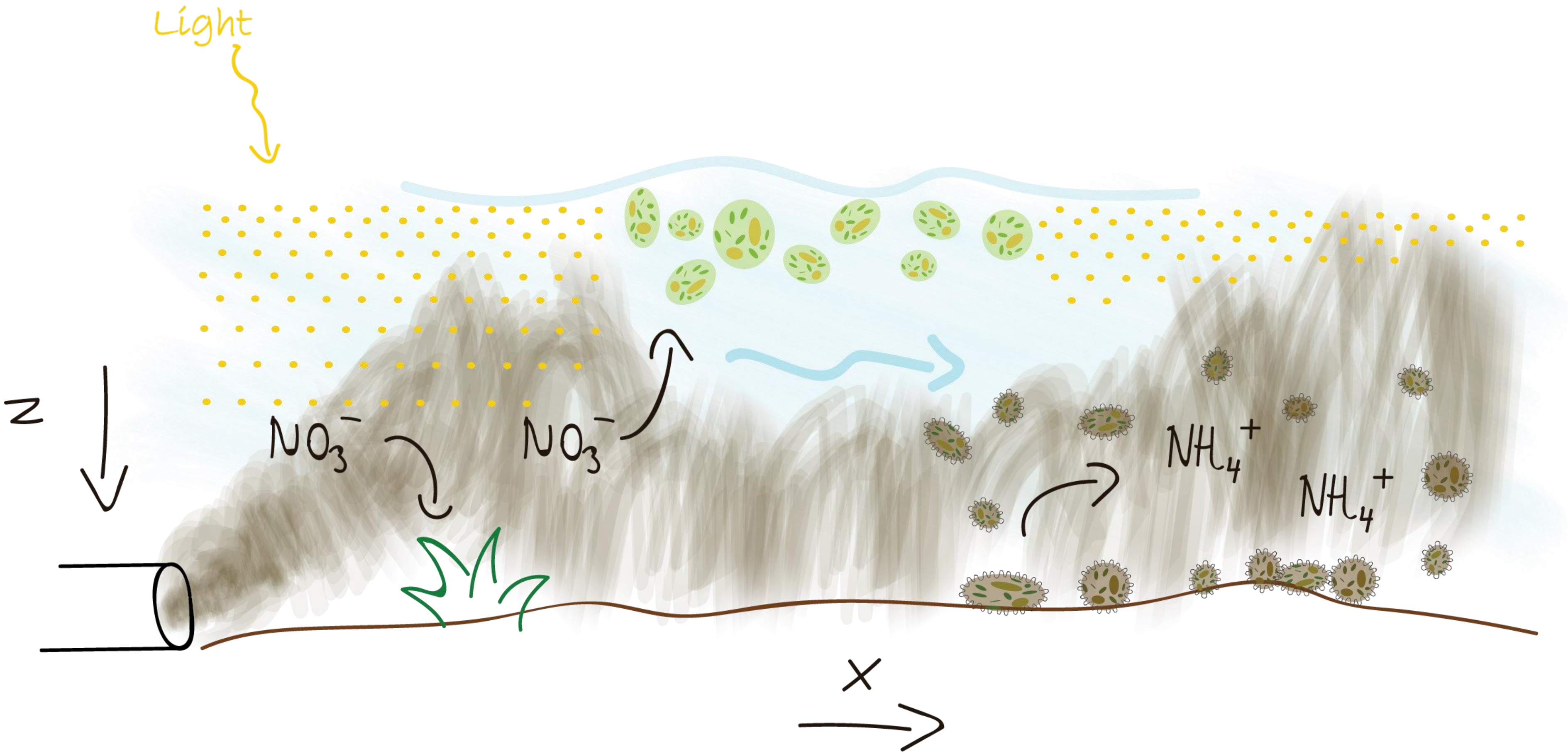
Towards **spatially resolved** models

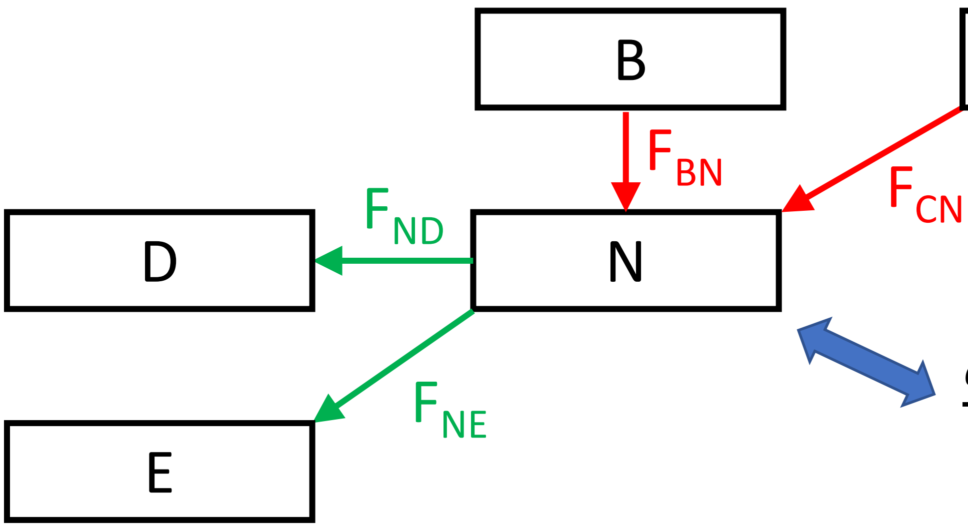


How do we include transport?

Conceptual level & mass balance equations

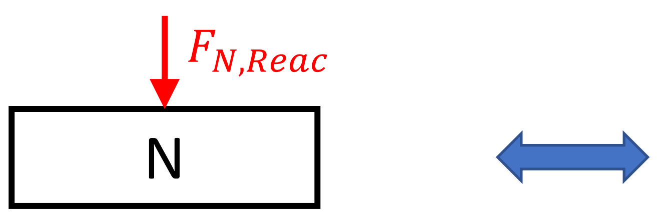
Until now:

- **Homogeneous** distribution of the system components (state variables)



$$\frac{d[\mathrm{N}]}{dt} = \underbrace{F_{BN} + F_{CN} - F_{ND} - F_{NE}}$$

Lump into **net reaction flux (rate)**



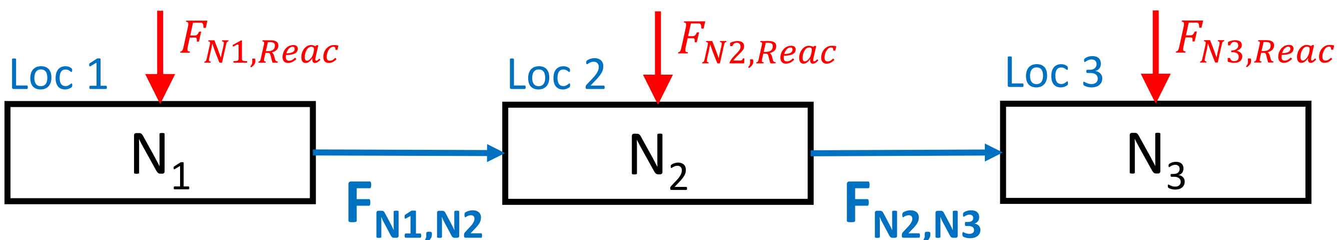
$$\frac{d[\mathrm{N}]}{dt} = F_{N,Reac}$$

How do we include transport?

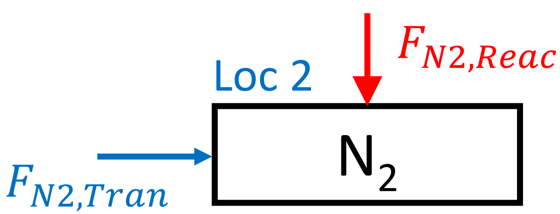
Conceptual level & mass balance equations

Now:

- State variable **varies in space**



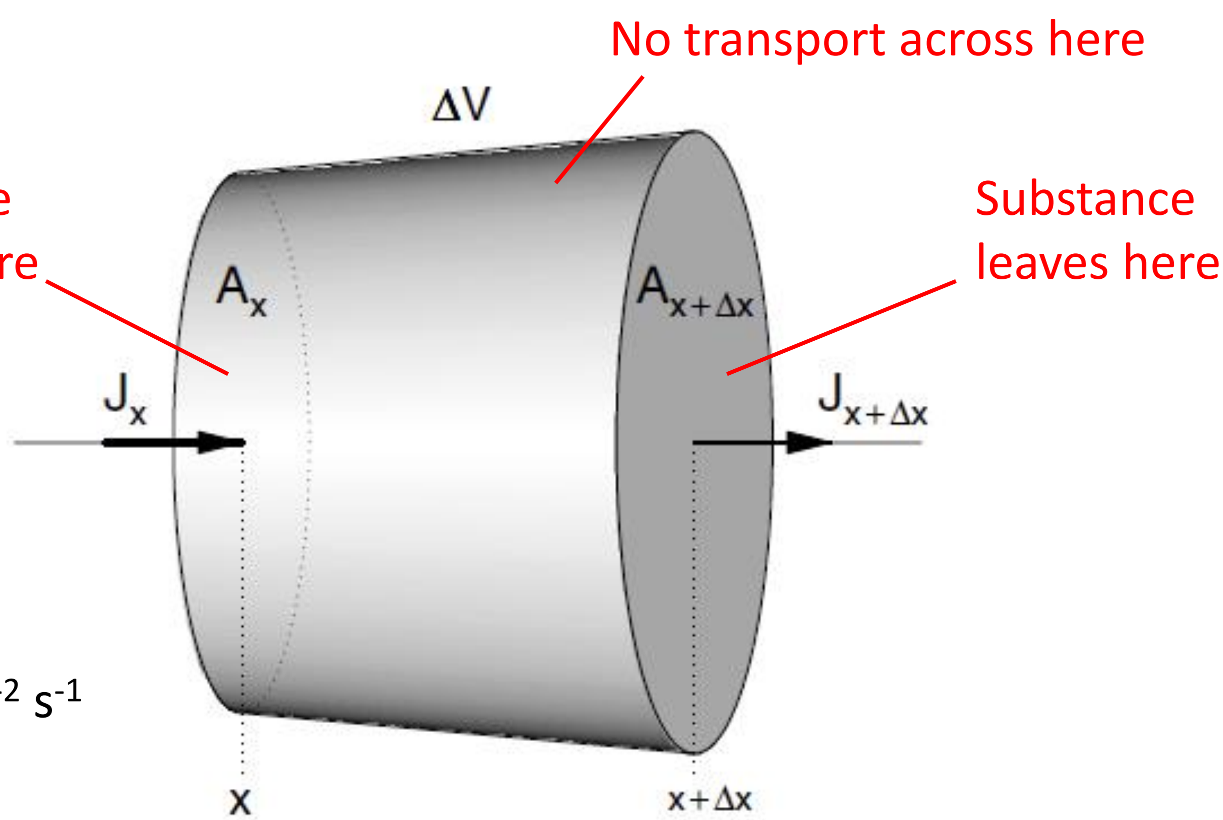
$$\frac{d[\mathrm{N}_2]}{dt} = F_{N2,Reac} + \underbrace{F_{N1,N2} - F_{N2,N3}}_{\text{Lump into \textbf{net transport flux (rate)}}}$$



$$\frac{d[\mathrm{N}_2]}{dt} = F_{N2,Reac} + F_{N2,Tran}$$

Mathematical formulation of transport

Transport flux: **J**



- Areas in m^2
- Fluxes in mol m^{-2} s^{-1}
- Distance in m

Mass balance equation:

$$\frac{\partial Amount}{\partial t} = \text{Input} - \text{Output}$$

$$= A_x \cdot J_x - A_{x+\Delta x} \cdot J_{x+\Delta x}$$

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Mathematical formulation of transport

$$\frac{\partial Amount}{\partial t} = A_x \cdot J_x - A_{x+\Delta x} \cdot J_{x+\Delta x}$$

Divide by ΔV

$$\frac{\partial C}{\partial t} = \frac{A_x \cdot J_x - A_{x+\Delta x} \cdot J_{x+\Delta x}}{\Delta V}$$

Approximate ΔV = $A_{x+\Delta x/2} \cdot \Delta x$

$$\frac{\partial C}{\partial t} = \frac{A_x \cdot J_x - A_{x+\Delta x} \cdot J_{x+\Delta x}}{A_{x+\Delta x/2} \cdot \Delta x}$$

Make a limit $\Delta x \rightarrow 0$

Mass balance equation: $$\frac{\partial C}{\partial t} = -\frac{1}{A} \cdot \frac{\partial (A \cdot J)}{\partial x}$$

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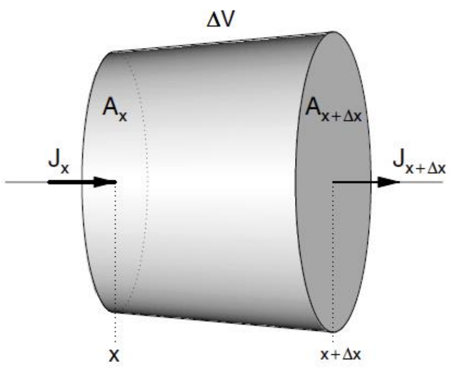
Mathematical formulation of transport

Mass balance equation (**1D**-transport):



Rate of change in concentration in **time**

$$\boxed{\frac{\partial C}{\partial t} = R_{Reac} - \frac{1}{A} \cdot \frac{\partial (A \cdot J)}{\partial x}}$$

Net rate of change due to **local reactions**

Rate of change in $A \cdot J$ in **space**

= **Net** rate of change due to **transport**

Similar mass balance equation for **each** component in the system

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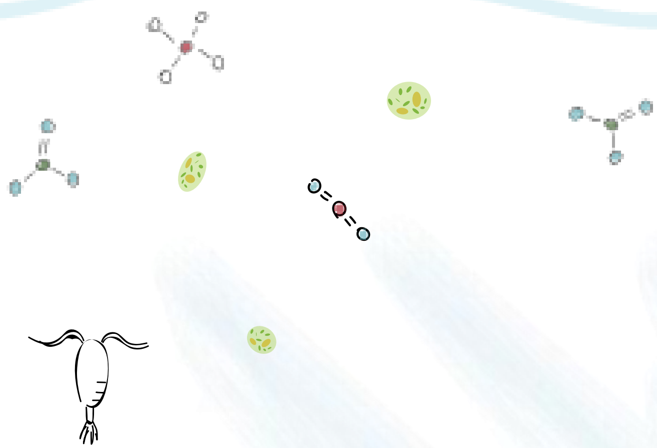

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