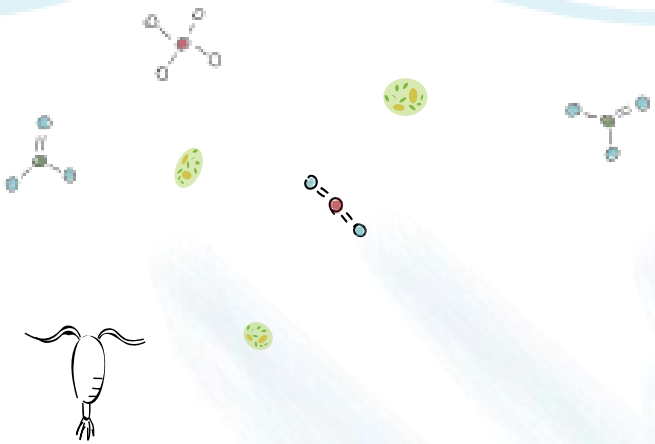

Reactive Transport in the Hydrosphere

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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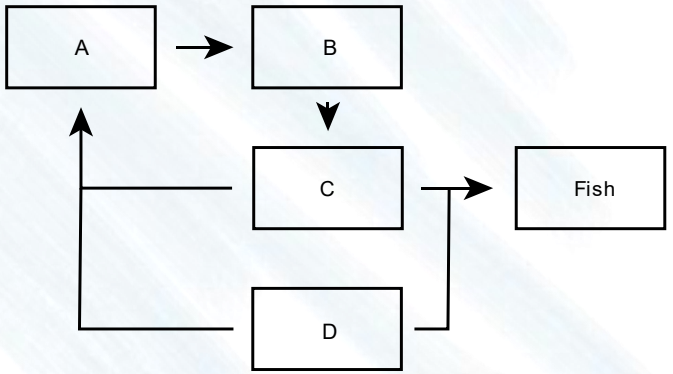
Model formulation

From a problem to a conceptual diagram



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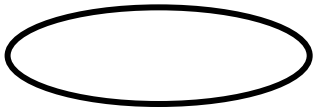
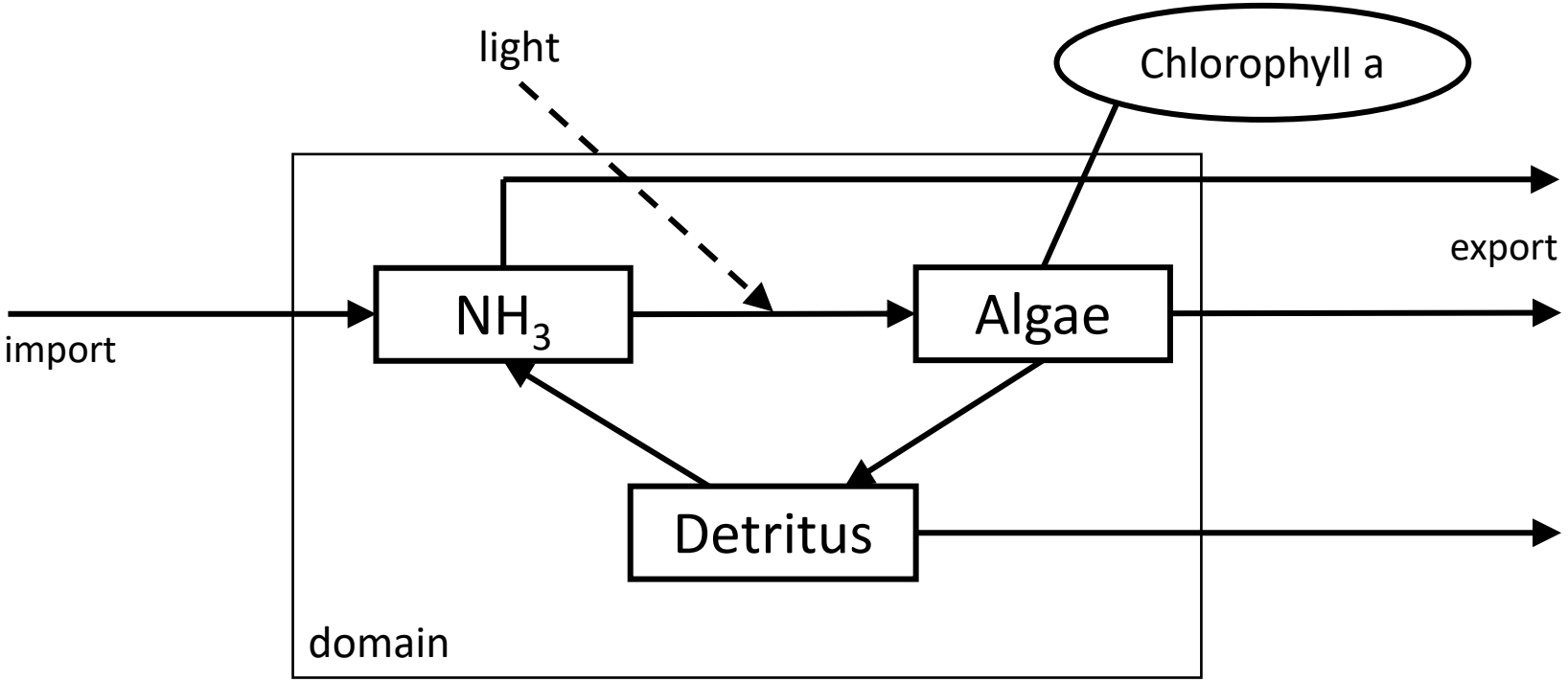
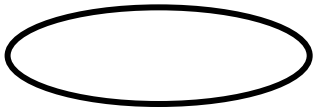
Model components

State variable	Process (incl. transport)	External forcing	Derived variable
			



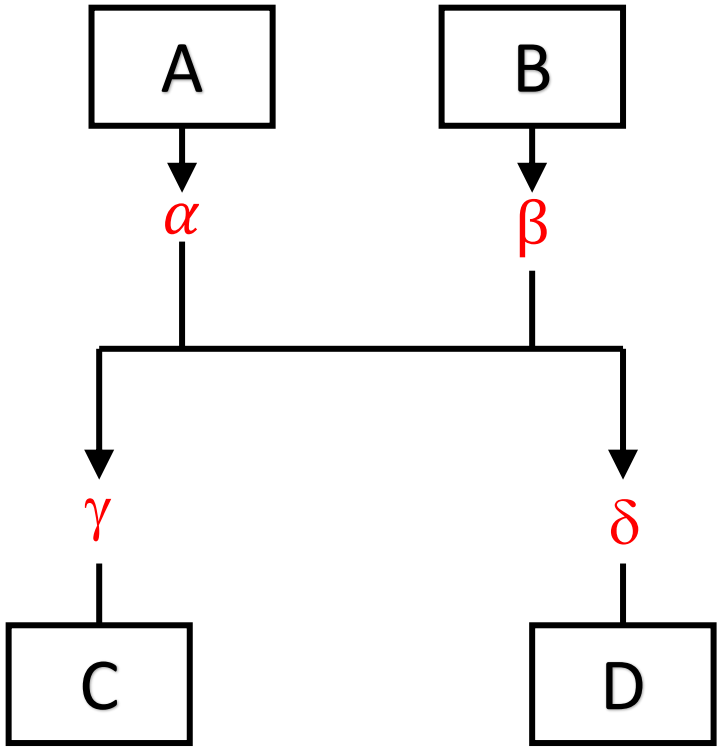
Model components

State variable	Process (incl. transport)	External forcing	Derived variable
			

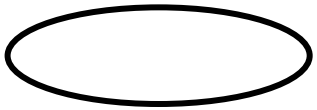
Chemical reactions

$$\alpha A + \beta B \rightarrow \gamma C + \delta D$$

Stoichiometric coefficients:
Moles of reactants and products
per mole reaction



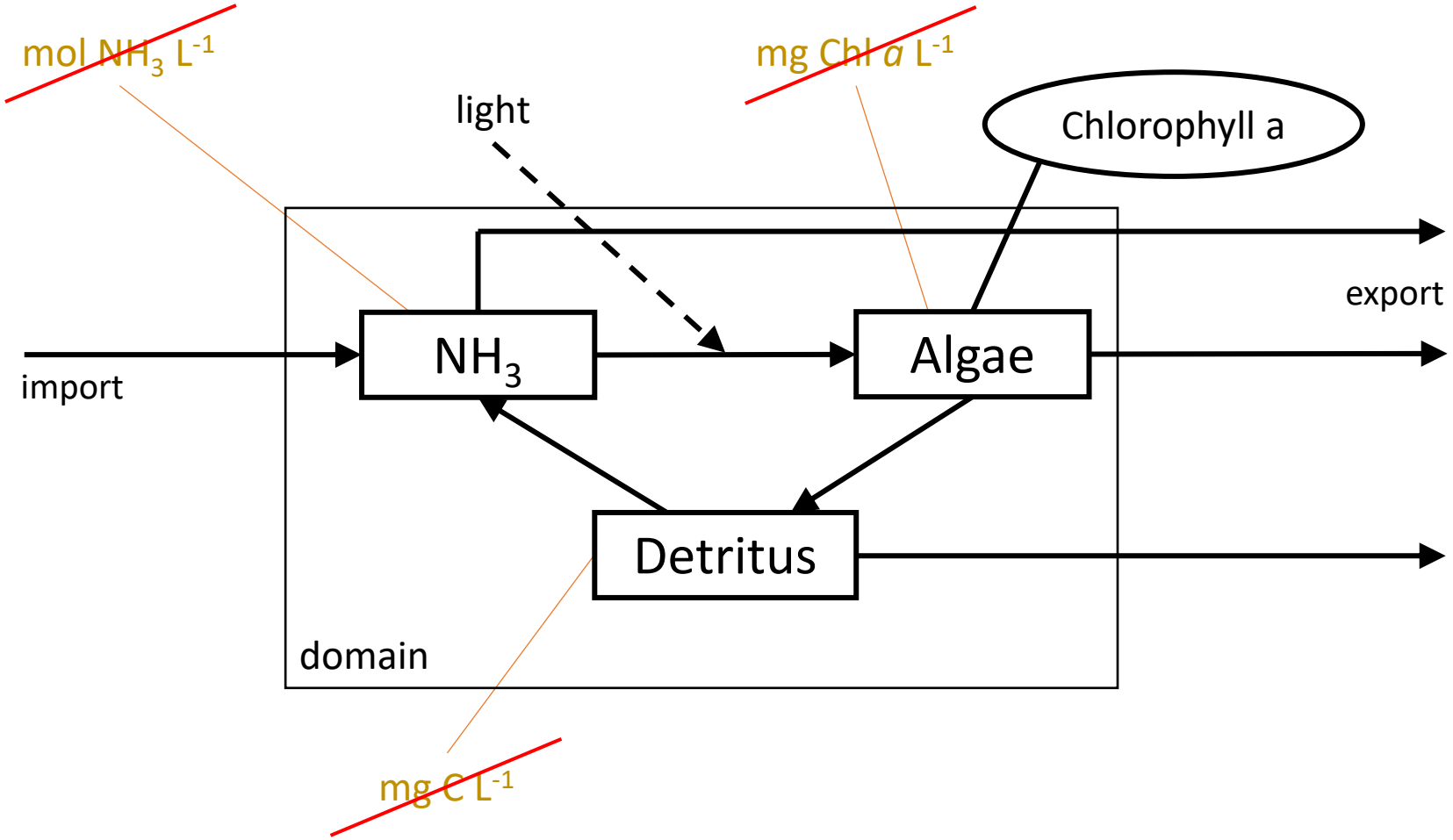
Model components

State variable	Process (incl. transport)	External forcing	Derived variable
			

Additionally:

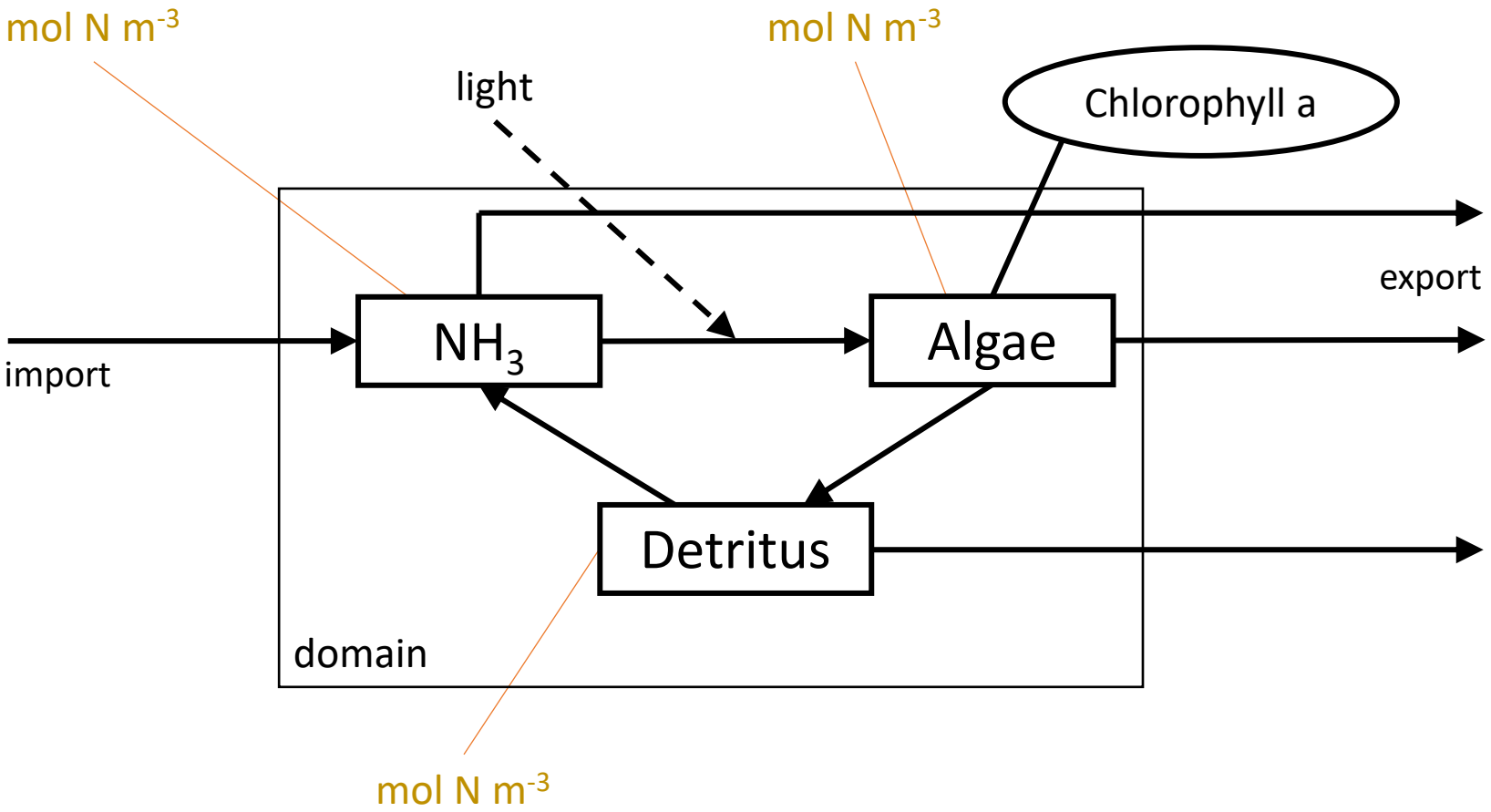
- Spatial and temporal **domain**
- Conditions at the domain boundaries (i.e., **boundary conditions**)
- Model **currency**
- **Units** of each state variable

Model currency and units of state variables



Common model currency: **N**

Model currency and units of state variables



Common model currency: **N**

Equal unit for each state variable: **mol N m^{-3}**

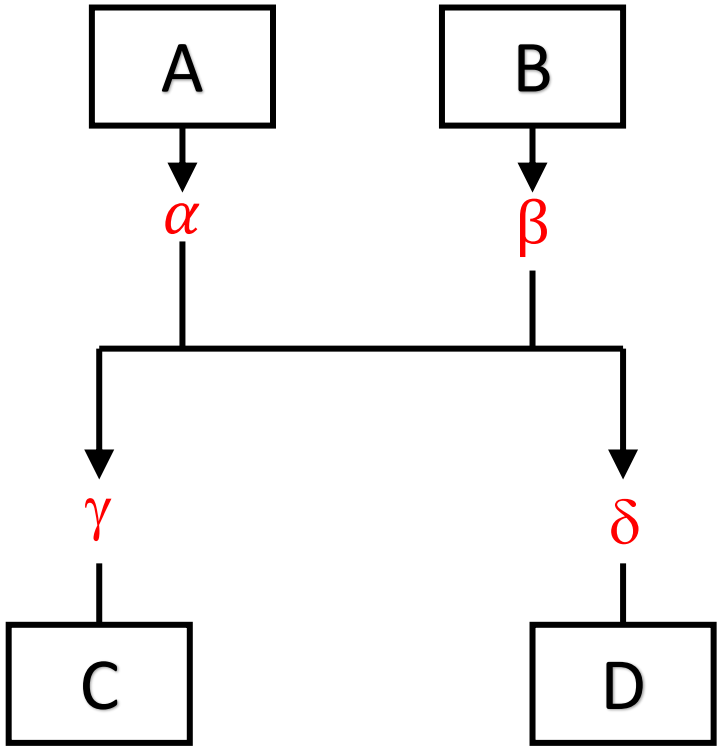
Model currency and units of state variables

Common model currency **not useful** for modeling chemical reactions.

Chemical reactions

$$\alpha A + \beta B \rightarrow \gamma C + \delta D$$

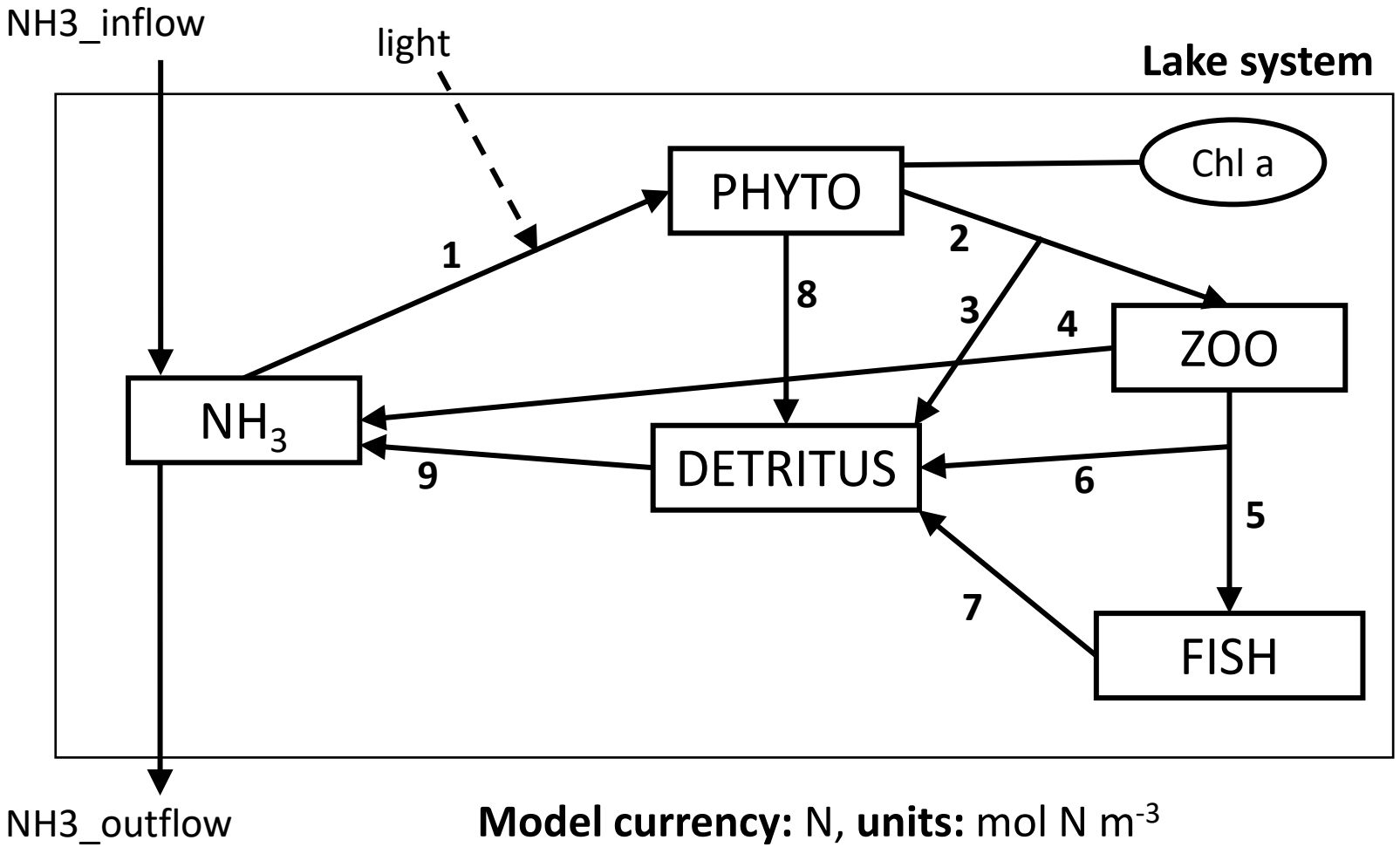
Stoichiometric coefficients:
Moles of reactants and products
per mole reaction



Better:

- Species A: **mol A L^{-1}**
- Species B: **mol B L^{-1}**
- Etc.

More complex example



Model currency: N, **units:** mol N m^{-3}
Spatial scale: entire lake
Temporal scale: annual
Processes: arrows 1-9
Domain boundaries: NH3_inflow, NH3_outflow