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Introduction to the Special Section in *Vadose Zone Journal*: Parameter Identification and Uncertainty Assessment in the Unsaturated Zone

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During the last few decades hydrologists have made significant progress toward applying physically based simulation models for the analysis and understanding of field-scale flow and transport phenomena in the vadose zone. This progress has been enabled in part by the development of advanced parameter estimation and uncertainty assessment methods such as statistically based pedotransfer functions and multidimensional inverse modeling techniques. However, even the most elaborate physically based model cannot capture the complex heterogeneity and interactions between spatially distributed water, plant, and atmospheric components of the unsaturated flow system. These will always need to be abstracted into models characterized by relatively simple mathematical expressions with a limited number of parameters. At the field scales of interest these parameters are difficult to evaluate directly and are represented by effective upscaled values instead. Due to the nonlinear nature of vadose zone processes, parameters vary strongly in space–time, even in the hypothetical case of a uniform soil. Considering further the difficulty of measuring state variables such as water content and pressure head at depth render the estimation of vadose zone parameters a special challenge.

Parameter estimates are inherently nonunique and prone to error due to insufficient and noisy data. Additional model uncertainty arises from inadequate conceptualization of system makeup and the underlying processes. There is a growing awareness among hydrologists for the need to articulate and quantify these uncertainties to properly inform decisions concerning data collection, model development, and operational issues. This is reflected in a growing number of technical publications and conference sessions devoted to parameter estimation and uncertainty in the recent past. The five papers in the special section "Parameter Identification and Uncertainty Assessment in the Unsaturated Zone" in this issue of the *Vadose Zone Journal* contribute to the debate by describing various methods and strategies for improved parameter estimation and treatment of uncertainty in subsurface flow and transport modeling. The contributions cover applications ranging from lysimeter to larger scale water flow and solute transport phenomena in the field.

Mertens et al. (2006) describe a multiobjective approach to subsurface parameter estimation, introducing an automatic computer-based optimization strategy to obtain a nondominated or Pareto set of solutions. Their multiobjective analysis of field lysimeter experiments using soil moisture content and leachate volume data from irrigated and nonirrigated treatments shows considerable differences in the Pareto optimal values of soil hydraulic parameters between two treatments. The tradeoff provides important insight into the issue of conceptual model uncertainty.

Kwicklis et al. (2006) couple a multiphase, multicomponent parameter estimation strategy with Monte Carlo uncertainty analysis approach for liquid and vapor fluxes in deep arid systems at the Nevada Test Site based on borehole measurements of water potential, saturation, and natural tracer concentration. Most of their parameter estimates exhibit significant correlations by calibration that impacts the prediction of uncertainty intervals.

Schoups and Hopmans (2006) evaluate the relationship between model complexity and input uncertainty for field-scale prediction of water flow and solute transport. Their methodology provides a straightforward approach to identifying an optimal level of model com plexity given the degree of field-scale heterogeneity and data availability.

Neuweiler and Eichel (2006) derive an upscaled model for Richards' equation in a layered porous medium using homogenization theory for small-scale capillary-dominated, intermediate, and large-scale gravity-dominated flow regimes. They find that effective parameter functions describing relative permeability and capillary pressure head versus saturation can be estimated with reasonable accuracy based on a capillary equilibrium assumption.

Kung et al. (2006) use three sets of four field-scale tracer mass flux breakthrough patterns measured under transient unsaturated flow conditions to evaluate the validity of an indirect method to quantify equivalent pore spectra of macropore preferential flow pathways. They conclude that the indirect method has predictive value and may be preferred to the lumped soil hydraulic conductivity approach in determining the impact of macropore preferential flow pathways on water movement and solute transport under transient unsaturated flow conditions.

Among emerging methods of comprehensive uncertainty assessment not addressed in this special section we include the Markov Chain Monte Carlo approach

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Abbreviations: BMA, Bayesian Model Averaging; EnKF, Ensemble Kalman Filter; MLBMA, Maximum Likelihood Bayesian Model Averaging.

(MCMC), Bayesian Model Averaging (BMA: Hoeting et al., 1999; Raftery et al., 2005; Vrugt and Robinson, unpublished data, 2006), its Maximum Likelihood version (MLBMA: Neuman, 2003; Ye et al., 2004, 2005), and recursive state space filtering methods such as the Ensemble Kalman Filter (EnKF: Evensen, 1994; Vrugt et al., 2005). BMA and MLBMA are particularly appealing because they are relatively easy to implement, accounting jointly for conceptual model and parameter uncertainty by considering a set of alternative models that may be very different from each other while being based on a common set of data. MLBMA is an approximate version of BMA, which incorporates standard maximum likelihood methods of parameter estimation (applicable to both deterministic and stochastic moment models), without requiring (though admitting) prior statistical information about the parameters. Furthermore, it obviates the need for computationally intensive Monte Carlo simulations to compute BMA weights, and honors the principle of parsimony by preferring simple over complex models if warranted by the data. All published applications of MLBMA thus far concerned models of spatially variable vadose zone properties. We are confident that the above methods, including those published in this issue of the *Vadose Zone Journal* will contribute to improved modeling of vadose zone processes in the future.

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REFERENCES

Evensen, G. 1994. Sequential data assimilation with a non-linear quasi-geostrophic model using Monte Carlo methods to forecast error statistics. J. Geophys. Res. 99(C5):10143–10162.

Hoeting, J.A., D. Madigan, A.E. Raftery, and C.T. Volinsky. 1999. Bayesian model averaging: A tutorial. Stat. Sci. 14(4):382–417.

Kwicklis, E.M., A.V. Wolfsberg, P.H. Stauffer, M.A. Walvoord, and M.J. Sully. 2006. Multiphase, multicomponent parameter estimation for liquid and vapor fluxes in deep arid systems using hydrologic data and natural environmental tracers. Available at www.vadosezonejournal.org. Vadose Zone J. 5:934–950 (this issue).

Kung, K.-J.S., E.J. Kladivko, C.S. Helling, T.J. Gish, T.S. Steenhuis, and D.B. Jaynes. 2006. Quantifying the pore size spectrum of macropore-type preferential pathways under transient flow. Available at www.vadosezonejournal.org. Vadose Zone J. 5:978–989 (this issue).

Mertens, J., R. Stenger, and G.F. Barkle. 2006. Multiobjective inverse modeling for soil parameter estimation and model verification. Vadose Zone J. 5:917–933 (this issue).

Neuman, S.P. 2003. Maximum likelihood Bayesian averaging of alternative conceptual-mathematical models. Stochastic Environ. Res. Risk Assess. 17(5):291–305. doi:10.1007/s00477-003-0151-7.

Neuweiler, I., and H. Eichel. 2006. Effective parameter functions for the Richards equation in layered porous media. Available at www.vadosezonejournal.org. Vadose Zone J. 5:963–977 (this issue).

Raftery, A.E., T. Gneiting, F. Balabdaoui, and M. Polakowski. 2005. Using Bayesian model averaging to calibrate forecast ensembles. Monthly Weather Rev. 133:1155–1174.

Schoups, G., and J.W. Hopmans. 2006. Evaluation of model complexity and input uncertainty of field-scale water flow and salt transport. Vadose Zone J. 5:951–962 (this issue).

Vrugt, J.A., B.A. Robinson, and V.V. Vesselinov. 2005. Improved inverse modeling for flow and transport in subsurface media: Combined parameter and state estimation. Geophys. Res. Let 32: L18408. doi:10.1029/2005GL023940.

Ye, M., S.P. Neuman, and P.D. Meyer. 2004. Maximum likelihood Bayesian averaging of spatial variability models in unsaturated fractured tuff. Water Resour. Res. 40(5):W05113. doi:10.1029/2003WR002557.

Ye, M., S.P. Neuman, P.D. Meyer, and K. Pohlmann. 2005. Sensitivity analysis and assessment of prior model probabilities in MLBMA with application to unsaturated fractured tuff. Water Resour. Res. 41:W12429. doi:10.1029/2005WR004260.