GEWaSC Modeling of the Rifle Floodplain Aquifer**:** Hydrological, Biogeochemical, and Microbial Controls on Carbon, Nitrogen, and Oxygen Fluxes

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The Genome Enabled Watershed Simulation Capability (GEWaSC) is being used to address the principal controls on carbon, nitrogen, and oxygen fluxes in the surface and subsurface portions of the Rifle floodplain. Previous studies have identified naturally reduced zones (NRZs) in the saturated alluvium associated with elevated organic carbon, Fe(II), sulfide, and U(IV). These reduced areas are important drivers of biogeochemical fluxes from the dominantly sub-oxic floodplain into the Colorado River. The seasonal rise and fall of the Rifle floodplain water table, as well as the seasonal variation in surface temperatures, creates transient conditions in which leaching and mixing of reactive vadose components into the groundwater exert an important control on biogeochemical conditions and reaction rates in the subsurface aquifer.

2-D and 3-D variably saturated flow and reactive transport models have been developed to address multiple terminal electron acceptor processes (TEAPs), kinetic and equilibrium mineral precipitation and dissolution, as well as spatially distinct pools of Fe and S minerals and functional microbial populations. New proteomics-informed metabolisms include nitrate-dependent Fe(II) oxidation, oxygen-dependent Fe(II) oxidation, fermentation of DOM, nitrate reduction and microaerophilic heterotrophy. Microbial contributions from chemo(litho)autotrophic processes (e.g., ammonia, sulfur and iron oxidation) appear to be prominent.

2-D model simulations, in which NRZs were self-organized from initially homogeneous conditions, focused on abiotic and biotic contributions to CO_2 fluxes along a well-instrumented transect. The dynamics of these fluxes were consistent with observed seasonal water table variations, temperature fluctuations, and isotopic systematics in the vadose zone. The modeling indicated that the observed CO_2 fluxes cannot be explained by abiotic reactions alone, but required contributions from chemo(litho)autotrophic microbial activity. In particular, ^{13}C profiles in the vadose zone points to a microbial rather than abiotic origin for the elevated CO_2 concentrations in the NRZ.

3-D floodplain modeling, incorporating geophysically-delineated NRZs, focused on the impact of NRZs and local vadose zone conditions on redox cycling involving Fe, O, S, N, and C. The descending water table limb brings O_2 and nitrate to depth, leading to the oxidation of FeS, which liberates Fe(II) and sulfate into solution. Arrivals in the groundwater of U(VI), Ca^{2+}, sulfate, and Sr^{2+} prior to the water table peak are associated with vadose zone remnants of mill tailings that were not replaced with fill material.

Both 2-D and 3-D simulations will eventually incorporate kinetic parameters derived from traitbased models, also developed under GEWaSC, which is expected to significantly reduce the limitations of current simulations.