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Simplifying the complexity of a coupled carbon turnover and pesticide degradation model

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The mechanistic one-dimensional model PECCAD (PEsticide degradation Coupled to CArbon turnover in the Detritusphere; Pagel et al. 2014, Biogeochemistry 117, 185-204) has been developed as a tool to elucidate regulation mechanisms of pesticide degradation in soil. A feature of this model is that it integrates functional traits of microorganisms, identifiable by molecular tools, and physicochemical processes such as transport and sorption that control substrate availability.

Predicting the behavior of microbially active interfaces demands a fundamental understanding of factors controlling their dynamics. Concepts from dynamical systems theory allow us to study general properties of the model such as its qualitative behavior, intrinsic timescales and dynamic stability: Using a Latin hypercube method we sampled the parameter space for physically realistic steady states of the PECCAD ODE system and set up a numerical continuation and bifurcation problem with the open-source toolbox MatCont in order to obtain a complete classification of the dynamical system's behaviour. Bifurcation analysis reveals an equilibrium state of the system entirely controlled by fungal kinetic parameters. The equilibrium is generally unstable in response to small perturbations except for a small band in parameter space where the pesticide pool is stable. Time scale separation is a phenomenon that occurs in almost every complex open physical system. Motivated by the notion of "initial-stage" and "late-stage" decomposers and the concept of r-, K- or L-selected microbial life strategies, we test the applicability of geometric singular perturbation theory to identify fast and slow time scales of PECCAD. Revealing a generic fast-slow structure would greatly simplify the analysis of complex models of organic matter turnover by reducing the number of unknowns and parameters and providing a systematic mathematical framework for studying their properties.