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A generalized optimization model of microbially driven aquatic biogeochemistry based on thermodynamic, kinetic, and stoichiometric ecological theory

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ABSTRACT

We have developed a mechanistic model of aquatic microbial metabolism and growth, where we apply fundamental ecological theory to simulate the simultaneous influence of multiple potential metabolic reactions on system biogeochemistry. Software design was based on an anticipated cycle of adaptive hypothesis testing, requiring that the model implementation be highly modular, quickly extensible, and easily coupled with hydrologic models in a shared state space. Model testing scenarios were designed to assess the potential for competition over dissolved organic carbon, oxygen, and inorganic nitrogen in simulated batch reactors. Test results demonstrated that the model appropriately weights metabolic processes according to the amount of chemical energy available in the associated biochemical reactions, and results also demonstrated how simulated carbon, nitrogen, and sulfur dynamics were influenced by simultaneous microbial competition for multiple resources. This effort contributes an approach to generalized modeling of microbial metabolism that will be useful for a theoretically and mechanistically principled approach to biogeochemical analysis.

1. Introduction

Aquatic ecosystems are currently subject to complex changes in external forcing due to changes in land use (Allan, 2004) and climate (Poff et al., 2002). In light of these multivariate changes, empirical data and assumptions of temporal stationarity (in the sense of Milly et al., 2008) are an insufficient basis for understanding the potential biogeochemical trajectories of these ecosystems. Furthermore, empirical work alone may reveal little about feedback effects (Stone and Weisburd, 1992; Singh et al., 2010) that may ultimately cause non-linear or discontinuous system behavior. Therefore, mechanistic simulation models of microbial metabolism are critical to understand the potential changes in aquatic biogeochemical cycles that may emerge from novel and dynamic mixtures of available metabolic reactants.

Use of thermodynamic theory in biogeochemical models relies on a non-equilibrium perspective (Schrödinger, 1944) of microbial metabolism. More specifically, accumulation of microbial biomass requires that the system must be far from equilibrium (Jørgensen et al., 1992), conservative of mass and energy (Patten et al., 1997), dissipative in the generation of entropy from available energy (Straškraba et al., 1999), and open to external sources and sinks of energy and matter (Jørgensen et al., 1999). This perspective assumes that microbial metabolism is inherently adapted to a state of disequilibrium, because the structure and function of a microbial assemblage is sustained by exergy (energy capable of work) provided by external factors (e.g., incoming solar or chemical energy). Starting from this premise, the non-equilibrium thermodynamic theory of ecology has led to several proposed goal

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functions that lead to the emergence of system complexity from imposed exergy sources (Fath et al., 2001). These goal functions include: maximum dissipation potential (Schneider and Kay, 1994), maximum exergy storage (Jørgensen et al., 2000), and maximum entropy production (Vallino, 2010). A model that maximizes microbial biomass using the available chemical potential is generally consistent with these goal functions, and provides a method by which thermodynamic ecological theory can be applied to (and tested by) field or lab studies of biogeochemical dynamics driven by microbial metabolism (Jessup et al., 2004; Prosser et al., 2007; Hall et al., 2011).

A non-equilibrium perspective alone would suggest that an appropriate metabolic model would be strictly rate-limited by kinetics, as opposed to equilibrium-limited, and the potential for kinetic drivers to control rates of metabolic activity is, indeed, an important consideration for any biochemical system. However, a generalized metabolic model also requires simulation of the effects of microbial competition for resources (Kalyuzhnyi and Fedorovich, 1998; Cherif and Loreau, 2007; van de Leemput et al., 2011). For example, a strictly rate-limited model for each heterotrophic metabolic reaction would predict that all terminal electron acceptors (TEAs) used for oxidizing dissolved organic carbon (DOC) would be consumed simultaneously, according to the relative magnitude of each predicted reaction rate. But in reality, exclusive separation of TEA consumption is commonly observed over space and time when chemical energy in the form of DOC is limiting (Hedin et al., 1998; Tesoriero et al., 2000; Zarnetske et al., 2011). This separation is typically attributed to competition for DOC among microbes capable of different heterotrophic metabolic pathways (e.g., aerobic respiration, denitrification, or sulfate reduction), and thermodynamic principles predict that microbes capable of higher energy-yielding metabolic reactions outcompete those capable of lower yielding reactions (Hedin et al., 1998). Therefore, we suggest that an effective generalized model of biogeochemistry should account for the potential occurrence of both kinetic and thermodynamic drivers (Jin and Bethke, 2003). Our use of the term “thermodynamic driver” does not refer to the more conventional definition of a system limited by reaching equilibrium, which would require death or dormancy for all life inhabiting that system (Schrödinger, 1944). Here, thermodynamic driver refers to an optimization algorithm that selects the metabolic processes that use the highest available energy yields from the available biochemical reactions.

The requirements for computer software supporting both our current and future modeling efforts are driven by the scientific needs of an adaptive hypothesis testing cycle. To initiate the cycle, a modular model that can be easily extended is constructed with a foundational set of hypotheses representing maximum parsimony. We define maximum parsimony as the simplest mechanistic explanation for a given set of observations. The initial model is configured and parameterized to simulate behavior of a real study system under a given experimental scenario. Comparison of the simulation with observations from the study system suggest how hypotheses encapsulated within the model need to be adapted to explain residual error. To maintain parsimony, complexity is added to the model only when it explains a statistically significant portion of the residual error. Further statistical analyses with the adapted model can then be used to suggest optimal designs for future laboratory or field experimentation, thus starting the next iteration of the cycle.

Here, we present a model framework designed to initiate this cyclic and adaptive approach for an assessment of biogeochemical trajectories of aquatic microbial ecosystems. Our objective was to develop an extensible biogeochemical modeling tool based on the metabolism of aquatic microbial assemblages, where the application of thermodynamic, kinetic, and stoichiometric theory is generalized to a level appropriate for simulating whole-system solute dynamics. We demonstrate a version of the model that incorporates the minimum conceptual complexity (or maximum parsimony) necessary to simulate system behavior that is consistent with modern thermodynamic and stoichiometric interpretations of microbially driven biogeochemistry.

2. Model description

Many models of microbial metabolism and growth have been based on some combination of thermodynamic, stoichiometric, and kinetic principles (Menkel and Knights, 1995; Vallino et al., 1996; Jin and Bethke, 2003; Franklin et al., 2011; van de Leemput et al., 2011). We build on these examples with a model implementation that has sufficient extensibility to be used in hypothesis testing against data from the typical aquatic ecosystem field or lab study. We designed a model where the suite of potential biogeochemical reactions was configurable at run time, allowing the researcher to define the appropriate simulation for a particular system or particular hypothesis of interest (similar to Flynn (2001)). The code was implemented in a highly modular, object-oriented framework for the purposes of (1) facilitating implementation of code to address new hypotheses that may arise from continued field and lab studies, and (2) allowing future integration with a hydrologic model to simulate physical transport of solutes.

We implemented the microbial ecosystem model using the Network Exchange Objects (NEO) modeling framework (Izurieta et al., 2012), coded in Java (v. 1.7, Oracle Corporation, Redwood Shores, California, USA). Critical NEO features include: (1) a shared name space for state variables within node and link objects based on a network-based data structure and (2) a dependency manager that automatically determines the appropriate execution order for calculating the new values for each state during a simulation time step. In this fashion, the NEO framework is designed to integrate the results of a collection of relatively simple individual calculations, in order to simulate the relatively complicated emergent interactions that may occur in the ecosystem.

We defined a functional unit of the microbial ecosystem with three nodes, where each node represents a particular physical location or conceptual structural component of the ecosystem (Fig. 1). The characteristics of these nodes are similar to model compartments proposed by Franklin et al. (2011), though less detailed in their ability to track variation of biomass stoichiometry. The nodes track the storage of compounds in various locations or forms, including: (1) the aqueous node, which tracks the amount and concentration of each simulated compound in the aqueous environment; (2) the biologically available node, which tracks the amounts of compounds that are in immediate proximity with enzymes driving metabolic processes; and (3) the biomass node, which tracks the amounts of elements that comprise living biomass (in this case, C and N).

NEO code is highly modular, where classes are organized within specific “behavior packages” that each define how a specific compound will behave in a given type of node or link. Model boundary conditions are implemented as one-sided links (henceforth called “boundary links”) that conceptually tie a single node to the exterior of the model domain. In this fashion, we describe how compounds and elements are moved and transformed within the microbial ecosystem by describing the general “behavior” of compounds in a given two-sided link between nodes, and we define the relationship between the ecosystem and external entities (e.g., driving data, compound source/sinks, etc.) by describing the behavior of compounds in one-sided boundary links connected to a single node.