Simplifying the Complexity of a Coupled Carbon Turnover and Pesticide Degradation Model

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Motivation

- Biogeochemical models that explicitly consider functional traits and physiology of microorganisms are **complex**
- Mathematical analysis provides a leverage point to **reduce the complexity of models** and fosters understanding of qualitative system behavior
- We analyze the PECCAD model applying methods from the field of **dynamic systems theory** in order to gain a holistic understanding of microbial dynamics and matter cycling in soil

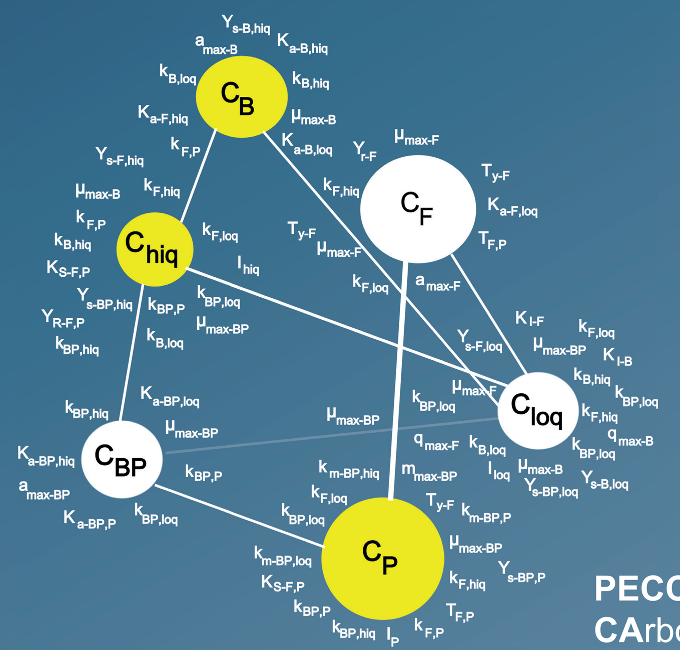
PECCAD Main Feature

Direct Pesticide Utilization

$$\mu_{BP,P} = \frac{\mu_{max-BP} k_{BP,P} C_P}{\mu_{max-BP} + k_{BP,P} C_P + k_{BP,hiq} C_{hiq} + k_{BP,loq} C_{loq}}$$

Cometabolic Degradation

$$q_{F,P} = \left(T_{y-F} \cdot \left(\mu_{F,hiq} + \mu_{F,loq}\right) + k_{F,P}\right) \cdot \frac{C_P}{K_{s-F,P} + C_P}$$



PECCAD (**PE**sticide degradation **C**oupled to **CA**rbon turnover in the **D**etritusphere (Pagel et al. (2014)) has a 51 dim. parameter space

Bifurcation Theory

A bifurcation occurs when a small change made to parameter values in the model leads to a qualitative change in dynamic behavior of the system

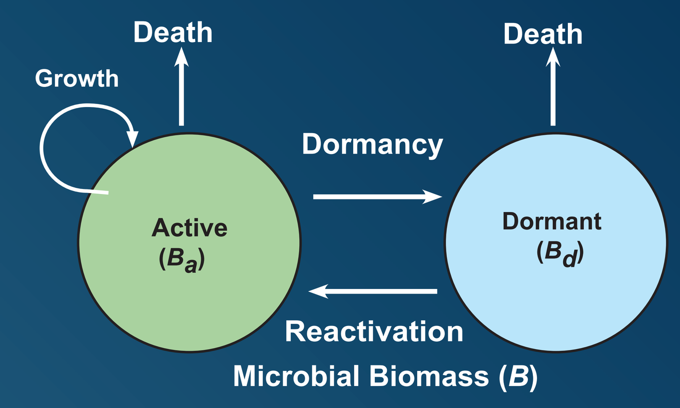
Results

Exponential dependence of microbial reactivation rate leads to complex model dynamics

Multiple time scales in the PECCAD model make a bifurcation analysis possible

Physiological Activity

Active microbial biomass is a driver of biogeochemical cycles, but existing minimal models representing physiological states lack experimental validation.
How can we distinguish between models?



Modified from Jones & Lennon (2010)

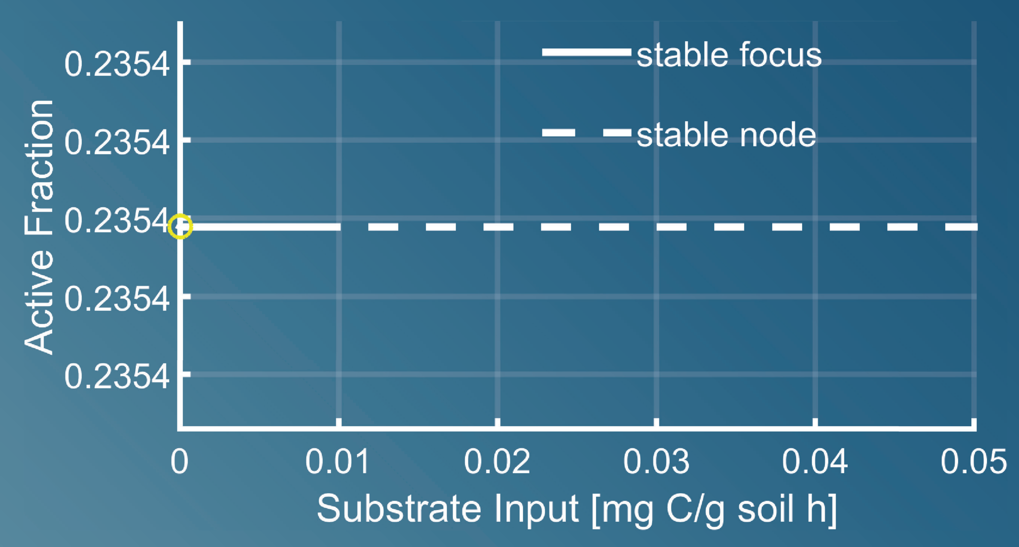
Wang et al. (2014)

Transition term

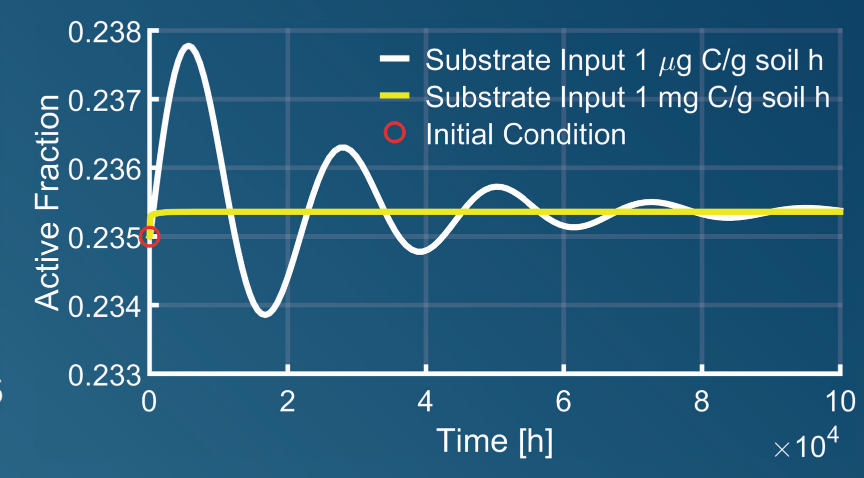
$$(1-\phi)\, m_R B_a + \phi m_R B_d$$

Substrate saturation

$$\phi = \frac{S}{K_s + S}$$



System shows simple relaxation oscillations

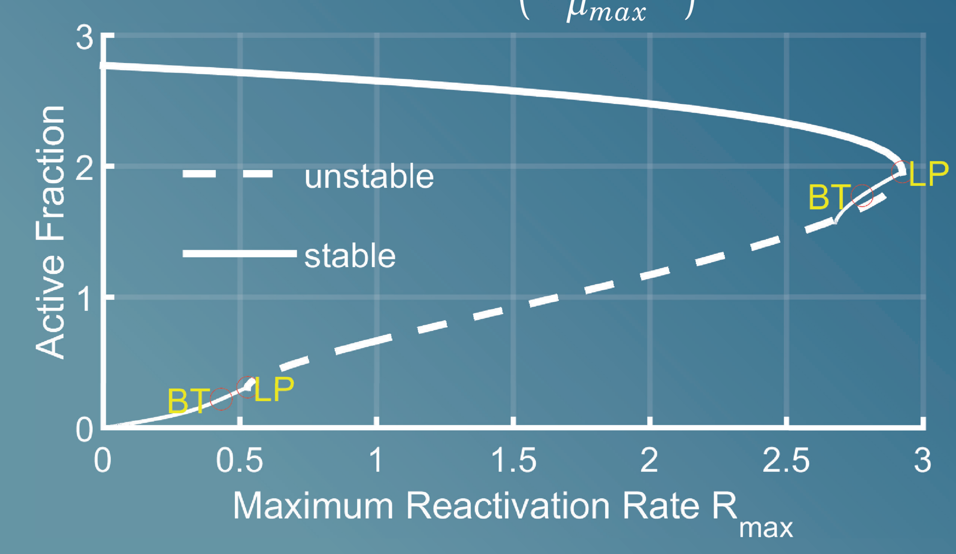


Jones & Lennon (2010)

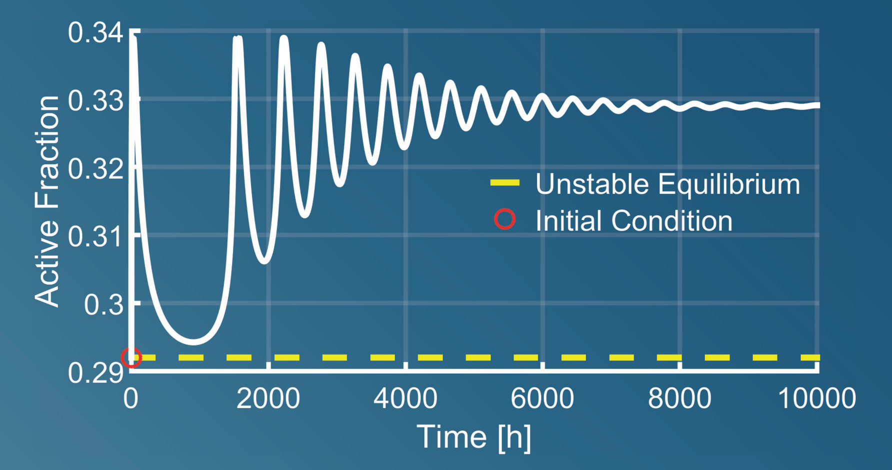
$$R = R_{max} \exp - \left(\frac{\mu_{max} - \mu}{\mu_{max}}\right)^2$$

Transition term

$$(1-R) B_a - R B_d$$



System driven away from unstable equilibrium



PECCAD has Three Distinct Time Scales

Based on dimensional analysis, it is possible to propose a **hierarchy of variables** according to the time scales on which they evolve. Such a **fast-slow system** is amenable to bifurcation analysis: in the singular limit, two 3 dimensional systems can be analyzed separately.

Superfast Pesticide

$$\varepsilon \frac{dc_p}{d\tau} = c_P \left[-\frac{\tilde{\mu}_{BP,P}(k_c c_i)}{Y_{s-BP,P}} - \tilde{m}_{BP,P}(k_c c_i) \right] - c_P \tilde{q}_{F,P}(k_c c_i) + \tilde{I}_P$$

Fast High Quality Carbon

$$\sqrt{\varepsilon} \frac{dc_{hiq}}{d\tau} = f_2\left(k_c c_{hiq}, k_c c_{loq}, k_c c_P, k_c c_B, k_c c_{BP}, k_c c_F\right)$$

Fast Bacterial Biomass

$$\sqrt{\varepsilon} \frac{dc_B}{d\tau} = f_3\left(k_c c_{hiq}, k_c c_{loq}, k_c c_P, k_c c_B, k_c c_{BP}, k_c c_F\right)$$

$$0 < \varepsilon = 1/(k_t \tau_x) \ll 1$$

Slow

$$\frac{dc_{loq}}{d\tau} = g_1\left(k_c c_{hiq}, k_c c_{loq}, k_c c_P, k_c c_B, k_c c_{BP}, k_c c_F\right)$$

$$\frac{dc_F}{d\tau} = g_2\left(k_c c_{hiq}, k_c c_{loq}, k_c c_P, k_c c_B, k_c c_{BP}, k_c c_F\right)$$

$$\frac{dc_{BP}}{d\tau} = g_3\left(k_c c_{hiq}, k_c c_{loq}, k_c c_P, k_c c_B, k_c c_{BP}, k_c c_F\right)$$

References

Pagel, H., et al. Biogeochemistry 117.1 (2014): 185-204
Wang et al., PloS one 9.2 (2014): e89252
Jones, Stuart E., and Jay T. Lennon, Proceedings of the National Academy of Sciences 107.13 (2010): 5881-5886
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Time Scales and Dimensional Analysis

The complexity of coupled soil models has to be reduced in order to conduct a stability analysis. This is achieved by identifying **multiple time scales**.

Kinetic Functions give the Time Scale of a Variable

As part of a nondimensionalization procedure, three scaling constants are introduced. The **scale** of a variable provides an estimate of its maximum order of magnitude.

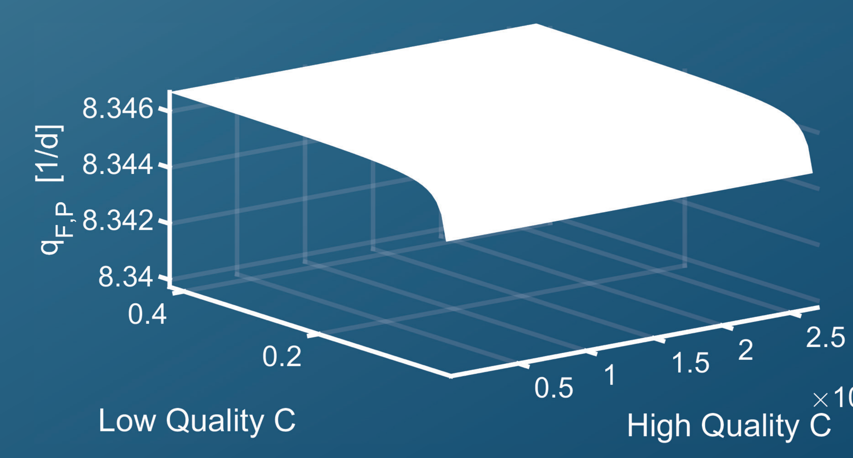
Carbon concentrations: $C_i = k_c \cdot c_i, \quad i = \{hiq, loq, P, B, BP, F\}$

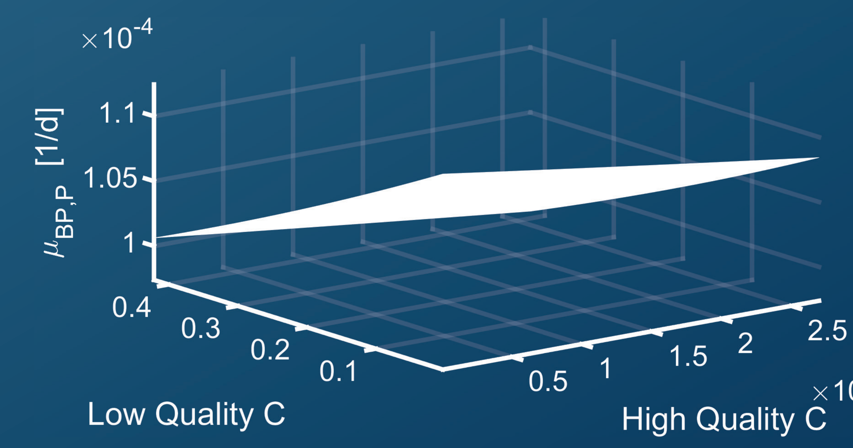
Time: $t = k_t \cdot \tau$

Kinetic functions: $\tau_x = \max_{0 \le c_i \le 1} \tau_x(k_c c_i)$

Example: Pesticide Concentration

$$\frac{dc_p}{d\tau} = c_P \left[-\frac{\tilde{\mu}_{BP,P}(k_c c_i)}{Y_{s-BP,P}} - \tilde{m}_{BP,P}(k_c c_i) \right] - c_P \tilde{q}_{F,P}(k_c c_i) + \tilde{I}_P$$





Examples of kinetic functions that define characteristic time scales for the pesticide variable. Cometabolic degradation $q_{F,P}$ is the dominant process.