Uncertainty and Upscaling in Porous Media Flow

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Processes associated with fluid flow through porous rocks and sediments are at the core of problems in groundwater flow, contaminant migration, and petroleum production. A rigorous understanding of these processes is necessary to optimize our water resources, reduce environmental risk, and exploit fossil fuel most cost-effectively. Our objective is to develop partial differential equations for the moments of single- and two-phase fluid flow in heterogeneous porous media under realistic conditions as an alternative to the commonly used Monte Carlo simulation approach.

The workable moment equations have some important benefits over the traditional Monte Carlo approach. First, there are a small number of equations to be solved: one equation for the mean, and one each for a small number of variances and co-variances. Second, the coefficients of the equations, as averaged quantities, are smooth; thus, these equations can be solved on a relatively coarse grid. Third, the moment equations are available in analytic form, even though they are solved numerically in applications. This feature holds the potential for increased physical understanding of the mechanisms of uncertainty.

Extending from one scale to a larger one requires "upscaling," which allows the essence of physical processes at one level to be summarized at the coarser level. For upscaling from the local scale to the field scale, there are usually two kinds of approaches.

The first begins with the macroscopic equations and assumes that they are valid at all (larger) length scales but with different coefficients. At a larger scale, the coefficients such as permeability and porosity are obtained based on finer-scale information.

The second is the stochastic approach, which derives equations governing the statistical moments of the variables of interest from the macroscopic equations. This approach provides not only the prediction but also the associated uncertainty.

In the first section of this report, we describe a stochastic approach and some key results for flow and transport at field scale. Flow and transport at field scale is of practical interest, for example, for problems associated with water resources, groundwater remediation, and oil recovery. The process of upscaling from the macroscopic to the field scale, however, relies heavily on accurate description of flow at the macroscopic scale.

The second section of this article describes our ongoing research project to develop upscaling methods to predict constitutive relationships and other macroscopic coefficients based on some statistical parameters of pore-scale structures.

Although natural porous media are heterogeneous at all length scales, our observations and theoretical treatments are usually limited to a few distinct scales. For example, we commonly associate flow in porous media with three different scales: pore (microscopic), local (lab, macroscopic), and field. Fluid flow may have to be described by different equations at different scales.

At the pore scale, the minute pore structure and detailed occupation of space by different fluids are important; the equations of fluid motion are the Navier-Stokes equations, whereas diffusion and heat conduction are governed by the molecular Fick and Fourier laws. Because of the difficulty in describing the complicated geom-

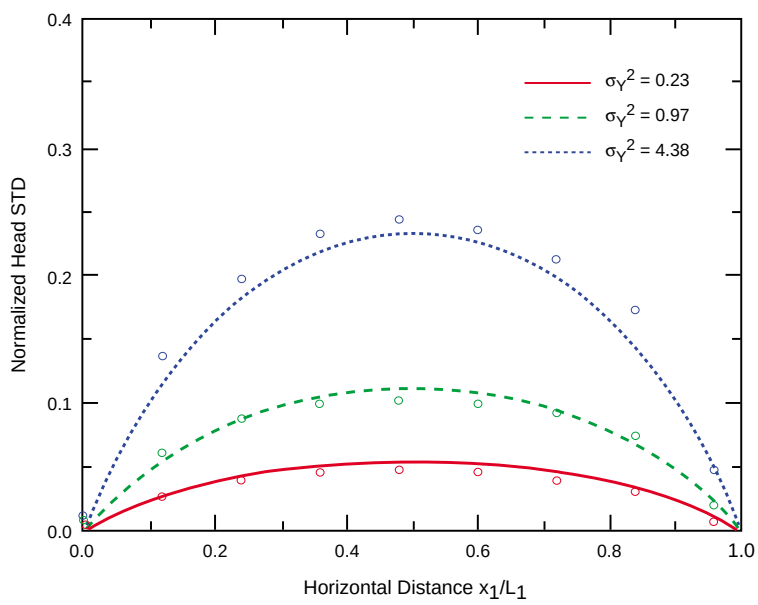

Figure 1. Model Validation.
The graph compares head standard deviations from the moment equation approach (curves) to the published Monte Carlo simulation results (circles).

etry of the individual pores and the fluid interphase boundaries coupled with the complex nature of the physical processes at this scale, the traditional focus has been on the larger lab scale.

At the lab scale, the macroscopic variables are defined by averaging the microscopic variables over a volume containing many pores. Because this volume is large compared to individual pores but extremely small compared to the lab scale, the macroscopic variables become point values, and the pore-scale details may be ignored. In turn, at this intermediate scale, the fluid motion satisfies macroscopic equations (for example, Darcy's law). The coefficients in the macroscopic equations are somehow related to the microscopic structures, and the fluid interphase boundaries may be determined through laboratory experiments. The lab scale is on the order of 10^{-1} to 10^{0} m, whereas the scale of interest can be as large as 10^{4} to 10^{5} m in hydrology and petroleum engineering; we usually refer to the large scale as "field scale."

Uncertainty Analyses of Flow at Field Scale

Despite the fact that geologic media exhibit a high degree of spatial variability, medium properties, including fundamental parameters such as permeability and porosity, are usually observed only at a few locations because of the high cost associated with subsurface measurements. This combination of significant spatial heterogeneity with a relatively small number of observations leads to uncertainty about the values of medium properties and, thus, to uncertainty in predicting flow and solute transport in such media.

The theory of stochastic processes provides a natural method for evaluating the prediction uncertainty. In stochastic formalism, uncertainty is represented by probability or by related quantities like statistical moments. Medium properties, boundary conditions, and initial conditions are treated as random fields whose values are determined by probability distributions. In turn, dependent variables such as pressure and flux are random fields, and the equations governing porous flow become stochastic differential equations whose solutions are probability distributions of pressure and flux. In general, we cannot solve a stochastic differential equation exactly but can only estimate the first few moments of the corresponding probability distribution, especially its mean, variance, and covariances. However, these moments usually suffice to approximate confidence intervals for the flow quantities.

We have developed moment equations for steady-state and transient single-phase flow in bounded domains of nonstationary media. The results from these models are the first two moments of flow quantities. The first moment (mean) can be used to estimate the field of the flow quantity of interest, and the second moment (standard deviation) measures the associated uncertainty (error). These two moments can be used to construct confidence intervals for the flow quantities. These models have been partially validated with Monte Carlo simulations (Figure 1). These flow models may be applied to both groundwater and gas reservoirs.

We have also developed and solved the moment equations for steady-state and transient unsaturated flow and solute transport in the vadose zone. In unsaturated media, water and air coexist in the pore systems. Unsaturated flow is treated as a special case of two-phase flow. We found that the boundary

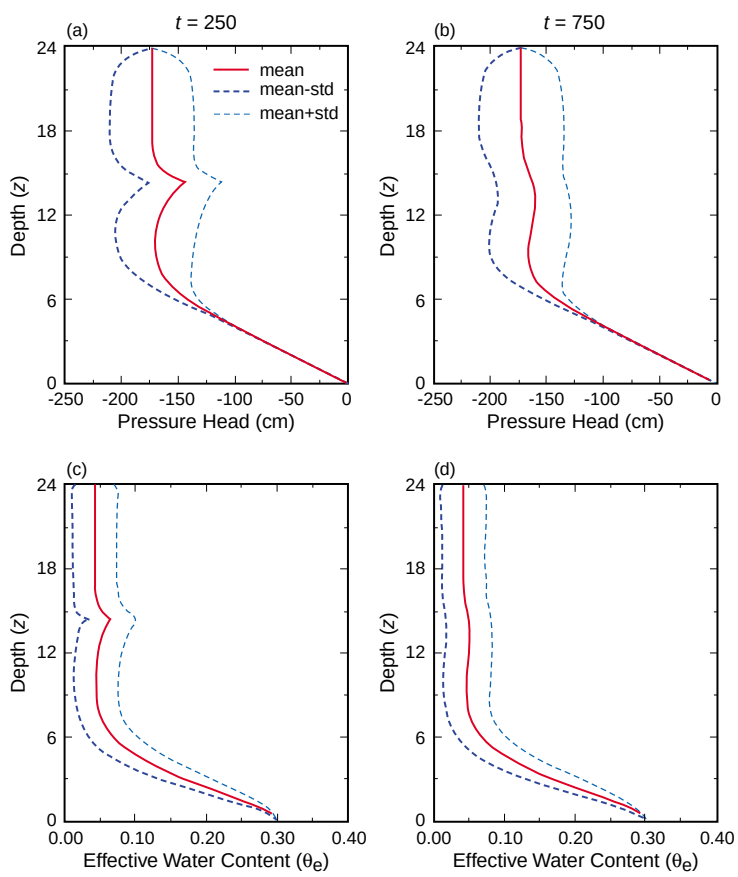

Figure 2. Unsaturated Flow.
The expected values and confidence intervals for pressure head and effective water content at two different times in the presence of an internal source for unsaturated flow in random porous media. The water table is at $z = 0$.

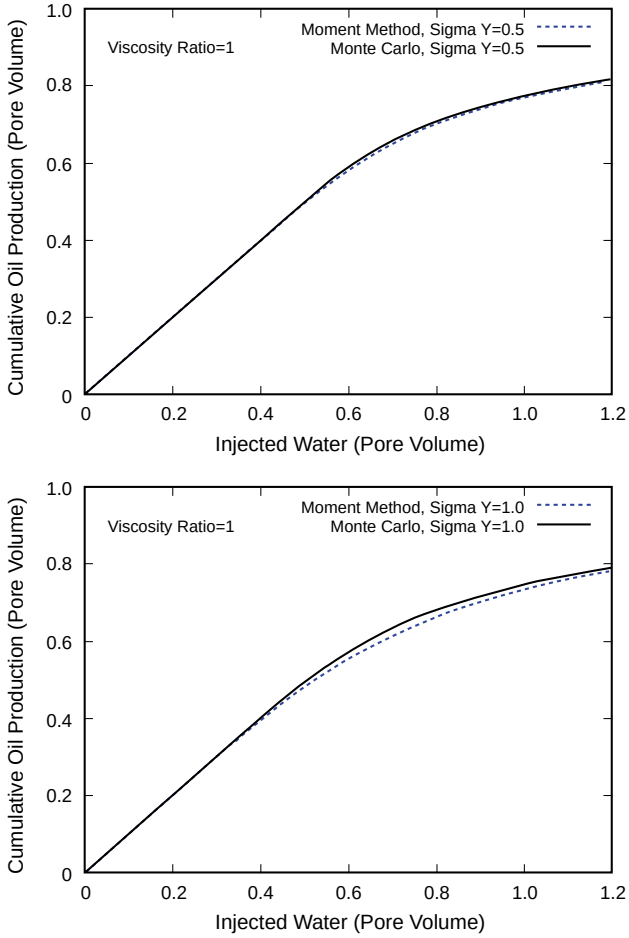

Figure 3. Two-Phase Flow.
The graphs show the cumulative oil production obtained from the moment equation approach and from Monte Carlo simulations for the two-phase case of water displacing oil.

conditions, especially the water table boundary, have a significant impact on the stochastic behaviors of unsaturated flow in random porous media (Figure 2).

For a true two-phase case of water displacing oil, we developed moment equations under both simplified and more realistic boundary conditions. We have compared the stochastic model of two-phase flow with Monte Carlo simulations and have found a very good agreement (Figure 3).

Upscaling from Pore to Macroscopic Scale

The objective of this project is to investigate fundamental issues of multiphase flow systematically at the microscopic and macroscopic scales and to develop upscaling methods for predicting macroscopic quantities and characteristic relationships based on some statistical parameters of microscopic quantities. We do so by applying recently developed computational tools and theoretical frameworks and by comparing these with experimental results. A successful upscaling approach would lead to a greatly increased efficiency and accuracy in simulating multiphase flows in porous media at the lab and field scales.

This past year we used an enhanced lattice Boltzman permeameter to study single-phase flow through pore-scale geometries obtained through high-resolution computed microtomography of rock cores. The permeameter allowed us to investigate some fundamental issues, such as the existence of representative elementary volume (REV), the scale dependence of porosity, specific surface area and permeability, and the relationship of these quantities. We found that although REV may not be well defined in a deterministic sense, it does exist statistically (Figure 4). The figure shows that at each scale, each quantity is computed by averaging over a window of this scale centered at a certain location. These values, obtained at different locations within the domain, are then analyzed to obtain the statistics. The expected values become constant, and the standard deviations approach zero with scale. The behaviors of these quantities indicate the existence of statistical REV. A similar observation is found for a computed microtomography of a sample of Berea sandstone.

The concept of statistical REV is weaker than the deterministic REV but is more useful in applications. We also found that the size of REV may be different for different quantities.

Conclusion

Based on our computational results, we found that rock permeability may not be predicted accurately with existing relationships such as the Kozeny-Carman relation, which is based only on porosity and specific surface area, the lower moments of rock geometry. A more accurate upscaling method would have to involve higher moments of pore geometry, and we will focus the remainder of the project on those. ■

Further Reading

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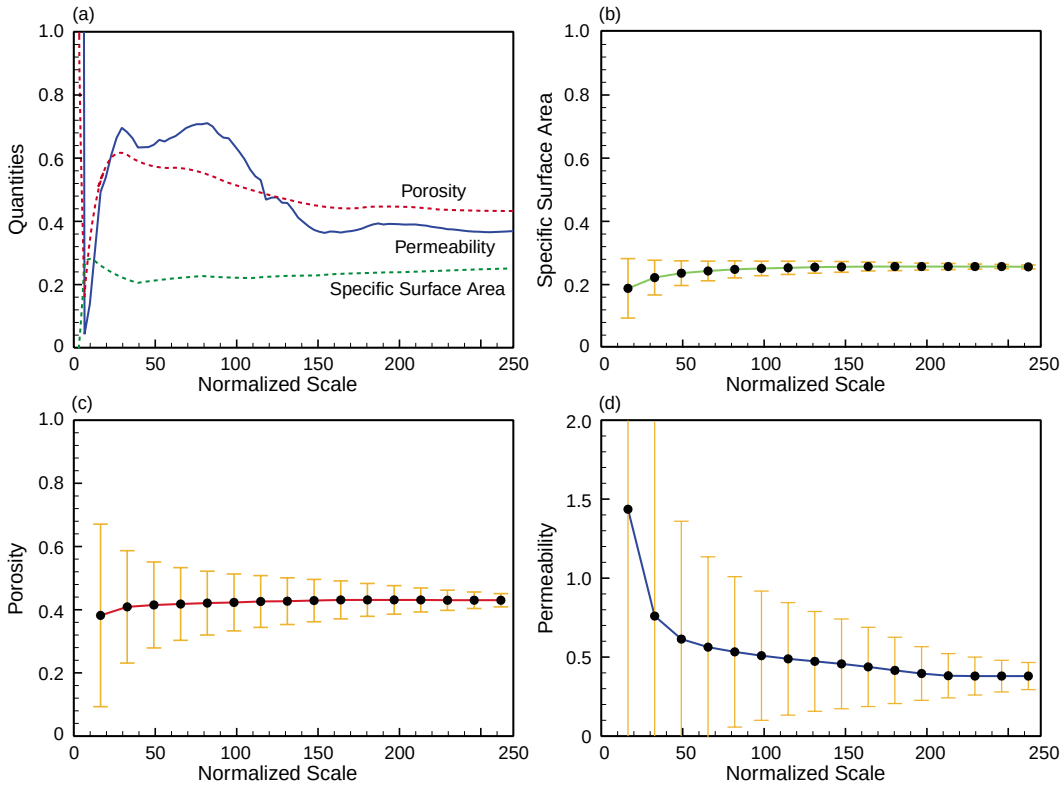

Figure 4. Study of Representative Elementary Volume.
Specific surface area, porosity, and permeability are shown in (a) for the point at the domain center, and their expected values as a function of lattice scale are given in (b), (c), and (d). The expected values are obtained with simulations performed on a computed-microtomography geometry of crushed glass beads divided into a 180 x 256 x 256 lattice structure with a resolution of 17.5 µm. The confidence intervals in these plots are plus or minus one standard deviation.

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