

## Uncertainty quantification in modeling flow and transport in porous media

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This special issue of *Stochastic Environmental Research and Risk Assessment* in honor of Shlomo P. Neuman presents recent developments in uncertainty quantification in predictions of flow and transport in heterogeneous porous media. It covers subjects as diverse as stochastic hydrogeology, aquifer characterization, effective (average) descriptions of subsurface processes, inverse modeling, and scaling theory, all of which benefited from the insightful contributions of Shlomo P. Neuman. We hope that this volume will become a reference point for students learning these subject, scientists pursuing innovative research, and professionals and water resources planners looking to quantify predicting uncertainty arising from the intrinsic complexity of the subsurface environment.

S. P. Neuman is one of the pioneers in the use of stochastic modeling as a means of dealing with uncertainty in hydraulic and transport parameters of heterogeneous subsurface environments. This special issue contains a number of contributions in this field. *Riva et al.* introduce a stochastic approach to interpret field-scale tracer tests conducted in heterogeneous aquifers. By using Monte Carlo simulations, the authors demonstrate that directly linking porosity and permeability distribution to the spatial variability of soil particle sizes renders the best prediction of the

observed heavy tailing of measured breakthrough curves. *Zhang et al.* compare the performance of Monte Carlo and stochastic collocation methods to evaluate the probability of the concentration of a conservative solute attaining a given threshold. Their analysis shows that Latin Hypercube sampling and Quasi Monte Carlo outperform standard Monte Carlo simulations, and that a sparse-grid collocation and a probabilistic collocation method provide an accurate and efficient alternative to Monte Carlo simulations. *Broyda et al.* develop partial differential equations satisfied by the probability density function (PDF) of the concentration of solutes undergoing heterogeneous reactions in porous media with uncertain chemical properties. The authors obtain a semi-analytical solution for the concentration PDF and demonstrate that its shape and evolution are significantly affected by both spatial variability of advective velocity and the Damköhler number. *Tartakovsky* presents a novel Lagrangian particle model based on smoothed particle hydrodynamics (SPH). His analysis reveals the advantages of Lagrangian methods for the stochastic analysis of miscible density-driven fluid flows in the presence of Rayleigh-Taylor instability. When used in the context of Monte Carlo simulations, the method can provide reliable estimated of the probability of occurrence of rare events.

Two papers are concerned with the estimation of hydrogeological parameters governing groundwater flow. *Liu et al.* present an approach to efficient and accurate parameter estimation for nonlinear flow and transport problems in porous media. They discuss the relative merits and weaknesses of different schemes, including Maximum a posteriori (MAP) and Monte Carlo based methods, used to parameterize a DNAPL dissolution/transport model. Methods to diagnose Markov Chain Monte Carlo (MCMC) samples are introduced, compared and discussed in the context of computationally demanding parameter estimation

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procedures. *Harp and Vesselinov* discuss a stochastic inversion approach to identify lithofacies distribution within a three-dimensional, large scale heterogeneous porous medium. Their approach embeds the Markov Chain based geostatistical framework into stochastic inversion of groundwater flow. This enables one to incorporate features associated with the internal architecture of facies into inverse modeling efforts.

*Zhang and Yang* and *Hsu and Chen* discuss various aspects of fractal interpretations of groundwater flow systems. The numerical simulations of *Zhang and Yang* improve our understanding of the nature of observed temporal fluctuations of hydraulic head in response to interactions with surface water. Their results show that groundwater level fluctuations can be interpreted as a temporal fractal in low to moderately permeable aquifers. *Hsu and Chen* explore the idea that hydraulic conductivity can be interpreted as a three-dimensional fractal random field, which displays a high degree of variability and exhibits one-point statistics of Levy-stable distribution and the two-point statistics of fractional Levy motion (fLm). The authors demonstrate that their fractal model can be used to simulate flow and solute transport under various scenarios by adjusting the Levy index and cutoffs of fLm.

*Di Federico et al.* explores the concept of effective permeability for non-Newtonian flow in a randomly

heterogeneous porous medium. Randomness is associated with the permeability coefficient, which is treated as a spatially correlated lognormal process. The authors start from a one-dimensional scenario for which they derive expressions for effective permeability under uniform (in the mean) flow. They then extend their findings to two- and three-dimensional systems upon conjecturing the effective permeability to be a power-average of one-dimensional scenarios. Their key findings are that the effective permeability depends on flow dimensionality, domain heterogeneity, and flow behavior index.

*Blasch et al.* studied a problem involving interaction between surface water and groundwater. The authors analyze the occurrence of vertical drainage through streambed sediments after the cessation of an ephemeral streamflow event. They analyze the drainage response of an alluvial stream channel located in Tucson, Arizona. The study is supported by a comprehensive set of data, including soil moisture and temperature measurements at various depths within the upper 2.5 m collected with a high temporal frequency during several flow events from 2000 and 2002. The authors frame their analysis in the context of management schemes for riparian areas. The results of the study demonstrate the need for combining quantitative, physically based modeling and data synthesis.