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Hybrid machine learning/adjoint sensitivity model for source zone sampling optimization

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Modeling DNAPL source zone plume evolution using traditional flow and transport models is a computationally intensive process that requires specification of a large number of material properties and hydrologic/chemical parameters. Given its computational burden, Monte Carlo simulation using such models is particularly ill-suited for uncertainty assessment and/or subsurface sampling optimization in real field applications. In this work, we present an innovative approach that couples machine learning, adjoint sensitivity theory, and statistical analysis to optimize borehole sampling for quantification of the evolution of down gradient flux-averaged concentration.

Probabilistic models, based on discriminative random fields (DRF), are first employed to synthesize stochastic realizations of a subsurface source zone consistent with known, limited, site characterization data. Using a suite of full scale simulations as training data, a statistical model is developed to predict the spatial distribution and uncertainty associated with key features (i.e. permeability and sequestered contamination [aqueous, sorbed, and NAPL]) that control plume evolution and persistence. Given an initial spatial distribution of contaminant mass, conditioned on measured field data, the adjoint state sensitivity method is then employed to quantify the importance of local system properties on down gradient flux-averaged concentration. The optimal sampling design problem is then addressed using first-order second-moment uncertainty analysis. In the decision process, the costs of additional measurements are justified by a sufficient decrease in the uncertainty, selecting measurements associated with the highest expected worth.

The utility of this probabilistic statistical modeling approach is demonstrated using numerically generated, two-dimensional, heterogeneous DNAPL source zones. Results reveal that down gradient flux-averaged concentration sensitivities to initial contaminant mass compartments are strongly affected by local permeability values. In addition, initial aqueous and sorbed concentrations and their corresponding variances have a major impact on down gradient flux-averaged concentration at early times, while the influence of initial NAPL saturation persists for a longer period. This innovative sampling strategy, coupling sensitivity analysis and uncertainty quantification, shows promise for enhancement of our ability to guide characterization of source zones under realistic field conditions.

References

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Primary authors: TANG, Tian (Tufts University); Dr ARSHADI, Masoud (Tufts University); Dr MILLER, Eric (Tufts University); Dr ABRIOLA, Linda (Tufts University)

Presenter: TANG, Tian (Tufts University)

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