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Myron B. Allen Richard E. Ewing

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Myron B. Allen and Richard E. Ewing
Department of Mathematics
University of Wyoming
Laramie, Wyoming

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1. INTRODUCTION.

One can argue that the nature of heterogeneities in an underground formation is the most influential factor limiting the success of mathematical models of flow or transport in the aquifer. Lack of adequate knowledge of aquifer heterogeneity and the attendant difficulty in assessing the realism of a model's predictions make the modeler's job a frustrating one.

The importance of heterogeneity elicits discomfort among many of us whose research concerns new numerical techniques for groundwater modeling. Part of the uneasiness over heterogeneity arises from a widely shared view of its importance. The valid premise of this view is that difficulties in accurately quantifying underground heterogeneity impose constraints on the accuracy of mathematical models, owing to limitations in the quality of the input data. The argument then proceeds as follows: Since poorly quantified heterogeneity is the dominant source of prediction error in most groundwater models, there is little point in focusing research on improved numerical techniques. After all, even if we use more accurate numerics, the deleterious effects of inadequate input data will still be present, swamping any improvements to be gained through mathematical refinements. The natural conclusion is that research into methods for detecting and characterizing underground heterogeneity have much more potential for improving mathematical models than does research into the numerical techniques themselves.

We offer a different perspective. No one would deny that improved methods for quantifying heterogeneity are crucial to advances in the realism and utility of groundwater models, in accordance with the popular maxim, "garbage in, garbage out." However, we contend that the most commonly used mathematical methods are inadequate to model heterogeneous aquifers. As we review in Section 3, even in the ideal case when the heterogeneities are "perfectly" known, standard methods can perform poorly, suggesting a new adage: "heterogeneity in, garbage out."

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* Department of Mathematics, University of Wyoming, Laramie, WY 82071.

** Departments of Mathematics, Petroleum Engineering, and Chemical Engineering, University of Wyoming, Laramie, WY 82071.

In a more realistic scenario, where one relies on detailed statistical characterizations of heterogeneous aquifers, existing mathematical techniques are largely inadequate at answering the hydrologist's questions. Here, quantifiable control over the uncertainties in aquifer parameters can fail to yield reasonable control over the reliability of the numerical solution. We illustrate this problem in Section 4. This observation suggests the even more distressing adage: "statistics in, garbage out."

In what follows, we examine these notions and briefly indicate promising avenues for overcoming the difficulties. We hope to affirm the importance of continued research into mathematical techniques used in numerical models of groundwater flow and transport, thereby rebutting the conclusions of the conventional wisdom.

2. GOVERNING EQUATIONS.

To clarify what we mean by aquifer heterogeneity, it is useful to review the governing equations used in groundwater models. We begin with the equations describing groundwater flow. Groundwater obeys a mass balance,

$$S_s \frac{\partial H}{\partial t} + \nabla \cdot \mathbf{v} = Q, \tag{1}$$

where S_s is the specific storage, H is the hydraulic head, $\mathbf{v}$ denotes the superficial velocity, and Q accounts for sources and sinks (Huyakorn and Pinder, 1983, Section 4.2). According to Darcy's law, $\mathbf{v}$ is related to the hydraulic head by the equation

$$\mathbf{v} = -\frac{\rho g k}{\mu} \nabla H = -K \nabla H. \tag{2}$$

Here, ρ is the density of water; g is the gravitational acceleration; k is the permeability of the rock matrix, and μ is the water's dynamic viscosity. Hydrologists typically use the lumped parameter K, called the hydraulic conductivity. In many contexts, Equation (2) is too restrictive, and k (and hence K) must be a tensor to accommodate anisotropies in the aquifer's flow characteristics. This consideration can have practical importance, but it imposes complications that are not essential to our thesis.

Heterogeneity, in this context, refers to spatial variations in the aquifer parameters $S_s(x, y, z)$ and $K(x, y, z)$. For simplicity, we focus on variations in K. A wide array of phenomena associated with the rock's deposition and diagenesis contribute to these variations, which may occur smoothly or

discontinuously. One point that is all too easy to neglect in this connection is that Darcy's law describes the *macroscopic* velocity of fluids, which in some sense represents an average of the velocity in the tortuous, microscopic interstices of the rock that are essentially inaccessible to observation. Thus spatial variations in K reflect what we might call *macroscopic heterogeneity*, as opposed to the microscopic variability in pore geometry that Equations (1) and (2) cannot explicitly model, even in principle.

In formulating numerical models of groundwater flow, people commonly substitute Equation (2) into Equation (1) to get the groundwater flow equation,

$$S_s \frac{\partial H}{\partial t} - \nabla \cdot (K \nabla H) = Q. \tag{3}$$

As we discuss in Section 3, discretizing Equations (1) and (2) separately can yield significant advantages over the usual approaches to discretizing Equation (3).

When the modeler is interested in how a dissolved contaminant moves in a flowing aquifer, it is necessary to solve a transport equation. In the absence of chemical reactions and interphase mass transfer, the equation governing the concentration $c(x, y, z, t)$ of solute has the form

$$\frac{\partial(\phi c)}{\partial t} + \nabla \cdot (\mathbf{v}c) - \nabla \cdot (\phi \mathbf{D} \nabla c) = q. \tag{4}$$

Here, ϕ stands for the porosity of the rock matrix, q accounts for sources and sinks of contaminant, and $\mathbf{v}$ is the velocity computed using a flow model. $\mathbf{D}$ denotes the hydrodynamic dispersion tensor, which is a crude attempt to account for a variety of microscopic phenomena that cause the macroscopically observed concentration to diffuse with respect to the advective field $\mathbf{v}$.

We shall not delve into the controversial physics of $\mathbf{D}$ (see Fried, 1975, Chapter 2, for the standard model). We note, though, that techniques for evaluating $\mathbf{D}$ in actual fieldwork are quite poor and are possibly sensitive to what length scales the measurer identifies as microscopic. Notwithstanding, $\mathbf{D}$ can exhibit macroscopic spatial variations attributable, in the standard model, both to variations in the rock matrix and to variations in $\mathbf{v}$. Thus heterogeneity affects the transport equation (4) through the variability in $\mathbf{v}$ inherited from flow models, through spatial variations in porosity ϕ, and through the intrinsic variability in $\mathbf{D}$.

These equations suffice to illustrate our views on heterogeneity; however, more complicated underground flows have attracted considerable recent attention among hydrologists. Noteworthy are flows involving several fluid

phases with interphase mass transfer, as commonly occurs when nonaqueous liquid contaminants percolate through partially saturated soils. Heterogeneity plays no less important a role in these flows. In fact, heterogeneity can exacerbate several types of instability that arise from the nonlinearity of the equations that govern these more complicated flows. The physics here are by no means well understood; we refer to Schwille (1984) for an overview.

3. HETEROGENEITY IN, GARBAGE OUT.

Having established how heterogeneity enters into groundwater models, we now examine how it leads to poor performance in standard numerical models of groundwater flow. For the remainder of this section we assume, for the sake of argument, that the modeler has "perfect" knowledge of an aquifer's heterogeneities. By this, we mean that the modeler knows the values of $K(x,y,z)$ and $S_s(x,y,z)$ at every point (x,y,z) in the aquifer. Notice that such knowledge does not imply any detailed knowledge about the *microscopic* heterogeneities associated with the tortuous interstices of the rock. We consider the case when significant spatial variations in K occur on a scale that is small compared with the size of the domain to be modeled, and for simplicity we neglect spatial variations in S_s.

The small-scale structure of K forces the modeler to use a fine discretization of the spatial domain. For example, if one uses finite differences to approximate the flow equations, then the maximum dimension h of the grid cells must be small enough to resolve the significant fluctuations in hydraulic conductivity. Finite-difference and finite-element schemes for solving the flow equation (3) yield large matrix equations to be solved for nodal values of head H at each time level in the model. Thus, smaller values of the grid mesh h lead to larger numbers of nodal heads and hence to larger and computationally more expensive matrix equations.

What is worse, smaller values of h yield more *poorly conditioned* matrices. For typical discretizations having spatial error $O(h^2)$, for example, the condition number of the matrix at each time level is $O(h^{-2})$ (see Johnson, 1987, Section 7.7). If one uses direct solution techniques such as the Cholesky decomposition, this large condition number can lead to enormous roundoff errors in the matrix solution, yielding unacceptably inaccurate values of head H. Numerically differentiating these heads to compute transport velocities via Equation (2) compounds the inaccuracies, and the result can be a useless velocity field $\mathbf{v}$ computed from a "perfectly" known hydraulic conductivity.

One can ameliorate the accumulation of roundoff by using iterative techniques, such as variants of relaxation schemes or conjugate gradients. Here

again, large condition numbers lead to difficulties, this time in the form of slow iterative convergence. One attractive property of conjugate-gradient techniques is that they are readily amenable to preconditioning, which can reduce this effect. Research into preconditioners that eliminate the slow convergence associated with fine discretizations is an active field of research; see Golub and O'Leary (1989) for a review.

Still, fine grids do not tell the entire story. When K varies spatially, there is a contribution to poor conditioning attributable simply to the discrepancy between the largest and smallest values, say $K_{\max}$ and $K_{\min}$, occurring in the model's domain. In fact, when one uses an iterative scheme to solve the matrix equations, the factor by which each iteration reduces the error in the approximate solution typically has the form $1 - O(K_{\min}/K_{\max})$ (see, for example, Allen et al., in preparation). Thus the convergence rate can be close to 1, and therefore prohibitively slow, when $K_{\min}$ differs from $K_{\max}$ by several orders of magnitude, independent of the grid mesh h.

Research by many investigators indicates that there is hope for this problem. Our own work, for example, suggests that a profitable first step is to isolate the two sources of poor conditioning by solving Equations (1) and (2) as a coupled system, using mixed finite-element methods (see, for example, Allen et al., 1985). The effects of highly variable conductivity K then influence only the discrete analog of Equation (2), which one can attack using any of several preconditioning schemes that effectively adapt to the heterogeneity. One can then address the effects of small grid mesh h by developing appropriate preconditioners for the conjugate-gradient method, as in Ewing et al. (to appear), or by exploiting multigrid techniques, as in Allen et al. (in preparation).

As an illustration of the potential for success in this area, we present iterative convergence rates for two schemes applied to steady-state flows in a set of fictitious aquifers (Allen et al., in preparation). The functional forms used for K in these experiments, listed in Table 1, are clearly contrived, yet in their spatial variability they can be just as troublesome as many occurring in nature. Figure 1 shows plots of iterative convergence rate versus grid mesh for each realization of K, using a scheme whose convergence rate is theoretically independent of h owing to a peculiar splitting of the mixed-method equations. This scheme overcomes sensitivity to small h but remains sensitive to spatial variations in K, as the slow convergence rates for the realization K_V attest. Table 2 displays iterative convergence rates for a modified version of the splitting scheme. Here, we precondition the discrete Darcy equations arising from the mixed method to mitigate sensitivity to

heterogeneity. Theory estimates a convergence rate of 0.5, independent of h and K, an estimate that the computed rates confirm. The methods used to generate these results by no means offer a final solution to the poor conditioning arising from heterogeneity, but they demonstrate that heterogeneity actually heightens the need for advances in numerical analysis.

The proper use of mixed finite-element methods offers the further advantage of avoiding the deterioration in accuracy that occurs when one numerically differentiates heads to compute Darcy velocities. As Ewing and Wheeler (1983) explain, mixed methods can generate approximate heads and velocities that have equal-order accuracy, a property that is especially attractive in the context of contaminant transport modeling.

Still, problems remain. We have not considered the effects of spatial variability in specific storage. Moreover, considerable work remains to be done to make mixed finite-element models truly efficient and flexible. Issues such as adaptive local grid refinement, exploitation of parallel computing architectures, and the treatment of nonlinearities associated with multiphase flows are prime examples of ongoing work along these lines.

4. STATISTICS IN, GARBAGE OUT.

In reality, heterogenities will never be "perfectly" known. The best we are likely to achieve are fairly detailed statistical descriptions of heterogeneities below some scale, which is likely to be large in practice. Thus it may suffice to use models to generate suites of scenarios yielding statistical predictions of aquifer behavior. For this strategy to be successful, ensembles of "statistically equivalent" realizations of a given heterogeneous aquifer must yield predictions that are "statistically similar." In other words, the model's predictions should be "stable," in some sense, against changes in heterogeneous structure that preserve the detailed statistics of the aquifer. Otherwise, a given statistical description of an aquifer might be consistent with a large and wildly varying class of model predictions. The notions of statistical equivalence, statistical similarity, and stability lack rigorous definition at this point, but we contend that there is considerable work to be done to make this strategy practical.

As evidence for our contention, we consider a set of numerical experiments involving coupled underground flow and solute transport. The coupling consists of the usual dependence of the solute transport coefficients on the output of a flow model, together with a dependence of the dynamic viscosity μ on the concentration c predicted by the transport model. This

model has its origin in oilfield applications, where injection of miscible fluids less viscous than oil is a common form of enhanced oil recovery. Nevertheless, there are clear analogies to be drawn with the physics of groundwater contamination and remediation. The experiments suggest that statistically similar heterogeneous porous media can yield flow fields that are qualitatively dissimilar in significant respects.

In the cases modeled, μ is a decreasing function of c, so the injected fluid is more mobile than the displaced fluid. This adverse mobility ratio makes the displacement unstable: Small perturbations in the geometry of the displacement front can lead to large differences in the fraction of the pore space contacted by the injectant. One manifestation of the instability is the occurrence of viscous fingers in the displacement front. It is not clear physically how small the perturbations can be and still trigger these fingers, but it is conceivable that they could arise from heterogeneities at the microscopic scale as well as the macroscopic scale. In this case, no model based on Equations (1) through (4) can possibly resolve all of the instabilities occurring in macroscopic flows. With this caveat in mind, we examine the effects of fine-scale but macroscopically resolvable heterogeneities on miscible displacement.

Figure 2 shows concentration isopleths for simulated displacements in two random porous media, with fluid being injected in the lower left corner and produced at the upper right (Ewing et al., 1989). The two media are independent realizations of the same lognormal spatial permeability distribution, and they have the same correlation length. The predicted displacement patterns show that the flows in the two model media yield qualitatively different concentration fields. In fact, the flows differ significantly even with respect to relatively coarse measures, such as the pore volumes of resident fluid produced after one pore volume of injection. The result for Figure 2a is 0.6921, while that for Figure 2b is 0.4968 – a decrease of over 28 percent. Clearly, these statistically similar media have dissimilar flow characteristics, at least for the physics modeled here.

Overcoming the difficulties associated with statistical characterizations of heterogeneity will require new modeling techniques and perhaps to wholly new ways of using models. Among the promising avenues for the near term are methods for scaling up fine-scale information to produce realistic models using coarse, computationally affordable grid cells. Homogenization theory (Bourgeat, 1984), flux-based averaging (White and Horne, 1987), and effective macroscopic dispersion tensors (Ewing et al., 1989) are three such approaches.

In the long run, the issue of uncertainty arising from aquifer heterogeneity has a direct bearing on the uses of deterministic models, since some uncertainty will doubtless remain as numerical analysis progresses. The inherently statistical nature of the problem reflects, in part, the discrepancy between the scales at which Equations (1) through (4) apply and the scales at which aquifers are accessible to measurement. This discrepancy implies a need for broader research into the relationships between fundamental physics, model formulation, numerical analysis, and parameter identification in groundwater modeling.

5. CONCLUSIONS.

The adages, "heterogeneity in, garbage out," and "statistics in, garbage out," are probably too pessimistic. We really intend the first adage as a caution: Modelers should not assume that all is settled on the numerical front, and that all we need are better measurements to feed into existing models. Numerical methods that are standard engineering practice today will become increasingly inadequate as better measurements of heterogeneous aquifer parameters become available. The second adage is a caution of a different sort. It suggests that the problems associated with uncertainty in heterogeneous aquifers may not be amenable to solution via straighforward discretization of the standard governing equations. Instead, these problems may require new approaches, in which rigorous numerical work contributes to the development of model formulations appropriate to the scales at which the models will actually be run.

6. ACKNOWLEDGMENTS.

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TABLE 1. CONDUCTIVITY FIELDS USED IN NUMERICAL EXPERIMENTS FOR ITERATIVE SOLUTIONS OF MIXED FINITE-ELEMENT MODELS FOR STEADY-STATE GROUNDWATER FLOW.

$$K_{\mathrm{I}}(x,y) = 1;$$

$$K_{\mathrm{II}}(x,y) = e^{-x-y};$$

$$K_{\mathrm{III}}(x,y) = \begin{cases} 1, & \text{if } x < y, \\ 0.1, & \text{if } x \geq y; \end{cases}$$

$$K_{\mathrm{IV}}(x,y) = K_{\mathrm{II}}(x,y) \cdot K_{\mathrm{III}}(x,y);$$

$$K_{\mathrm{V}}(x,y) = \begin{cases} 1, & \text{if } x < y, \\ 0.01, & \text{if } x \geq y. \end{cases}$$

TABLE 2. CONVERGENCE RATES FOR A UNIFORMLY CONDITIONED ITERATIVE SCHEME APPLIED TO PROBLEMS IDENTIFIED IN TABLE 1.

	GRID MESH h				
COEFFICIENT	2^{-4}	2^{-5}	2^{-6}	2^{-7}	2^{-8}
K_{I}	0.4933	0.4988	0.4993	0.4995	0.4999
K_{II}	0.4966	0.4995	0.4988	0.4997	0.4999
K_{III}	0.4948	0.4982	0.4991	0.4998	0.4999
K_{IV}	0.4947	0.4980	0.4992	0.4998	0.4999
K_{V}	0.4939	0.4978	0.4989	0.4999	0.5000

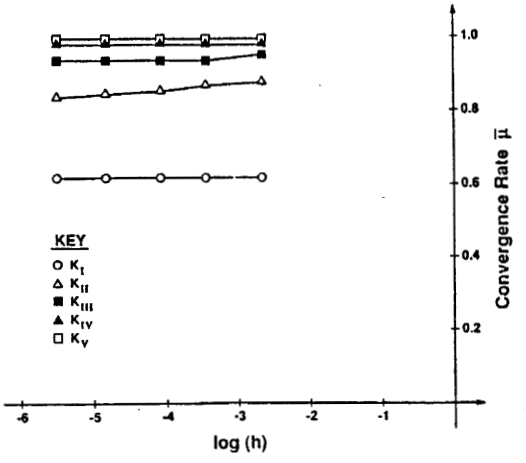

Figure 1. Convergence rates for an h-independent iterative scheme applied to problems identified in Table 1.

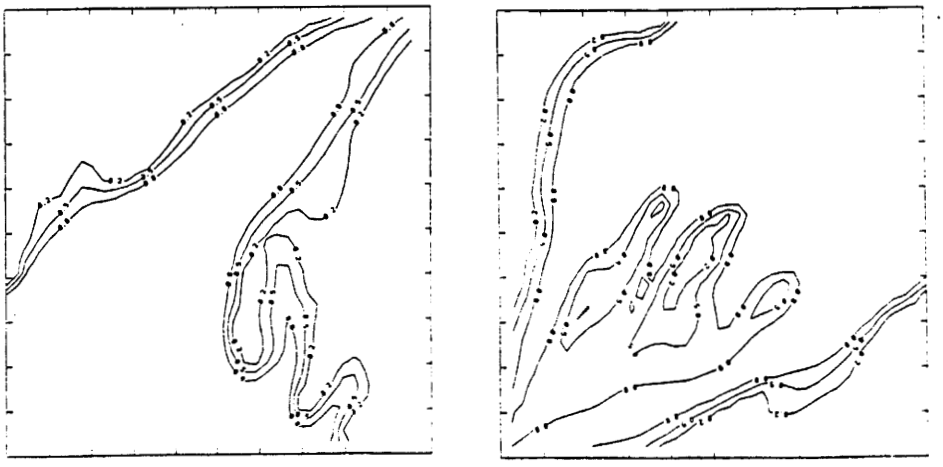

Figure 2. Concentration isopleths after injection of one pore volume for model miscible displacements in two random media having similar statistics.