

Understanding microscale isotopic patterns in pyrite using a two-dimensional reaction-diffusion model

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As high resolution analyses of individual sedimentary pyrites becomes increasingly common [1], complex patterns of sulfur isotope composition ($\delta^{34}\text{S}$) among and within single grains are often observed. These distinct isotopic variations, which form during diagenesis, encode information on past sedimentary environments. Deciphering the controls over these patterns may be used to reconstruct past environmental parameters, such as microbial rates of sulfate reduction, iron and organic matter abundance and reactivity in the sediment, sedimentation rate, and the efficiency of diffusive exchange between the water column and sediments during diagenesis [2,3].

To understand these isotopic patterns, we developed a two-dimensional model of sedimentary sulfur cycling, which simulates a suite of abiotic and microbially-driven solid-solution interactions in a cm-scale spatial domain. Using a finite-difference scheme, the model solves the pore-scale mass transport, (bio)chemical reactions and isotopic mass balance of dissolved sulfur, inorganic carbon and iron. Dissolution and precipitation of solids associated with these species (e.g., iron oxides, iron sulfides) cause changes to the pore geometry, which are applied using the “volume of pixel” method [4]. We prescribe the initial pore geometry and sediment composition, including the abundance and form of organic matter and reactive iron, and account for the evolving bulk chemical and isotopic composition of pore fluids by changing the simulation domain’s boundary conditions, using the results of a unidimensional diagenetic model [3]. For each combination of model parameters (sedimentation rate, organic matter and iron oxide concentrations and spatial distributions, porosity, etc.), simulations yield micrometer-resolution pyrite $\delta^{34}\text{S}$ patterns, which can be compared quantitatively to natural pyrite grains. The model provides a powerful new theoretical tool to link observed patterns of pyrite $\delta^{34}\text{S}$ to the properties of the depositional environments in which the pyrite formed and the dominant processes during diagenesis in those environments.

[1] Fike et al., 2015, *Annu. Rev. Earth Planet. Sci.* 43, 593–622. [2] Bryant et al., submitted (2019). [3] Halevy et al., submitted (2019). [4] Kang et al., 2007, *Water Resour. Res.* 43, 1–12.