Modelling Global Biogeochemical Cycles Part I

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Chapter 4: Modeling Biogeochemical Cycles
Outline

- Mass balance equations
- Matrix representation
- Diagnostic times
Earth system models

- Movement and transport of energy and matter across Earth’s main reservoirs
- Use for climate change simulations
- Help us understand connections among Earth system processes
Biogeochemical elements follow conservation laws

- Mass cannot be created or destroyed. The change of mass $M$ over time is the result of inputs minus outputs of mass.

\[
\frac{dM}{dt} = \text{Inputs} - \text{Outputs}
\]
Compartmental theory

Definitions:

- Compartment/reservoir/pool: an amount of material defined by certain physical, chemical, or biological characteristics and is kinetically homogeneous. We characterize compartments by their mass.

- Flux: amount of material transferred from one compartment to another per unit of time, i.e. \([\text{mass time}^{-1}]\)

- Rate: relative speed of change of the mass of a reservoir in units of inverse time, i.e. \([\text{time}^{-1}]\)
Steps for modeling biogeochemical cycling

- Define the boundaries and structure of the system through a conceptual diagram
- Define a mathematical model that captures the structure of the conceptual diagram
- Find the best set of parameters of the model
- Manipulate the mathematical model to observe its dynamics over time and compute other interesting diagnostics
Simple example: radioactive decay
Conceptual model: radioactive decay

Total number of $^{14}$C atoms (N)

Loss by radioactive decay

Question: How much mass remains after $x$ units of time?
Mathematical model

\[
\frac{dx}{dt} = Inputs - Outputs
\]

or

\[
\frac{dx}{dt} = Sources - Sinks
\]
Conceptual model: radioactive decay

\[
\frac{dN}{dt} = -\lambda \cdot N
\]
Mathematical solution

Initial value problem (IVP)

\[
\frac{dN}{dt} = -\lambda \cdot N, \quad N(t = 0) = N_0
\]
Mathematical solution

Initial value problem

\[
\frac{dN}{dt} = -\lambda \cdot N, \quad N(t = 0) = N_0
\]

Solution:

\[
N(t) = N_0 \exp(-\lambda \cdot t)
\]
Libby half-life for radiocarbon is 5568 years!

\[ t_{1/2} = 5568 = \frac{\ln 2}{\lambda}, \]

Then,

\[ \lambda = 0.0001244876 \text{ years}^{-1} \]
How much radiocarbon would be available after 10,000 years of radioactive decay if the initial amount of $^{14}$C atoms $N_0 = 100$?

$$N(t = 10000) = 100 \exp(\lambda \cdot 10000)$$

$$= 28.8$$
The one pool model

The mass balance equation:

\[
\frac{dx}{dt} = I - O
\]
\[= I - k \cdot x\]

- **I**: External flux from outside the system \([\text{mass} \cdot \text{time}^{-1}]\).
- **O = k \cdot x**: Flux leaving the system.
- **k**: Rate at which mass leaves the system \([\text{time}^{-1}]\).
Analytical solution of the one pool model

\[ x(t) = \frac{I}{k} - \left( \frac{I}{k} - x(0) \right) e^{-k \cdot t} \]

With initial condition \( x(0) = 0 \) Pg, \( I = 10 \) Pg \( \text{yr}^{-1} \), and \( k = 0.5 \) \( \text{yr}^{-1} \).
Effect of the initial conditions

Steady-State:
At steady-state, inputs are equal to outputs ($I = O = k \cdot x$), and

$$x = \frac{I}{k}$$
Turnover time

At steady-state, the ratio of the stock and the input or output flux is defined as the turnover time $\tau$

$$\tau = \frac{x}{I} = \frac{x}{k \cdot x}$$

$$\tau = \frac{1}{k}$$

Turnover time is usually interpreted as the time it would take to renew all mass in the reservoir, or the time it would take to fill or empty the reservoir.
Heterogeneous interconnected systems
Concept to math: balance equations

\[
\frac{dS_{V1}}{dt} = F_0 - F_1
\]
\[
\frac{dS_{V2}}{dt} = F_1 - F_2
\]
Example: a lake ecosystem

C cycle

\[
\begin{align*}
\frac{d\text{PHYTOC}}{dt} &= f_1 - f_2 - f_8 - f_9 \\
\frac{d\text{ZOOOC}}{dt} &= f_2 - f_3 - f_4 - f_5 - f_{13} \\
\frac{d\text{DETritusc}}{dt} &= f_3 + f_8 + f_6 + f_{12} + f_{13} - f_7 - f_{10} \\
\frac{d\text{FISHC}}{dt} &= f_5 - f_6 - f_{12} - f_{14} \\
\frac{d\text{BottomDetritusc}}{dt} &= f_7 + f_9 - f_{11}
\end{align*}
\]
The matrix with fluxes among compartments

\[ F = \begin{pmatrix}
-f_{1,1} & f_{1,2} & \cdots & f_{1,n} \\
 f_{2,1} & -f_{2,2} & \cdots & f_{2,n} \\
 \vdots & \vdots & \ddots & \vdots \\
 f_{n,1} & f_{n,2} & \cdots & -f_{n,n}
\end{pmatrix} \]
Mathematical formulation for the fluxes

The law of mass action:

\[
\text{Reaction Rate} = k \cdot [A]^\alpha \cdot [B]^\beta
\]

*The rate of the reaction is proportional to a power of the concentrations of all substances taking part in the reaction*
Reaction order

- **Zero order**: $k_0$
- **First order**: $k_1 \cdot [A]$
- **Second order**: $k_2 \cdot [A] \cdot [B]$
- **Third order**: $k_3 \cdot [A]^2 \cdot [B]$
First order models are very common

\[
\begin{align*}
\frac{dC_1}{dt} &= I - k_1 C_1 \\
\frac{dC_2}{dt} &= \alpha k_1 C_1 - k_2 C_2
\end{align*}
\]
Nomenclature of pool models

<table>
<thead>
<tr>
<th>No. Pools</th>
<th>1</th>
<th>2</th>
<th>3</th>
</tr>
</thead>
<tbody>
<tr>
<td>Parallel</td>
<td></td>
<td></td>
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<tr>
<td>Series</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Feedback</td>
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</tbody>
</table>
General matrix representation

Any model using first-order reaction terms with constant coefficients of the form

\[
\begin{align*}
\frac{dx_1}{dt} &= I_1 + \sum \alpha_{1,j} k_j x_j - k_1 x_1 \\
\frac{dx_i}{dt} &= I_i + \sum \alpha_{i,j} k_j x_j - k_i x_i \\
\frac{dx_n}{dt} &= I_n + \sum \alpha_{n,j} k_j x_j - k_n x_n
\end{align*}
\]

can be expressed as a system of the form

\[
\frac{dx}{dt} = I + A \cdot x
\]
Analytical solution

The system

\[ \frac{dx}{dt} = I + A \cdot x, \]

with initial conditions \( x(t = 0) = x_0 \), has solution

\[ x(t) = e^{A \cdot (t-t_0)} x_0 + \left( \int_{t_0}^{t} e^{A \cdot (t-\tau)} d\tau \right) I. \]

At steady-state:

\[ x_{ss} = -A^{-1} \cdot I \]
The ratio of all stocks over all inputs is defined as the turnover time of the system

$$\tau = \frac{\sum x_{ss}}{\sum I}$$
Numerical solutions

Calculate the solution of the IVP taking advantage of the known values of the derivatives and the initial value. For the IVP

\[ x'(t) = f(t, x(t)), \quad x(t_0) = x_0, \]

an approximation to the solution is

\[ x(t + h) \approx x(t) + hf(t, x(t)). \]

This leads to a recursion of the form

\[ x_{n+1} = x_n + hf(t_n, x_n). \]
Run multiple-pool models numerically

- Parallel: no exchange of matter among pools
- Series: Progressive transfer of matter among pools
- Feedback: Multiple exchange of matter among pools.
Mathematical form

- **Parallel:**

\[
\frac{dx(t)}{dt} = I \begin{pmatrix} 1 & 0 & 0 \\ \gamma_1 & \gamma_2 & 1 - \gamma_1 - \gamma_2 \end{pmatrix} + \begin{pmatrix} -k_1 & 0 & 0 \\ 0 & -k_2 & 0 \\ 0 & 0 & -k_3 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix}
\]

- **Series:**

\[
\frac{dx(t)}{dt} = I \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} + \begin{pmatrix} -k_1 & 0 & 0 \\ a_{21} & -k_2 & 0 \\ 0 & a_{32} & -k_3 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix}
\]

- **Feedback:**

\[
\frac{dx(t)}{dt} = I \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} + \begin{pmatrix} -k_1 & a_{12} & 0 \\ a_{21} & -k_2 & a_{23} \\ 0 & a_{32} & -k_3 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix}
\]
Effect of model structure: same inputs and rates
**Model properties: Ages and transit times**

- **System age** is a random variable that describes the age of particles or molecules within a system since the time of entry.
- **Pool age** is a random variable that describes the age of particles or molecules within a pool since the time of entry.
- **Transit time** is a random variable that describes the ages of the particles at the time they leave the boundaries of a system; i.e., the ages of the particles in the output flux.
Age and transit time are not always equal

- Mean transit time > mean age: human population
- Mean transit time = mean age: Uranium, Radiocarbon
- Mean transit time < mean age: Ocean water

Bolin & Rodhe (1973, Tellus 25: 58)
Formulas for transit times and ages

For the autonomous system $\dot{x}(t) = A \, x(t) + I$

- **System age**
  - $f(a) = z^T \, e^{a \, A} \, \frac{x^*}{\|x^*\|}$
  - $\mathbb{E}[a] = -1^T \, A^{-1} \, \frac{x^*}{\|x^*\|} = \frac{\|B^{-1} x^*\|}{\|x^*\|}$

- **Pool age**
  - $f(a) = (X^*)^{-1} \, e^{a \, A} \, I$
  - $\mathbb{E}[a] = -(X^*)^{-1} \, A^{-1} \, x^*$

- **Transit time**
  - $f(\tau) = z^T \, e^{\tau \, A} \, \frac{I}{\|I\|}$
  - $\mathbb{E}[\tau] = -1^T \, A^{-1} \, \frac{I}{\|I\|} = \frac{\|x^*\|}{\|I\|}$

Three-pool model example

- One pool model:
  \[ \frac{dx}{dt} = 100 - \left( \frac{1}{16} \right) x \]

- Three-pool model in parallel:
  \[ \frac{d\mathbf{x}(t)}{dt} = \begin{pmatrix} 70 \\ 20 \\ 10 \end{pmatrix} + 
  \begin{pmatrix} -\frac{1}{4} & 0 & 0 \\ 0 & -\frac{1}{25} & 0 \\ 0 & 0 & -\frac{1}{100} \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} \]

- Three-pool model in feedback:
  \[ \frac{d\mathbf{x}(t)}{dt} = \begin{pmatrix} 70 \\ 30 \\ 0 \end{pmatrix} + 
  \begin{pmatrix} -\frac{1}{4} & \frac{20}{90 \cdot 4} & \frac{20}{55 \cdot 25} - \frac{1}{100} \\ \frac{20}{90 \cdot 4} & -\frac{1}{25} & \frac{1}{100} \\ 0 & \frac{5}{55 \cdot 25} & -\frac{1}{100} \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} \]
Three-pool model example

- **One pool model:**
  - Turnover time: 16 yrs
  - Mean Age: 16 yrs
  - Mean transit time: 16 yrs

- **Three-pool model in parallel:**
  - Turnover time: 16 yrs
  - Mean Age: 63.8 yrs
  - Mean transit time: 17.8 yrs
  - Mean pool ages: 4, 25, 100 yrs.

- **Three-pool model in feedback:**
  - Turnover time: 16 yrs
  - Mean Age: 60.5 yrs
  - Mean transit time: 22.35 yrs
  - Mean pool ages: 13, 43, 143 yrs.
Three-pool model example

\[ k = \frac{1}{16} \text{ yr}^{-1} \]
\[ k = \frac{1}{4} \text{ yr}^{-1} \]
\[ k = \frac{1}{25} \text{ yr}^{-1} \]
\[ k = \frac{1}{100} \text{ yr}^{-1} \]
Three-pool model example

Pool age distributions: Parallel and feedback model structures
A simple carbon cycle model

\[
\begin{bmatrix}
120 \text{ Pg C yr}^{-1} & 120 \text{ Pg C yr}^{-1} & 70 \text{ Pg C yr}^{-1} & 70 \text{ Pg C yr}^{-1} \\
600 & 900 & 2300 & 0
\end{bmatrix}, \quad \begin{bmatrix}
0 \\
55 \\
0
\end{bmatrix}
\]

\[
\frac{dx_A}{dt} = F_{AT} + F_{AS} - F_{TA} - F_{SA}
\]

\[
\frac{dx_S}{dt} = F_{SD} + F_{SA} - F_{DS} - F_{AS}
\]

\[
\frac{dx_T}{dt} = F_{TA} - F_{AT}
\]
System of differential equations

\[
\begin{align*}
\frac{dx_A}{dt} &= x_T k_{AT} + x_S k_{AS} - x_A (k_{TA} + k_{SA}) \\
\frac{dx_S}{dt} &= I_S + x_A k_{SA} - x_S (k_{DS} + k_{AS}) \\
\frac{dx_T}{dt} &= x_A k_{TA} - x_T k_{AT}
\end{align*}
\]
System of differential equations

\[
\frac{dx_A}{dt} = x_T k_{AT} + x_S k_{AS} - x_A(k_{TA} + k_{SA})
\]

\[
\frac{dx_S}{dt} = I_S + x_A k_{SA} - x_S(k_{DS} + k_{AS})
\]

\[
\frac{dx_T}{dt} = x_A k_{TA} - x_T k_{AT}
\]

\[
\begin{pmatrix}
\frac{dx_A}{dt} \\
\frac{dx_S}{dt} \\
\frac{dx_T}{dt}
\end{pmatrix} = \begin{pmatrix} 0 \\ I_s \\ 0 \end{pmatrix} + \begin{pmatrix} -(k_{TA} + k_{SA}) & k_{AS} & k_{AT} \\ k_{SA} & -(k_{DS}k_{AS}) & 0 \\ k_{TA} & 0 & -(k_{AT}) \end{pmatrix} \cdot \begin{pmatrix} x_A \\ x_S \\ x_T \end{pmatrix}
\]

\[
\frac{dx}{dt} = I + A \cdot x
\]
Summary

- We use compartmental/reservoir/pool models to represent biogeochemical cycling.
- Compartmental models are build using information about stocks and fluxes among reservoirs.
- Models can be expressed in matrix form, explicitly representing connections among pools.
- Major model diagnostics are turnover time, system age, and transit time.
- For a single homogeneous pool at steady-state, all diagnostic times are equal.
- Ages and transit time change according to the connectivity of the system.