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MATHEMATICAL CHALLENGES IN GROUNDWATER CONTAMINANT MODELING

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The use of computer models to simulate groundwater flow and contaminant transport has burgeoned in the past few years. There are good reasons for this phenomenon: Natural aquifers tend to have complicated geometries and highly variable rock properties, and there is a pressing societal need for quantitative predictions of contaminant movements in these complex geologic settings. Computer models offer the only realistic hope for meeting this need.

Despite the apparent power of computer models, many technical problems conspire to reduce their accuracy in field studies. Obvious to most water resources professionals are difficulties associated with aquifer characterization and the "garbage in, garbage out" syndrome. More subtle, however, are several mathematical issues that require adequate resolution before we can expect realistic aquifer simulations. This abstract is a brief summary of our research into these issues.

Three concepts are common to all numerical models of underground flows. First, one must make some assumptions about the physics and chemistry of the flows. These assumptions give rise to complicated and often nonlinear sets of partial differential equations that govern fluid velocities, movements and fates of contaminant plumes, and other variables of interest. Second, to solve the governing equations, one must approximate them, usually by converting the differential equations to discrete algebraic analogs. Among the most common "discretization" methods are finite-difference and finite-element techniques. These methods partition the aquifer into grid cells or nodes, associating with each cell or node algebraic equations analogous to the mass or momentum balance for that zone. The results are systems of algebraic equations, characterized by matrices that can have tens of thousands or even millions of entries. Third, given such large matrix analogs of the original flow and transport equations, one must devise efficient ways to solve them on digital computers.

Some of our work focuses on the first phase of the modeling enterprise, the derivation of governing equations. Although the physics of flows in porous media are well established at small scales, they are poorly understood at scales where the natural heterogeneities of the rock matrix are prominent. Such heterogeneities arise from variations in depositional environment, diagenetic changes in the pore geometry of the rock, and structural events that cause fracturing and faulting. To the modeler, these heterogeneities pose a severe challenge: How can we scale our knowledge, gained from measurements on cores, well tests, and wireline data, to the scale of typical grid cells?

As an example of the utility of numerical models in answering scaling problems, consider the small-scale fingering and channeling of water-soluble contaminants through an aquifer that has high-conductivity streaks distributed irregularly in space. Capturing the precise geometry of such plumes in a model is typically infeasible: It simply requires too much fine-scale knowledge of an aquifer's properties, and this knowledge is expensive even in bench-scale studies. However, one can use numerical models to investigate connections between well understood, small-scale physics and the large-scale movement of plumes in the presence of heterogeneities. We have explored techniques for modeling the average behavior of such plumes by incorporating "effective hydrodynamic dispersivities" in the governing equations. To incorporate geologic and petrologic information into the calculation of the new effective dispersivity parameters, though, we need help from engineers and hydrogeologists, who have detailed knowledge of the types of measurements that are feasible and a sense of the statistical structure of the conductivity fields that occur in particular formations.

We have also devoted considerable effort to the development of finite-difference and finite-element approximations to the equations governing groundwater flow and contaminant transport. For example, we have explored the calculation of accurate fluid velocities from the groundwater flow equations, the resolution of steep concentration gradients in moving contaminant pluses, and the efficient discretization of multiphase flows, such as those that occur beneath leaking gasoline tanks, TCE spills, and other nonaqueous liquid sources.

Among the most promising methods for approximating the groundwater flow equation are *mixed finite-element methods*. These methods solve the coupled system comprising the mass balance for water and Darcy's law. By choosing appropriate shape functions, one can generate approximate solutions for the water velocity having the same order of accuracy as the approximate hydraulic head. In contrast, standard finite-element and finite-difference methods, which differentiate numerical heads to compute Darcy velocities, yield approximate velocities that are less accurate than the heads and therefore less useful in modeling contaminant transport.

In the realm of transport equations, we have focused much of our attention on cases where advective transport dominates the effects of hydrodynamic dispersion — a case of prime interest in many sandstone and unconsolidated aquifers. Plumes in this regime tend to have persistent, steep concentration gradients that are difficult to resolve numerically with coarse-celled grids. One strategy that we have used to overcome this difficulty is the use of *adaptive local grid refinement*. The idea is to assign smaller grid cells to regions of the plume needing greater numerical resolution. However, the fact that the plume is moving makes implementation of the idea on the computer a delicate task. Among the algorithmic difficulties that we have tried to address are the disruption of efficient matrix structures associated with regular, coarse grids and the poor numerical conditioning that results from the use of cells

having widely disparate sizes.

We have employed a variety of other techniques in this arena. For example, it is possible to adopt a "hybrid" coordinate system in discretizing the contaminant transport equation, measuring temporal rates of concentration change along the paths of fluid particles, not at fixed spatial points. This *modified method of characteristics* allows more accurate timestepping than the usual formulation. Also, we have investigated the use of *finite-element collocation*, a high-accuracy discretization technique, to reduce the numerical smearing associated with many low-order finite-element and finite-difference methods.

In modeling multiphase flows, we have developed a variety of improvements to the standard discretizations. Among these are mass-conserving formulations of the time derivatives in vadose-zone flows, splittings of the nonlinear fractional flow in saturation equations to facilitate the use of the modified method of characteristics, and the analysis of finite-element methods in the mathematically difficult case when capillary pressure gradients are negligible or degenerate. By no means has our work settled all of the important issues in this class of flows. Nonaqueous-phase contaminant flow promises to remain a significant challenge for modelers and engineers for years to come.

Finally, our research has led to the development of several new approaches for solving the large matrix equations associated with discretizations of the governing equations. For example, we have examined iterative schemes for solving the mixed finite-element equations that use conjugate-gradient and multigrid techniques to overcome the slow convergence associated with highly heterogeneous conductivity fields. We have also explored alternating-direction methods for decomposing multidimensional problems to one-dimensional structures that can be solved efficiently on parallel-processing computers. We have also developed efficient ways to decompose locally refined grids into coupled coarse-grid problems and fine-grid problems, thereby overcoming the disruption of regular coarse-grid structures and the conditioning problems associated with local grid refinement.

Mathematicians often unwittingly give the impression that numerical problems associated with groundwater modeling are under control and that the remaining difficulties are attributable to poor input data. However, poor data constitute only part of the problem. Many of the standard numerical techniques are blunt instruments in the presence of the mathematically difficult features of groundwater flow and transport. We aim to sharpen these instruments.

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