

A Field-Scale Omics-Enabled Groundwater Reactive Transport Model

Y. Wang^{1*} (yajiao.wang-1@ou.edu), D. Ning¹, G. Wang¹, N. Xiao¹, Z. Shi¹, P. Zhang¹, Z. He¹, J.D. Van Nostrand¹, L. Wu¹, T.C. Hazen^{2,3}, J-Z. Zhou¹, A.P. Arkin^{4,5} and **P.D. Adams**^{4,5}

¹University of Oklahoma, Norman; ²University of Tennessee, Knoxville; ³Oak Ridge National Lab, Oak Ridge; ⁴Lawrence Berkeley National Lab, Berkeley; ⁵University of California, Berkeley.

<http://enigma.lbl.gov>

Project Goals: ENIGMA -Ecosystems and Networks Integrated with Genes and Molecular Assemblies use a systems biology approach to understand the interaction between microbial communities and the ecosystems that they inhabit. To link genetic, ecological, and environmental factors to the structure and function of microbial communities, ENIGMA integrates and develops laboratory, field, and computational methods.

Microbial activity substantially impacts the temporal and spatial distribution of contaminants through diverse reactions and transport in groundwater. The reactive transport model (RTM) in groundwater is aimed to quantitatively describe and predict the distribution of chemicals, which integrates various active hydrological, geochemical, and microbial processes. However, current groundwater reactive transport models are limited in the ability to predict microbial activity, especially when the structure and functions of the microbial community are dynamic due to variations of environmental conditions. The increasing availability of the meta-omics data makes it feasible to quantitatively simulate and predict the dynamics of microbial community structure and functions in groundwater. Our idea is to refine the biotic reactions in the reactive transport processes by incorporating the microbial functional group information through omics measurements to explicitly represent microbially-mediated biogeochemical reactions.

The primary flow field and solute transport model were built using the commonly applied MODFLOW and MT3D-USGS models. In addition, we modified MT3D-USGS to incorporate multiple (i.e., 22) microbial functional groups, which mediate the critical metabolic processes in anaerobic fermentation of organic matter, methanogenesis, methane oxidation, oxic/anoxic degradation of organic matter, uranium (VI) reduction, denitrification, nitrification, nitrogen fixation, dissimilatory sulfate reduction and oxidation, dissimilatory iron (III) reduction and oxidation. In addition, the new model development will include the assimilatory processes of methane oxidation, nitrate reduction, sulfate reduction, and iron (III) reduction, microbial mortality, abiotic iron (II) oxidation and iron (III) reduction, immobilization of uranium (IV) and iron (II, III), and sorption of various substances.

The measurements of chemical concentrations and functional gene abundances will be used to constrain and validate the new model. However, since the groundwater reactive transport process

combines various complex processes, it is challenging to estimate the key parameters. Therefore, we developed an parameter optimization procedure for field-scale groundwater RTM based on the Shuffled Complex Evolution (SCE) algorithm. To enhance the computation efficiency, we developed the parallel computation program with the OpenMPI interface on the supercomputer. We considered multiple objectives in the calibration of model parameters. Each objective evaluates the goodness-of-fit of a specific observed variable, e.g., water table, concentrations of ammonium/nitrate/nitrite, sulfate/sulfide, iron (II/III), uranium (VI), gases (N₂O, NO, CH₄, CO₂, H₂), microbial biomass, functional gene/enzyme abundances. The overall objective function is the weighted average of multiple objective functions.

This new model was applied to the Emulsified Vegetable Oil (EVO) injection project in 2009 at the ORIFRC site. Here we present the updates of the modeling results on the model development and parameterization. The total area of the modeling zone was around 3700 m², which contains the main flow path of injected chemicals. The modeling area was discretized into grids with 0.5 m × 0.5 m × 2 m for the finite-difference calculation. At first, we used the MODFLOW and PEST pilot point method to estimate the spatial distribution of flow-related parameters, i.e., hydraulic conductivity and recharge rate, and simulated the transient flow field after EVO injection. The mean residual of the water heads in the optimization was <0.01 m. Then we estimated the porosity and dispersivity with tracer concentration due to its weak reactivity. To build the baseline RTM, we estimated the reactive parameters and simulated the chemical transport process with biomass-based microbial reaction rate. Next, we will integrate the omics data into the reaction rates and use functional gene abundances to constrain the model. By comparing with the baseline RTM, we will evaluate the omics-informed reactive transport model to see if we could improve modeling performance and reduce uncertainty by introducing necessary functional enzymes/genes.

This new model could help better understand how different microbial functional groups contribute to the transformations of the contaminants in groundwater after EVO injection in the complex interactions between microbial, hydrological, and geochemical processes. It can also be extended to quantitatively and systematically predict the fate of contaminants in groundwater under different scenarios (e.g., extreme flood, low temperature, the dosage of different carbon sources).

This material by ENIGMA- Ecosystems and Networks Integrated with Genes and Molecular Assemblies a Science Focus Area Program at Lawrence Berkeley National Laboratory is based upon work supported by the U.S. Department of Energy, Office of Science, Office of Biological & Environmental Research under contract number DE-AC02-05CH11231