A CONSTRAINT-BASED, COMPOUND SPECIFIC APPROACH TO MODELING LINKED BIOGEOCHEMICAL CYCLES

A. M. Reinhold
Department of Land Resources and Environmental Sciences, Montana Institute on Ecosystems, Montana State University – Bozeman
G. C. Poole
Department of Land Resources and Environmental Sciences, Montana Institute on Ecosystems, Montana State University - Bozeman
A. M. Helton
Department of Natural Resources and the Environment & the Center for Environmental Sciences and Engineering, University of Connecticut
C. I. Izurieta
Department of Computer Science, Montana Institute on Ecosystems, Montana State University - Bozeman
R. A. Payn
Department of Land Resources and Environmental Sciences, Montana Institute on Ecosystems, Montana State University - Bozeman
E. S. Bernhardt
Department of Biology, Duke University

We developed a "generic algorithm for nutrient, growth, stoichiometric, and thermodynamic analysis" (GANGSTA) that automates the creation of user defined, constraint-based, compound specific biogeochemical models. Such models are founded in thermodynamic theory and simulate microbial metabolism, growth, and linked elemental cycling in user-specified *in silico* biogeochemical systems subject to stoichiometric constraints. We present a series of GANGSTA-derived models that simulate linked C, H, O, N, and S cycling and reproduce realistic patterns of aerobic heterotrophy, denitrification, nitrification, methane oxidation, sulfate reduction, hydrogen sulfide oxidation, and methanogenesis. Our models illustrate the advantages of representing compound limitation rather than elemental limitation when simulating linked elemental cycles. Further, and perhaps counterintuitively, our models reveal that tracking O and H cycling through specific compounds provides a more complete representation of C, H, O, N, and S biogeochemistry than tracking any other pair of elements through those same compounds.