

Quantifying Subsurface Parameter and Transport Uncertainty Using Surrogate Modeling and Environmental Tracers

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September 25, 2021

Abstract

We combine physics-based groundwater reactive transport modeling with machine learning techniques to quantify hydrogeologic model and solute transport predictive uncertainties. We train an artificial neural network (ANN) on a dataset of groundwater hydraulic heads and ^3H concentrations generated using a high-fidelity groundwater reactive transport model. Using the trained ANN as a surrogate model to reproduce the input-output response of the high-fidelity reactive transport model, we quantify the posterior distributions of hydrogeologic parameters and hydraulic forcing conditions using Markov-chain Monte Carlo (MCMC) calibration against field observations of groundwater hydraulic heads and ^3H concentrations. We demonstrate the methodology with a model application that predicts Chlorofluorocarbon-12 (CFC-12) solute transport at a contaminated site in Wyoming, USA. Our results show that including ^3H observations in the calibration dataset reduced the uncertainty in the estimated permeability field and infiltration rates, compared to calibration against hydraulic heads alone. However, predictive uncertainty quantification shows that CFC-12 transport predictions conditioned to the parameter posterior distributions cannot reproduce the field measurements. We found that calibrating the model to hydraulic head and ^3H observations results in groundwater mean ages that are too large to explain the observed CFC-12 concentrations. The coupling of the physics-based reactive transport model with the machine learning surrogate model allows us to efficiently quantify model parameter and predictive uncertainties, which is typically computationally intractable using reactive transport models alone.

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