Subsurface Flow and Transport Modeling: Upscaling, Inversion, and Model Complexity

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Bio: Ye Zhang received her B.S. degree in Hydrogeology from Nanjing University, People’s Republic of China; her M.S. degree in Hydrogeology from the University of Minnesota, with a M.S. Minor in Civil Engineering; and her Ph.D. in Hydrogeology from Indiana University, with a Ph.D. Minor in Scientific Computing. She is currently an Associate Professor in the Department of Geology and Geophysics, University of Wyoming. Her research interests include geologic modeling/geostatistics, upscaling, inversion, and uncertainty analysis for subsurface applications. Recent interest includes drilling, instrumentation, and modeling of interconnected surface and groundwater systems in mountain headwater regions.

Abstract: Numerical modeling is used to evaluate a variety of subsurface flow and transport phenomena, although significant uncertainty in model parameters, processes, and boundary conditions (BC) exists. This talk will first discuss parameter uncertainty, whereas due to data scarcity or computation limitation, simplified subsurface conceptual models are constructed without resolving smaller scale parameter variability. Because higher resolution models often incur greater characterization costs, for various modeling objectives, what kind of model(s) should be built, and at what resolution(s)? For a set of hierarchically coarsened conceptual models, a connectivity-based permeability and dispersivity upscaling technique is developed to calculate equivalent parameters, thus bulk flow and transport arising out of underlying heterogeneous parameter fields can be captured. In modeling geologic carbon sequestration, these models are compared within their full parameter space, yielding insights into optimal heterogeneity resolutions for meeting different prediction goals under uncertainty. To address BC uncertainty, a new and computationally efficient subsurface inverse theory is developed for confined and unconfined aquifers to simultaneously estimate parameters (e.g., permeabilities and storativities), state variables, and BC. Uncertainty in subsurface static data can be accounted for, while permeability structure can also be identified. The theory addresses model “structure errors”, either simplifying due to limited data or complexifying due to process uncertainty, by estimating equivalent parameters, thus providing a means of constructing optimally coarsened subsurface models if detailed measurements needed for upscaling do not exist. The theory has been successfully extended to inverting transient and unsaturated flows as well as for contaminant source identification under unknown transport initial and BC.
A Direct Method of Hydraulic Conductivity Structure Identification for Subsurface Transport Modeling

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Abstract: Solute transport in aquifers is strongly influenced by the spatial distribution of subsurface hydraulic conductivity ($K$), while limited drilling in data-sparse environments typically results in lack of data characterizing both the $K$ and the in-situ fluid flow boundary conditions (BC). To characterize such environments, we present an efficient direct inverse method to simultaneously identify aquifer $K$ pattern, its values, and the flow field [Jiao & Zhang, 2016]. The method ensures fluid flow continuity using local approximate solutions of the governing equation conditioned to limited hydraulic measurements, while physics of the flow is enforced making the inverse problem well-posed. A single system of equations is assembled and solved, from which parameters and BC can be simultaneously estimated. For problems with irregular and regular $K$ distributions, inversion is demonstrated for different measurement types, quality, and quantity. When measurement error is increased, the estimated $K$ pattern is largely insensitive to the error, although the inverted flow field suffers greater inaccuracy. Local conductivity and Darcy flux measurements are found to have similar information content, although subtle differences exist in the inverted flow fields when long-term contaminant release is simulated. Local conductivity measurements lead to better identification of conductivity pattern, values, and the hydraulic head field; Darcy flux measurements lead to more accurate estimation of the velocity field and thus improved transport predictions. Overall, the velocity fields estimated based on the hydraulic data alone can lead to reasonable predictions of contaminant migration and breakthrough curves under unknown aquifer BC. Depending on the desired accuracy, fine-scale heterogeneity can be recovered at increased sampling density. However, given the cost of field data acquisition, we argue that the goal of pattern inversion is to recover a sufficient level of detail to make approximately accurate transport prediction. Fine scale details may be ignored by employing appropriate upscaling techniques [Zhang et al., 2006; Zhang & Zhang, 2015]. Our recent work has successfully developed a sequential inversion technique whereas both hydraulic and tracer data are inverted [unpublished research]. Future work will (1) evaluate sample network design to optimize data collection and minimize cost; (2) develop joint inversion techniques using hydraulic, tracer, and geophysical data; (3) quantify uncertainty in inversion and forecast.

Reference:

