Simulation analysis of biogeochemical systems

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The behavior of biogeochemical systems is dictated by interactions amongst multiple elemental cycles, yet elemental cycles are easier to conceptualize in isolation than in concert. To assist thinking in terms of biogeochemical systems rather than individual cycles, we developed a thermodynamically-based model that simulates the co-occurrence of competing metabolic pathways based on (1) the availability of electron donors and acceptors required by each pathway, (2) the energetic yield of the pathway, (3) the energetic demand of microorganisms, and (4) microbial growth constraints imposed by ecological stoichiometry. We performed a model sensitivity analysis by systematically varying the availability of DOC, O_2, NO_3^-, SO_4^{2-}, and CH_4 in the model, and analyzed results with multivariate statistics to identify broad drivers of biogeochemical systems. Our results identify several hypotheses describing broad drivers of biogeochemical system behaviors, such as the implications of competition for electron donors versus acceptors and variation in the ratio of metabolic demand for energy versus free energy yield from potential metabolic pathways.