Theory and models of soil organic matter decomposition

Carlos A. Sierra
via Shane Stoner
Max Planck Institute for Biogeochemistry

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Outline

- History of soil organic matter models
- General models
- Practical exercise

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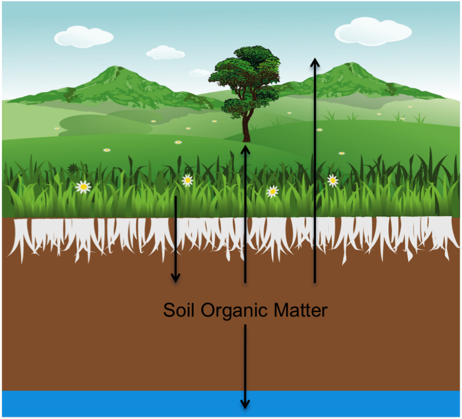
Soil organic matter decomposition



- Mineralization of biogeochemical elements
- Transfer of matter between biosphere, atmosphere, and hydrosphere
- Important implications for plant growth and climate

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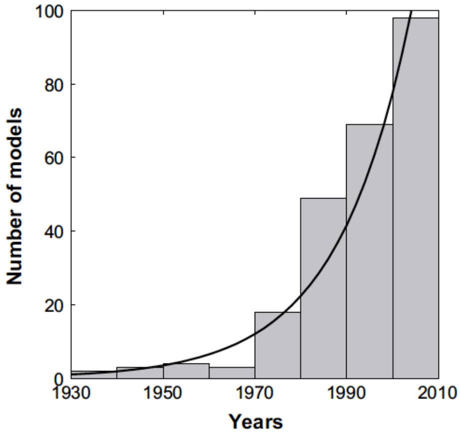
Models of soil organic matter decomposition



How decomposition should be modeled remains currently an unresolved issue

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Manzoni & Porporato (2009, Soil Biol Biochem 41, 1355)

van't Hoff's model of decomposition

MARCHE DE LA TRANSFORMATION CHIMIQUE.

PREMIÈRE PARTIE.

LA TRANSFORMATION CHIMIQUE NORMALE.

I. LA TRANSFORMATION UNIMOLÉCULAIRE (DÉCOMPOSITION DE L'ACIDE DIBROMOSUCCINIQUE).

La plus élémentaire des transformations chimiques simples est celle qui peut se produire dans la molécule isolée; c'est-à-dire, quand pour la réaliser, l'action mutuelle de plusieurs molécules n'est pas nécessaire. Que ce soit une transformation isomérique ou une décomposition, la marche en est caractérisée par la loi que nous allons faire connaître; c'est pour cela que j'appelle cet acte chimique la transformation unimoléculaire.

En effet l'expérience démontrera que, dans le cas décrit, il y a proportionnalité entre la quantité transformable et la quantité transformée, supposition que traduit la forme algébrique:

$$-\frac{\partial C}{\partial t} = k\,C$$

C concentration (quantité dans l'unité de volume),
t temps,
k constante.

van't Hoff (1884)

$$-\frac{\partial C}{\partial t} = k\,C$$

$$-\frac{\partial C_{\prime}}{\partial t} = k_{\prime}\, C_{\prime} C_{\prime\prime}$$
$$-\frac{\partial C_{\prime\prime}}{\partial t} = k_{\prime\prime}\, C_{\prime\prime}\, C_{\prime},$$

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The geometric series of Kostychev (1885-1886)

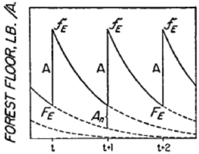

Fig. 10.

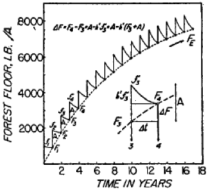

Fig. 11.

Fig. 10. Schematic Illustration of Rhythmic Variation of Forest Floor in a Deciduous Forest at Equilibrium

Fig. 11. Building up of a Forest Floor Under Conditions of Invariant k

We may develop the following simple geometrical series:

$$
\begin{aligned}
\mathfrak{F}_1 &= A \\
F_1 &= \mathfrak{F}_1(1-k') = A(1-k') \\
\mathfrak{F}_2 &= F_1 + A = A + A(1-k') \\
F_2 &= \mathfrak{F}_2(1-k') = A(1-k') + A(1-k')^2 \\
F(t) &= \frac{A(1-k')[1-(1-k')^t]}{k'} = F_E[1-(1-k')^t] \qquad (3)
\end{aligned}
$$

The series converges to:

$$F_n = \frac{A(1-k')}{k'}$$

Nikiforoff, 1937. SSSAJ 1: 333.; Jenny et al., 1949. Soil Sci. 68: 419

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The humification model of Henin & Dupuis (1945)

ESSAI DE BILAN
DE LA MATIÈRE ORGANIQUE DU SOL

PAR

S. HENIN et M. DUPUIS
(Versailles).

Introduction.

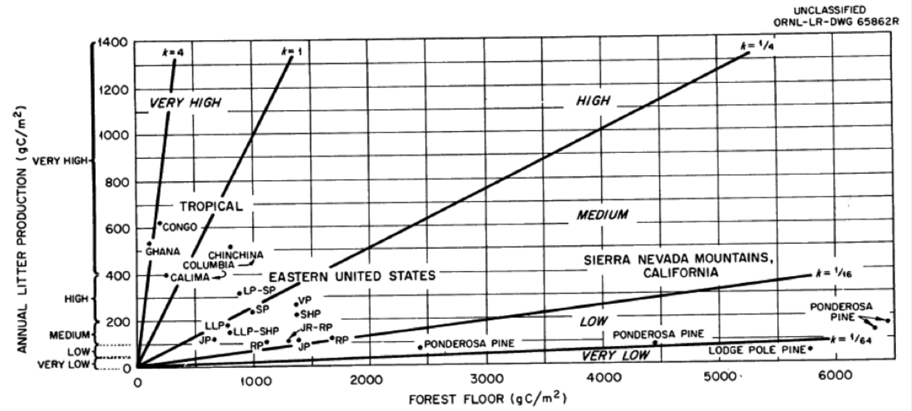
- Établissement de la formule d'interpolation.
- Détermination du coefficient de destruction apparent en supposant un apport nul.
- Détermination du coefficient iso-humique.
- Enrichissement en matières organiques par les résidus de récoltes.

Conclusions.

$$\frac{dX_1}{dt} = L - k_1 X_1$$
$$\frac{dX_2}{dt} = \alpha k_1 X_1 - k_2 X_2$$

Henin & Dupuis, 1945. Ann. Agron. 15: 17.

Olson's classic paper



$$\frac{dX}{dt} = L - kX$$

$$X_{ss} = \frac{L}{k}$$

Olson, 1963. Ecology 44: 322.

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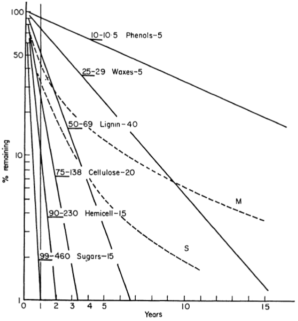
The need to account for SOM heterogeneity

Substrates with intrinsic rates

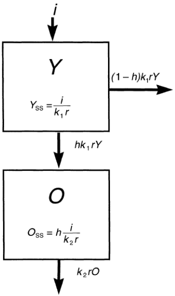
$$\frac{dX_1}{dt} = \gamma L - k_1 X_1$$
$$\frac{dX_2}{dt} = (1-\gamma)L - k_2 X_2$$



Minderman (1968). J Ecol 56: 355.

Humification concept

$$\frac{dX_1}{dt} = L - k_1 X_1$$
$$\frac{dX_2}{dt} = \alpha k_1 X_1 - k_2 X_2$$



Andren & Katterer (1997) Ecol Appl 7: 1226.

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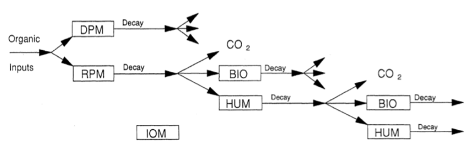
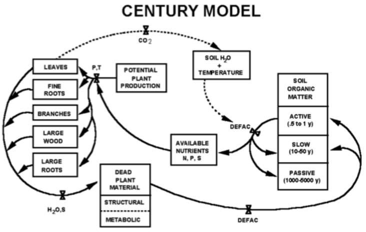
The multiple pool paradigm

Roth-C



Jenkinson & Rayner 1977. Soil Sci. 123: 298



Overall flow diagram for the CENTURY model.

Parton et al. 1987. SSSAJ 51: 1173

The multiple pool paradigm

Rothamsted

$$\frac{dX_1}{dt} = \gamma I - k_1 X_1$$

$$\frac{dX_2}{dt} = (1-\gamma) I - k_2 X_2$$

$$\frac{dX_3}{dt} = f_1 (k_1 X_1 + k_2 X_2 + k_4 X_4) - (1-f_1) k_3 X_3$$

$$\frac{dX_4}{dt} = f_2 k_5 X_5 - (1-f_1) k_4 X_4$$

$$\frac{dX_5}{dt} = f_3 (k_1 X_1 + k_2 X_2 + k_3 X_3 + k_4 X_4) - (1-f_4) k_5 X_5$$

$$\frac{dX_6}{dt} = 0$$

Century

$$\frac{dX_1}{dt} = \beta I - k_1 X_1$$

$$\frac{dX_2}{dt} = (1-\beta) I - k_2 X_2$$

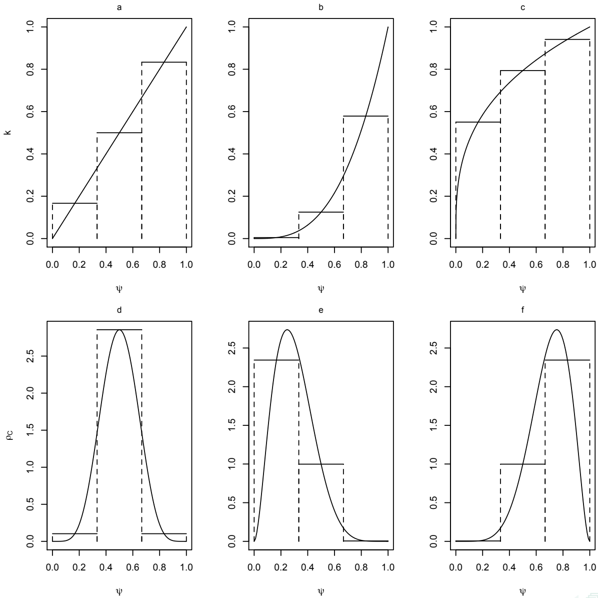
$$\frac{dX_3}{dt} = f_1 k_1 X_1 + f_2 k_2 (1-\lambda) X_2 + f_7 k_4 X_4 + f_8 k_5 X_5 - k_3 X_3$$

$$\frac{dX_4}{dt} = f_3 \lambda k_2 X_2 + f_4 k_3 X_3 - k_4 X_4$$

$$\frac{dX_5}{dt} = f_5 k_3 X_3 + f_6 k_4 X_4 - k_5 X_5$$

Paustian et al. 1997, Bolker et al. 1998

From multiple pools to continuous distributions



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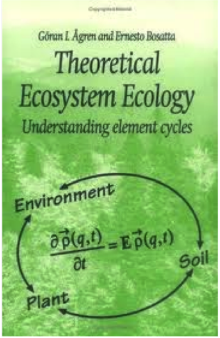
The continuous quality model

$$\frac{\partial \rho(q,t)}{\partial t} = L(q,t) - S(q,t) + \frac{\partial \Phi(q,t)}{\partial q}$$



Ågren & Bosatta, 1996. Cambridge Univ. Press.

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The continuous quality model

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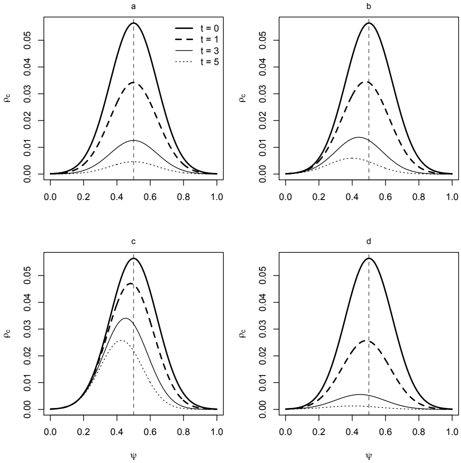

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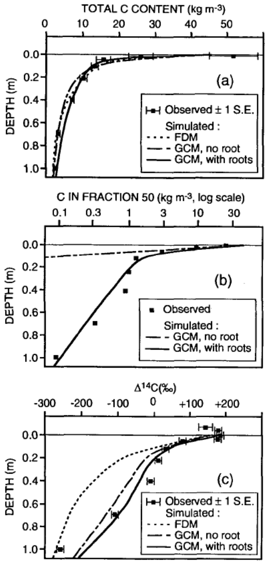
The vertical dimension



$$\frac{\partial X_i}{\partial t} = D\frac{\partial^2 X_i}{\partial z^2} - v\frac{\partial X_i}{\partial z} + L_i - k_i X_i + \sum_{j=1}^{n} \alpha_{i,i} k_j X_j$$

Elzein & Balesdent (1995) Soil Sci Soc Am J 59: 1328.

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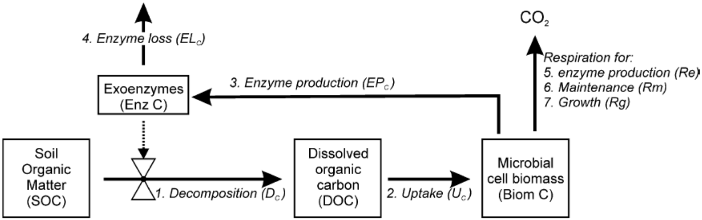
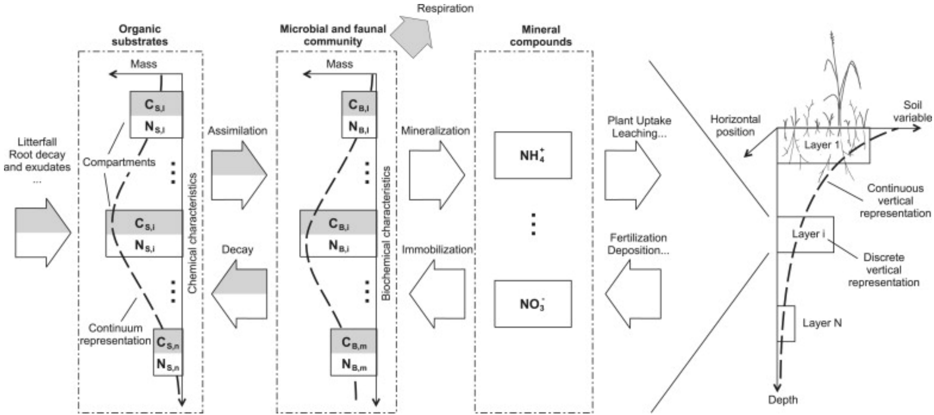
Microbial explicit models



$$\frac{dS}{dt} = -\frac{k_d \cdot E \cdot S}{E + K_M}$$

Schimel & Weintraub (2003) Soil Biol Biochem 35: 549

A landscape of SOM model structures



Manzoni & Porporato (2008). Soil Biol Biochem 40: 1137.

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A landscape of SOM model structures

$$\frac{\partial x}{\partial t} = f(z, \psi, x, t)$$

- z: Vertical dimension
  - Continuous
  - Discrete (layered)
- ψ: SOM heterogeneity
  - Continuous
  - Discrete (compartments)
- x: States
  - Rates and inputs x dependent: nonlinear systems
  - No x dependence: linear systems
- t: Time dependencies
  - Rates and inputs time-dependent: nonautonomous system
  - No time dependencies: autonomous system

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General models of SOM dynamics

CONCEPTS & SYNTHESIS
EMPHASIZING NEW IDEAS TO STIMULATE RESEARCH IN ECOLOGY

Ecological Monographs, 85(4), 2015, pp. 505–524

A general mathematical framework for representing soil organic matter dynamics

Carlos A. Sierra[1] and Markus Müller

Max Planck Institute for Biogeochemistry, Hans Knöll Straße 10, 07745 Jena, Germany

Abstract. We propose here a general mathematical framework to represent soil organic matter dynamics. This framework is expressed in the language of dynamical systems and generalizes previous modeling approaches. It is based on a set of six basic principles about the decomposition of soil organic matter: (1) mass balance, (2) substrate dependence of decomposition, (3) heterogeneity of the speed of decay, (4) internal transformations of organic matter, (5) environmental variability effects, and (6) substrate interactions. We show how the majority of models previously proposed are special cases of this general model. This approach provides tools to classify models according to the main principles or concepts they include. It also helps to identify a priori the general behavior of different models or groups of models. Another important characteristic of the proposed mathematical representation is the possibility to develop particular models at any level of detail. This characteristic is described as a modeling hierarchy, in which a general model of a high degree of abstraction can accommodate specific realizations of model structure for specific modeling objectives. This framework also allows us to study general properties of groups of models such as their qualitative behavior, timescale of application, and their dynamic stability. For instance, we find conditions under which models are asymptotically stable, i.e., converge to a stable steady state in the long term, but may approach this state with or without oscillations. We also expand the concept of dynamic stability for models that include time dependencies and do not converge to a fixed steady state, but rather to a region of stability in the state-space. As an example of the application of the concept of dynamic stability, we show how this framework helps to explain the acclimation of soil respiration fluxes in soil-warming experiments.

Key words: decomposition; dynamical systems; microbial carbon use efficiency; soil carbon models; soil microbial models; soil respiration; soil-warming experiments; stability analysis.

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1. Mass balance

Any mass of organic matter entering the soil must either leave or accumulate within the system

IN - OUT = ACCUMULATION.

Mathematically,

$$\frac{dX}{dt} = F_{in} - F_{out}$$
$$\frac{dX}{dt} = I - O$$

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2. Substrate dependence of decomposition

There is no decomposition without available substrate

$$F_{out} = f(x)$$

In the simplest case

$$F_{out} = f(x) = k \cdot x$$

therefore,

$$\frac{dx}{dt} = I - k \cdot x$$

3. SOM heterogeneity

SOM is heterogeneous in terms of its rates of decomposition

$$
\begin{aligned}
\frac{dx_1}{dt} &= I_1 - f_1(x_1, x_2, \cdots, x_m) \\
\frac{dx_2}{dt} &= I_2 - f_2(x_1, x_2, \cdots, x_m) \\
&\vdots \\
\frac{dx_m}{dt} &= I_m - f_m(x_1, x_2, \cdots, x_m)
\end{aligned}
$$

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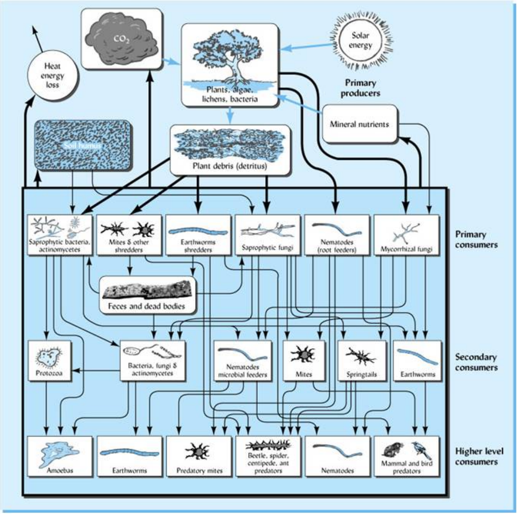
3. SOM heterogeneity



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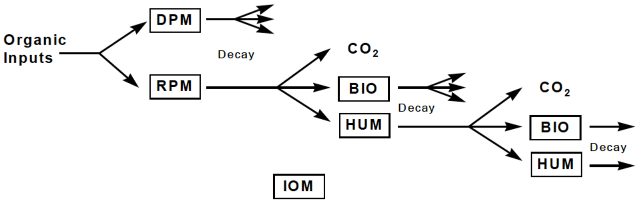
3. SOM heterogeneity

Figure 1 - Structure of the Rothamsted Carbon Model



RPM : Resistant Plant Material
DPM : Decomposable Plant Material
BIO : Microbial Biomass
HUM : Humified OM
IOM : Inert Organic Matter

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3. SOM heterogeneity

SOM is heterogeneous in terms of its rates of decomposition

$$
\begin{aligned}
\frac{dx_1}{dt} =& I_1 - f_1(x_1, x_2, \cdots, x_m)\\
\frac{dx_2}{dt} =& I_2 - f_2(x_1, x_2, \cdots, x_m)\\
&\vdots\\
\frac{dx_m}{dt} =& I_m - f_m(x_1, x_2, \cdots, x_m)
\end{aligned}
$$

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3. SOM heterogeneity

The m dimensional system can be expressed in vector form as

$$\frac{d\mathbf{x}(t)}{dt} = \mathbf{I} - f(\mathbf{x})$$

For first-order linear models without SOM transfers, we can write explicitly:

$$\frac{d\mathbf{x}(t)}{dt} = \mathbf{I} - \mathbf{K} \cdot \mathbf{x}$$

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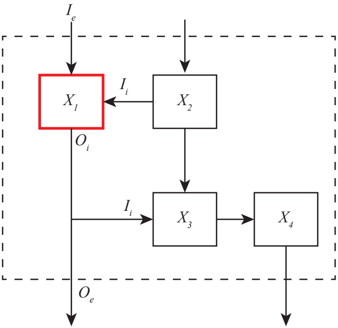
4. Transformations of organic matter



Portions of soil organic matter can be transformed in terms of their decomposition rates

$$\frac{dx_1}{dt} = I_1 - k_1 x_1 + \sum_{j=1}^{m} \alpha_{1j} k_j x_j$$

$$\vdots$$

$$\frac{dx_m}{dt} = I_m - k_m x_m + \sum_{j=1}^{m} \alpha_{mj} k_j x_j$$

This is equivalent to

$$\frac{d\mathbf{x}(t)}{dt} = \mathbf{I} - \mathbf{A} \cdot \mathbf{x}$$

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4. Transformations of organic matter

$$\frac{d\mathbf{x}(t)}{dt} = \mathbf{I} + \mathbf{A} \cdot \mathbf{x}$$

is equivalent to

$$\frac{d\mathbf{x}(t)}{dt} = \mathbf{I} + \mathbf{T} \cdot \mathbf{K} \cdot \mathbf{x}$$

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5. Environmental variability effects

Changes in the environment can either reduce or increase rates of SOM decomposition

$$\frac{d\mathbf{x}(t)}{dt} = \mathbf{I} - \xi(t) \cdot \mathbf{A} \cdot \mathbf{x}(t)$$

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More generally,

$$\frac{d\mathbf{x}(t)}{dt} = \mathbf{I}(t) - \mathbf{A}(t) \cdot \mathbf{x}(t)$$

6. SOM interactions

Different components of the SOM system may interact, synergistically increasing or decreasing decomposition rates

$$\frac{d\mathbf{x}(t)}{dt} = \boldsymbol{I}(t) + \mathbf{T}(\mathbf{x}, t) \cdot \mathbf{N}(\mathbf{x}, t) \cdot \mathbf{x}(t)$$

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The general model

$$\frac{d\mathbf{x}(t)}{dt} = \boldsymbol{I}(t) + \mathbf{T}(\mathbf{x}, t) \cdot \mathbf{N}(\mathbf{x}, t) \cdot \mathbf{x}(t)$$

- $\boldsymbol{I}(t)$ is a vector of time dependent functions representing external inputs to the system.
- $\mathbf{T}(\mathbf{x}, t)$ is a square matrix with -1 in the diagonal and functions in the off-diagonal representing transfers among pools.
- $\mathbf{N}(\mathbf{x}, t)$ is a square diagonal matrix containing the multiplicative nonlinear terms.

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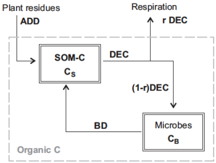
Examples: A nonlinear microbial model



$$\frac{dC_S}{dt} = I + k_B C_B - k_S C_B \frac{C_S}{K_M + C_S}$$
$$\frac{dC_B}{dt} = (1-r) k_S C_B \frac{C_S}{K_M + C_S} - k_B C_B$$

$$\begin{aligned} \frac{d\boldsymbol{C}}{dt} &= \boldsymbol{I} + \mathbf{T} \cdot \mathbf{N}(\boldsymbol{C}) \cdot \boldsymbol{C} \\ &= \begin{pmatrix} I \\ 0 \end{pmatrix} + \begin{pmatrix} -1 & 1 \\ 1-r & -1 \end{pmatrix} \begin{pmatrix} \frac{k_S C_B}{K_M + C_S} & 0 \\ 0 & k_B \end{pmatrix} \begin{pmatrix} C_S \\ C_B \end{pmatrix}. \end{aligned} \tag{1}$$

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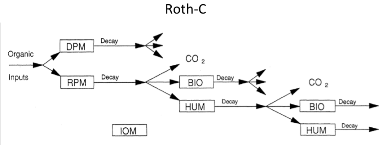
Examples: The RothC model



$$\frac{d\boldsymbol{C}}{dt} = \boldsymbol{I} + \xi(t) \cdot \mathbf{A} \cdot \boldsymbol{C}$$

$$\frac{d\boldsymbol{C}}{dt} = I \begin{pmatrix} \gamma \\ 1-\gamma \\ 0 \\ 0 \\ 0 \end{pmatrix} + \xi(t) \begin{pmatrix} -k_1 & 0 & 0 & 0 & 0 \\ 0 & -k_2 & 0 & 0 & 0 \\ \alpha_{1,3}k_1 & \alpha_{2,3}k_2 & -k_3(1-\alpha_{3,3}) & \alpha_{4,3}k_4 & 0 \\ \alpha_{1,4}k_1 & \alpha_{2,4}k_2 & \alpha_{3,4}k_3 & -k_4(1-\alpha_{4,4}) & 0 \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} C_1 \\ C_2 \\ C_3 \\ C_4 \\ C_5 \end{pmatrix}$$

$$\frac{d\boldsymbol{C}}{dt} = I \begin{pmatrix} \gamma \\ 1-\gamma \\ 0 \\ 0 \\ 0 \end{pmatrix} + \xi(t) \begin{pmatrix} -k_1 & 0 & 0 & 0 & 0 \\ 0 & -k_2 & 0 & 0 & 0 \\ a_{1,3} & a_{2,3} & -k_3 + a_{3,3} & a_{4,3} & 0 \\ a_{1,4} & a_{2,4} & a_{3,4} & -k_4 + a_{4,4} & 0 \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} C_1 \\ C_2 \\ C_3 \\ C_4 \\ C_5 \end{pmatrix}$$

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Some properties

The linear autonomous system

$$\frac{d\mathbf{x}}{dt} = \boldsymbol{I} + \mathbf{A} \cdot \mathbf{x}$$

converges to a steady-state given by

$$\mathbf{x}_{ss} = -\mathbf{A}^{-1} \cdot \boldsymbol{I}$$

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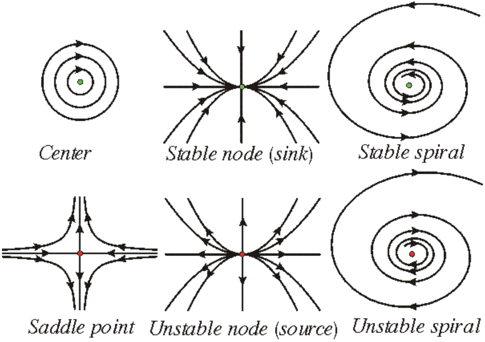
Some properties

The autonomous nonlinear models are generally stable



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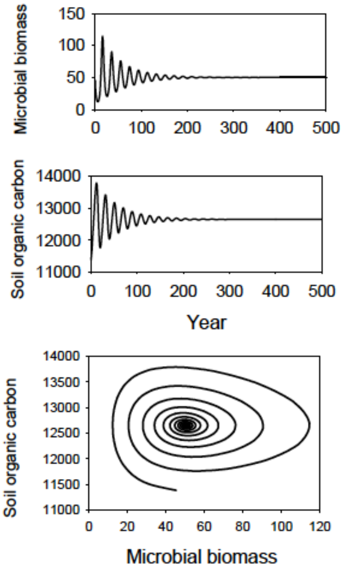
Oscillations in the two-pool microbial model



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Take-home messages

- There are a lot of SOM models out there!
- We can classify them according to their mathematical characteristics
- We can also group them in general classes that exhibit common behaviors
- Never ask what is the best model, ask what is the most useful model for a specific problem

Practical exercise

- Go to this site: `https://www.bgc-jena.mpg.de/TEE/software/soilr/`
- Click on First steps with R and SoilR to download and install
- Click on Run multiple-pool models and run the examples
- Click on Run the RothC model for a site and run part 1 of the example
- What is the value of C stocks per pool at steady-state? Can you calculate them using a simpler formula?
- How much does the steady-state value changes if you increase litter inputs by a factor of 2?
- How much does the steady-state value changes if you increase decomposition rates by a factor of 2?

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