Modeling of geochemical processes

Global Systems

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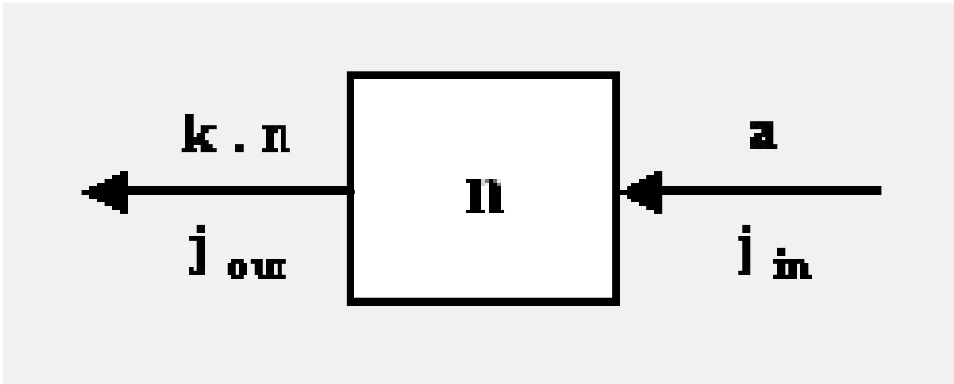
Dynamic models

Global systems

Reservoirs and fluxes



Flux into reservoir, $\mathbf{j}_{in}$, flux out from reservoir, $\mathbf{j}_{out}$, reservoir content **n**.
n [ton, kg, mol, mol/l ...], **j** [ton/year, mol/day ...]

Assumption: the flux from the reservoir is directly proportional to concentration or reservoir content. **k** is a constant.

Example: the flux of sulfates from ocean to sediments is proportional to sulfate content in ocean.
Example: a photosynthesis rate is proportional to CO_2-content in atmosphere

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If $\mathbf{j_{in}} \sim \mathbf{a}$ = const., it si valid for the reservoir content **n**: $+\frac{dn}{dt} = a - kn$

Steady state: reservoir content is constant $+\frac{dn}{dt} = 0$

Then **a – kn = 0** and $n = n_{ss} = \frac{a}{k}$

The solution of the differential equation ($t = 0$, $n = n_0$): $n = \frac{a}{k} - \left(\frac{a}{k} - n_0\right) e^{-kt}$

reorganizing gives: $n = n_0\, e^{-kt} + \frac{a}{k}\left(1 - e^{-kt}\right)$

Interpretation:

(1) Initial content of element $\mathbf{n_0}$ is transformed into steady state content $\mathbf{n_{ss} = a/k}$,

with decrease of the exponential term e^{-kt} with time. In time $t = 0$ is $e^{-kt} = 1$

(2) Initial content of element $\mathbf{n_0}$ decays in $t = \infty$ $(e^{-kt} = 0)$

the second term is **a/k** at this time! $\frac{a}{k}\left(1 - e^{-kt}\right)$

Infinite time is needed for reaching the steady state.

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However, significant decrease of the exponential term e^{-kt}

is reached at $t = \frac{1}{k}$ where $e^{-kt} = \frac{1}{e} = 0.3679$

This time is a *response time*

The residence time is given by

$$\tau_{res} = \frac{n_{ss}}{\dot{j}_{in}} = \frac{n_{ss}}{\dot{j}_{out}}$$ Substitution gives $$\tau_{res} = \frac{a/k}{a} = \frac{1}{k}$$

For simple linear model, *response time* equals *residence time*

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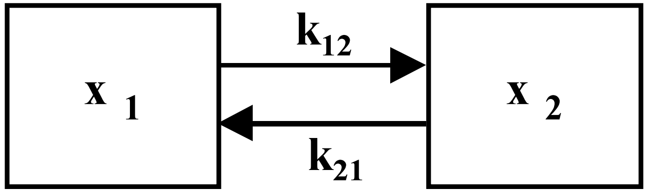
Two-reservoir model



The increments in reservoir contents are expressed by differential equations

$$+\frac{dx_1}{dt} = -k_{12}x_1 + k_{21}x_2 \qquad +\frac{dx_2}{dt} = \quad k_{12}x_1 - k_{21}x_2$$

In matrix form, it is $$\frac{d}{dt}\begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} -k_{12} & k_{21} \\ k_{12} & -k_{21} \end{bmatrix}\begin{bmatrix} x_1 \\ x_2 \end{bmatrix}$$

In vector form, it is $\frac{d\mathbf{x}}{dt} = \mathbf{K}\ \mathbf{x}$, where **x** is a vector of variables $\mathbf{x_i}$ and **K** is matrix of rate constants