PROGRAM ELEMENT 7

System Engineering, Integration, Prediction and Optimization

Simulating Bioremediation of Uranium Contaminated Aquifers; A Global Uncertainty Assessment of Model Parameters

Peter R. Jaffe, Sookyun Wang, Genyuan Li, Sheng-Wei Wang and Herschel A. Rabitz
Department of Civil and Environmental Engineering, Princeton University, Princeton, N.J.

Mobility of trace metals and radioisotopes in groundwater can be controlled to a significant extent via in-situ manipulation of key biogeochemical reactions that directly or indirectly alter their solubility. For this purpose, specified redox profiles need to be established in the groundwater. These redox profiles develop, in response to biostimulation schemes, from the availability and transport of different electron acceptors and their utilization by different bacteria during the degradation of an organic substrate. The objective of this research is to assess modeling techniques that are capable of simulating the fate of trace metals and radionuclides in the subsurface in response to different biostimulation schemes.

A time-dependent one-dimensional reactive transport model has been developed. The model consists of a set of coupled, steady state mass balance equations, accounting for advection, diffusion, dispersion and a kinetic formulation of the transformations affecting an organic substrate, electron acceptors, corresponding reduced species and contaminant metals of interest. This set of equations is solved numerically, using a finite element scheme. The redox conditions of the domain are characterized by estimating the pE, based on the concentrations of the dominant terminal electron acceptor and its corresponding reduced specie. This pE and the concentrations of relevant species are passed to a modified version of MINTEQA2, which calculates the speciation and solubilities of the species of interest. Kinetics of abiotic reactions are described as being proportional to the difference between the actual and equilibrium concentration. Simulations are performed to illustrate the effect of biostimulation on the transport of uranium in the subsurface.

In the model, the relationship between the various biological chemical variables and the model output may be nonlinear, and various interdependencies are expected to exist. It is important to identify all of these variable interactions, especially for the key model parameters, and use this information to: (1) develop more robust models; (2) identify the key coefficients that need to be specified with the highest precision; and (3) develop reliable bioremediation schemes.

A recently developed nonlinear analysis tool, RS-HDMR (Random Sampling-High Dimensional Model Representation) is employed to determine the relationship between the various model inputs and outputs. The RS-HDMR formulation provides a highly efficient and thorough sampling of the overall space of variables to identify those that are important and are acting either independently or cooperatively. An initial analysis has been performed to investigate the effect of 20 rate constants and transport parameters on the transport of four chemical species, including uranium. The global output uncertainties in the whole domain of 20 input variables was quantified by RS-HDMR, and the key model parameters were identified. A significantly higher variance was associated with outputs representing a given concentration in space and time than for outputs integrated over space and/or time such as cumulative flux at a given location.