Modeling Hydrobiogeochemical Dynamics in a Field Emulsified Vegetable Oil (EVO) Injection Test at the Oak Ridge IFRC

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A pilot test was conducted involving a one-time 2-hour injection of emulsified vegetable oil (EVO) into an aquifer to reduce long-term U discharge to a stream. The objective of this work was to develop a coupled hydrological, geochemical and microbiological model to better describe and understand the complex processes in the field, and identify knowledge and data gaps for field scale bioremediation predictive simulation.

First, we developed a comprehensive biogeochemical model to couple hydrolysis of EVO, production and oxidation of long-chain fatty acids (LCFA), glycerol, acetate, and hydrogen, reduction of nitrate, Fe(III), U(VI) and sulfate, and methanogenesis with growth and decay of multiple functional microbial groups. By estimating a consistent set of EVO, LCFA and glycerol degradation rate constants, and using growth rate parameter values from the literature, the model matched observed sulfate, U(VI), and acetate concentrations and described microbial population dynamics in various microcosms amended with ethanol, oleate, and EVO and different levels of sulfate.

Using a kinetic Langmuir isotherm to approximate EVO sorption, we then applied the biogeochemical model to simulate observed acetate, nitrate, Fe, U, and sulfate concentrations, and the activities of multiple microbial functional groups during and after EVO injection. While lab-determined parameters were generally applicable in the field-scale simulation, the rate coefficient for EVO hydrolysis was estimated to be an order of magnitude greater in the field than in microcosms. Assuming *Pelosinus* was grew via glycerol fermentation, the model predicted later and less biomass production for these fermentative microorganisms than observed, indicating potential alternative pathways for *Pelosinus* growth. A lag time of about 50 days or alternative inhibitory mechanisms for acetoclastic methanogenesis was necessary to simulate the observed sustained acetate concentration.

The model predicted substantial accumulation of denitrifiers and sulfate reducers, and U(IV) near injection wells and along the side boundaries of the treatment zone where produced electron donors (e.g., acetate) met electron acceptors in the groundwater. While EVO retention and hydrolysis characteristics were expected to control treatment longevity, modeling results indicated that electron acceptors such as sulfate may not only compete for electrons but also play a role in degrading complex substrates and enhancing U(VI) reduction and immobilization.