

## MULTIPHYSICS SIMULATION OF THE ELECTRICAL SIGNATURE OF DUAL-DOMAIN MASS TRANSFER AT THE PORE-SCALE

*Charles L. Dorchester, Colorado School of Mines, Golden, CO, USA*

*Kamini Singha, Colorado School of Mines, Golden, CO, USA*

*Frederick D. Day-Lewis, Pacific Northwest National Laboratory, Richland, WA, USA*

Dual-domain mass transfer (DDMT) is a conceptual model that interprets aquifer systems as being defined by a mobile porosity, an immobile porosity, and the mass-transfer rate coefficient that describes how easily solutes can move between these two domains. The mass-transfer rate coefficient describes the retention and release of solutes from immobile porosity, which has been shown to produce late-time concentration rebound and the slow release of solutes, otherwise known as anomalous tailing. Although DDMT techniques can describe contaminant storage and release more accurately than the advection-dispersion equation, they typically involve adjusting these model parameters until the model predictions fit observed data. To help constrain estimation of these parameters, electrical resistivity (ER) has been used in previous work; fluid electrical conductivity and bulk electrical conductivity show a hysteretic relationship in response to DDMT behavior because fluid sampling preferentially draws from the mobile domain, whereas ER methods are sensitive to the bulk composition. Here, we investigate the relationship between the mobile porosity, immobile porosity, and mass-transfer rate coefficient in a pore-scale numerical model by simulating solute concentration—converted to fluid electrical conductivity—and the subsequent bulk electrical conductivity. In particular, we study the application of ER to (1) constrain parameterization of a pore-scale DDMT model, and (2) assess spatial variability of effective parameters.

The pore-scale numerical model, developed in COMSOL Multiphysics, simulates fluid flow, transport of an electrically conductive solute, and direct-current electrical conduction in 2-D. We match an analytic solution of the 1-D DDMT equation to our simulated data using a nonlinear least-squares regression technique. We find that: (1) mobile domains and immobile domains are present, regardless of the system being explicitly defined with one versus two domains; and (2) the mobile porosity, immobile porosity, and mass-transfer rate can be estimated by analyzing the hysteretic relationship between fluid and bulk electrical conductivity, and perhaps meaningfully scaled to field systems. Overall, our findings support the hypothesis that hysteresis in ER data is a function of fast versus slow paths, even in the absence of pre-defined immobile porosity, so an open question is what “immobile” means in a macroscopic system with no explicit immobile pore space.