A mechanistic understanding of oxygen isotope effects during microbial sulfate reduction

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The sulfur and oxygen isotopic composition of sulfate provides key insight into the reconstruction of both modern and paleo-environments. Variability within the correlation between $^{34}S/^{32}S$ and $^{18}O/^{16}O$ in sulfate resulting from microbial sulfate reduction (MSR) indicates isotopically distinct effects, yet requires a shared intracellular biochemistry. Understanding this metabolic signature is crucial in order to apply these isotope measures to the reconstruction of modern and paleo-environments. Here we present oxygen isotope results from a series of continuous culture experiments with two strains of sulfate reducing bacteria (fresh water *Desulfovibrio vulgaris* str. Hildenborough, and marine *Desulfovibrio alaskensis* str. G-20) grown across a range of metabolic rates and ambient sulfate concentrations. In combination with an updated MSR biochemistry, we draw explicit relationships between intracellular reaction reversibiilty and associated kinetic isotope effects, intracellular ATP yields, and net isotope effect captured in residual sulfate. This model also conserves the flux balance required to satisfy sulfur isotope observations from the same expeirments. We use non-linear regression fitting tools to solve for unknown kinetic, step-specific oxygen isotope effects, and to identify the key reactions within the metabolic pathway. With this novel combination of experimental and statistical tools, we defined a new, calibrated framework for understanding oxygen isotope variability in sulfate. This biochemically informed, thermodynamically driven cellular-scale model can then be used in combination with pore water sulfate/sulfide concentration data to solve for $^{18}O/^{16}O$ in pore water sulfate as a function of cell-specific sulfate reduction rates. This fully independent approach to cellular behaviour predicts MSR cell

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counts to within a factor of 2 of more time intensive, direct biological measurements.