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Authors

Chen, Jinsong
Hubbard, Susan
Rubin, Yoram
et al.

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Geochemical Characterization Using Geophysical Data and Markov Chain Monte Carlo Methods

Jinsong Chen, Susan Hubbard, Yoram Rubin, Chris Murray, and Ernest Majer

Although the spatial distribution of geochemical parameters is extremely important for many subsurface remediation approaches, traditional characterization of those parameters is invasive and laborious, and thus is rarely performed sufficiently to describe natural hydrogeological variability at the field-scale. This study is an effort to jointly use multiple sources of information, including noninvasive geophysical data, for geochemical characterization of the saturated and anaerobic portion of the DOE South Oyster Bacterial Transport Site in Virginia. Our data set includes hydrogeological and geochemical measurements from five boreholes and ground-penetrating radar (GPR) and seismic tomographic data along two profiles that traverse the boreholes. The primary geochemical parameters are the concentrations of extractable ferrous iron Fe(II) and ferric iron Fe(III). Since iron-reducing bacteria can reduce Fe(III) to Fe(II) under certain conditions, information about the spatial distributions of Fe(II) and Fe(III) may indicate both where microbial iron reduction has occurred and in which zone it is likely to occur in the future. In addition, as geochemical heterogeneity influences bacterial transport, estimates of the geochemical parameters provide important input to numerical flow and contaminant transport models geared toward bioremediation.

Motivated by our previous research, which illustrated that crosshole geophysical data can be very useful for estimating hydrogeological parameters, we hypothesize in this study that geochemical and geophysical parameters may be linked through their mutual dependence on hydrogeological parameters such as lithofacies. We attempt to estimate geochemical parameters using both hydrogeological and geophysical measurements in a Bayesian framework. Within the two-dimensional study domain (12m x 6m divided into 0.25m x 0.25m pixels), geochemical and hydrogeological parameters were considered as data if they were available from direct measurements or as variables otherwise. To

estimate the geochemical parameters, we first assigned a prior model for each variable and a likelihood model for each type of data, which together define posterior probability distribution for each variable on the domain. Since the posterior probability distribution may involve hundreds of variables, we used a Markov Chain Monte Carlo (MCMC) method to explore each variable by generating and subsequently evaluating hundreds of realizations.

Results from this case study showed that although geophysical attributes are not necessarily directly related to geochemical parameters, through their joint and indirect connections with hydrogeological properties such as lithofacies, geophysical data could be very useful for providing accurate and high-resolution information about geochemical parameter distribution. This case study also demonstrated that MCMC methods were particularly useful for geochemical parameter estimation using geophysical data because they allow for incorporation of spatial correlation information as well as measurement errors and cross correlations among different types of parameters into the procedure.