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

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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.