

Biogeochemical simulations to assess the impact of redox processes on mercury cycling in sediments

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Methylmercury (MeHg) in the environment poses a significant threat to human and ecological health and is a major contaminant of concern for water quality. Biogeochemical models that simulate mercury (Hg) cycling in sediments are an emerging tool to aid management decisions. Such models can be used to assess driving processes and improve understanding of the complicated dynamics of Hg cycling. Redox cycling of sulfur (S) and iron (Fe) exert strong controls on Hg cycling and net MeHg production, whereas manganese (Mn) can be an indicator of redox conditions that are favorable for high MeHg production. A biogeochemical reaction model using the PHREEQC program was modified from prior studies to improve the model description of net MeHg production in sediments. The model connects Hg cycling with cycling of Mn, Fe, S, and organic matter by considering primary and secondary redox reactions, adsorption-desorption, and mineral dissolution and precipitation. Rate equations to describe mercury methylation were coupled to biogeochemical redox reactions. Simulations were compared to chemical conditions in incubations of wetland sediments with known amounts of organic matter and electron acceptors, which allowed rates of biogeochemical processes to be estimated. Subsequent comparison of simulations to field data collected in reconnaissance monitoring of wetlands in the Grasslands Ecological Area in Merced County, CA was used to estimate transport processes within wetland sediments. Simulations showed that Hg speciation and solubility were controlled by Fe and S cycling in addition to microbial Fe(III) and sulfate reduction being driving forces for Hg methylation. This shows the importance of coupling between Hg and redox-sensitive element cycles for predicting Hg fate.