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Discriminative Random Field Models for Subsurface Source Zone Characterization and Uncertainty Quantification

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Application of flow and transport simulators for prediction of the release, entrapment, and persistence of dense non-aqueous phase liquids (DNAPLs) and associated contaminant plumes is a computationally intensive process that requires specification of a large number of material properties and hydrologic/chemical parameters. Given its computational burden, this direct simulation approach is particularly ill-suited for quantifying both the expected performance and uncertainty associated with candidate remediation strategies under real field conditions. Prediction uncertainties primarily arise from limited information about contaminant mass distributions, as well as the spatial distribution of subsurface hydrologic properties. Application of direct simulation to quantify uncertainty would, thus, typically require simulating multiphase flow and transport for a large number of permeability and release scenarios to collect statistics associated with remedial effectiveness, a computationally prohibitive process.

The primary objective of this work is to develop and demonstrate a fast and effective methodology that employs measured field data to produce equi-probable stochastic representations of a subsurface source zone that capture the spatial distribution and uncertainty associated with key features that control remediation performance (i.e., permeability and contamination mass). Here we employ probabilistic models known as discriminative random fields (DRFs) to synthesize stochastic realizations of initial mass distributions consistent with known, and typically limited, site characterization data. Using a limited number of full scale simulations as training data, a statistical model is developed for predicting the distribution of contaminant mass (e.g., DNAPL saturation and aqueous concentration) across a heterogeneous domain. Markov chain Monte Carlo (MCMC) sampling methods are then employed, in conjunction with the trained statistical model, to generate realizations conditioned on measured borehole data. Performance of the statistical model is illustrated through comparisons of generated realizations (metrics) with the 'true'numerical simulations. Finally, we demonstrate how these realizations can be used to determine statistically optimal locations for further interrogation of the subsurface.

References

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