Energetics-based modeling of cryptic sulfur cycling in sediments

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Reactive sulfur in aquatic sediments spans the range of redox states from sulfate (+6) to sulfide (-2), and cycles through intermediate species (e.g., sulfite, thiosulfate, S^0) at concentrations that are often below detection. Fueled by mineralization of organic matter, microbially-catalyzed reaction pathways are selected by thermodynamic and kinetic constraints, and determine the concentrations of reactants and products and microbial abundances. We analyze the diagenetic reactions of sediment sulfur species with an energetics-based model, which considers distinct microbial populations, the energies needed for microbial catabolism and anabolism, and the thermodynamically-determined microbial growth yields. The structures of the reaction networks are analyzed under the contrasting conditions of marine vs. freshwater (low-sulfate) sediments, and account for the synthropic relationships between fermenting and respiring organisms. The results are interpreted to constrain the survival limits of sulfur-dependent microorganisms and to identify the differences in S cycling between the modern sulfate-rich oceans and the anoxic, ferruginous, low-sulfate oceans of the Archean and Proterozoic eons. Model results are compared against a limited dataset from modern lakes and coastal ocean environments.