

## **Genome-informed reactive transport simulations of CO<sub>2</sub> and carbon isotope dynamics in a flood plain aquifer**

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Although carbon fluxes in soils and groundwater are critical components of the global carbon budget, significant uncertainty is associated with their prediction due to the different hydrological and biogeochemical mechanisms that affect carbon turnover and distribution in the subsurface. In particular, redox reactions regulated by large and diverse soil microbial population exert an important control on soil CO<sub>2</sub> dynamics. The objectives of this study are to: (1) analyze spatio-temporal variability associated with CO<sub>2</sub> and carbon isotope profiles within the unsaturated zone of the Rifle site and (2) understand the importance of including microbial complexity in reaction networks.

A 2-D reactive transport model has been developed for the Rifle flood plain that couples hydrologic and biogeochemical processes to microbial functional distributions inferred from site-specific 'omic' data. The model includes microbial contributions from heterotrophic and chemolithoautotrophic processes. Monod based formulations are used to represent biomass formation and consider energy partitioning between catabolic and anabolic processes. We use this model to explore community emergence at the Rifle site and further constrain the extent and rates of nutrient uptake and CO<sub>2</sub> fluxes using stable carbon isotopes.

Results from 2D model simulations suggest that the genome-informed reaction network significantly improved predictions of biogeochemical cycling at the Rifle Floodplain. For example, not including chemolithoautotrophic pathways in the model resulted in 160% under-prediction of CO<sub>2</sub> fluxes to the atmosphere and 12% under-prediction of groundwater inorganic carbon exports to the Colorado River. Both CO<sub>2</sub> concentrations and δ<sup>13</sup>C profiles in the unsaturated zone point to spatially-variable sources and strong seasonal signatures.