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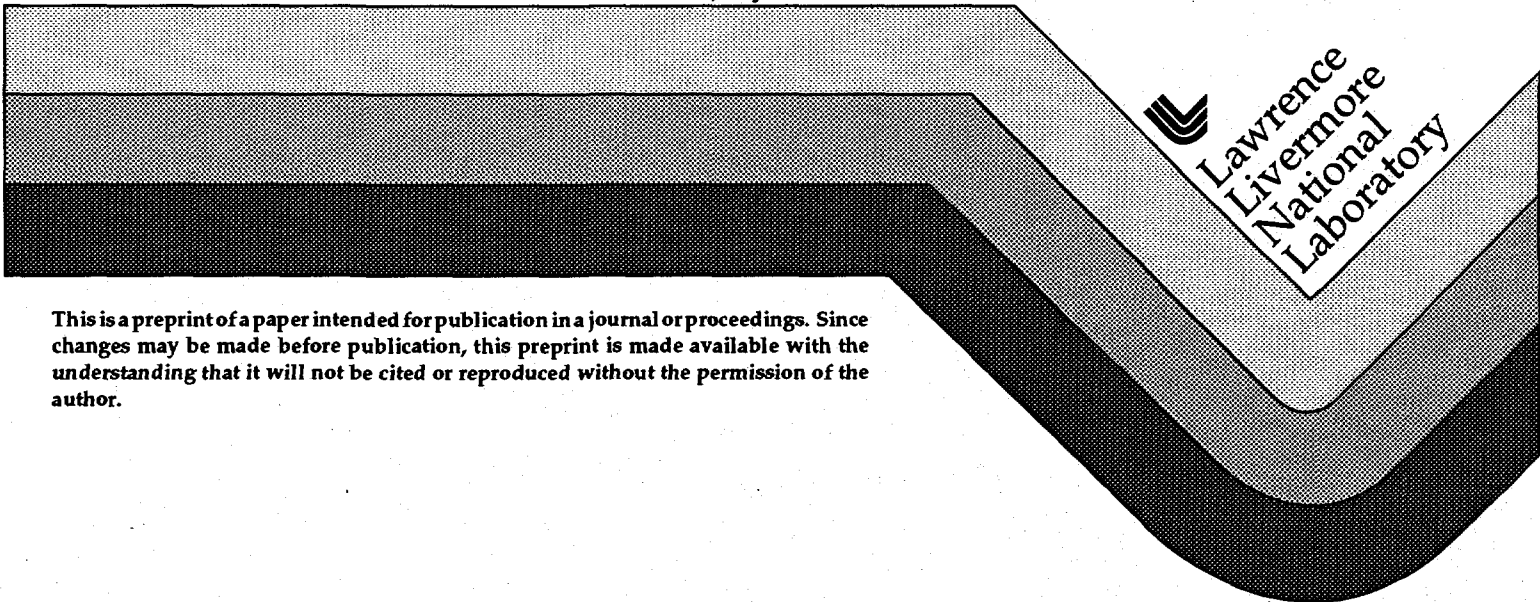
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A New Breed of Innovative Ground Water Modeling

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Sparse data is a critical obstacle in every ground water remediation project. Lack of data necessitates non-unique interpolations that can distort modeled distributions of contaminants and essential physical properties (e.g., permeability, porosity). These properties largely determine the rates and paths that contaminants may take in migrating from sources to receptor locations. We apply both forward and inverse model estimates to resolve this problem because coupled modeling provides the only way to obtain constitutive property distributions that simultaneously simulate the flow and transport behavior observed in borehole measurements. Innovations in multi-dimensional modeling are a key to achieving more effective subsurface characterizations, remedial designs, risk assessments, and compliance monitoring in efforts to accelerate cleanup and reduce costs in national environmental remediations. Fundamentally new modeling concepts and novel software have emerged recently from two decades of research on self-adaptive solvers of partial differential equations (PDEs). We have tested a revolutionary software product, *PDEase*, applying it to coupled forward and inverse flow problems. In the Superfund cleanup effort at Lawrence Livermore National Laboratory's (LLNL) Livermore Site, the new modeling paradigm of *PDEase* enables ground water professionals to simply provide the flow equations, site geometry, sources, sinks, constitutive parameters, and boundary conditions. Its symbolic processors then construct the actual numerical solution code and solve it automatically. Powerful grid refinements that conform adaptively to evolving flow features are executed dynamically with iterative finite-element solutions that minimize numerical errors to user-specified limits. Numerical solution accuracy can be tested easily with the diagnostic information and interactive graphical displays that appear as the solutions are generated. We have verified and validated the code for LLNL ground water flows and have compared the results with the standard industry codes, MODFLOW/MODINV, for coupled forward and inverse problems.

Introduction

A key problem in all ground water remediations is that contaminants may migrate to high-risk receptors with uncertain rates, paths, and concentrations. The migration is uncertain because data are always sparse when characterizing subsurface properties. At most cleanup sites, practical cost

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considerations preclude high sampling densities to acquire all desired statistics on contaminant concentrations as well as data on ground water, sediment, flow, transport, and geology. Therefore, it is extremely important to extract the maximum amount of information that is contained in all available data at every stage of remediation.

Inverse modeling methods are used in many scientific disciplines to help resolve the ever-present problems of undersampling. For example, computerized tomography (CT) scans and magnetic resonance imaging (MRI) use the patterns of electromagnetic rays transmitted through the human body to back-calculate high-resolution images of the body's internal structure. These procedures do so using inverse solution methods that are mathematically ill-posed (i.e., more than one admissible solution exists). Similarly, ground water flow and contaminants, as well as seismic signals, transmitted through the earth's subsurface can be back-calculated with various inverse solution methods to gain a better picture of critical properties that govern contaminant migration before, during, and after active remediation operations. Inverse solution methods for ground water aquifer properties, also known as parameter estimation and history-matching techniques, have been investigated and reported in the scientific literature for at least 25 years (Gelhar, 1993); they have also been used effectively for many years in the oil/gas industry. However, such methods are not yet practical when applied to remediation of ground water contaminants. One of the principal obstacles is the fixed-grid numerical solution methods commonly used in the remediation industry to solve the forward flow equation (an elliptic partial differential equation [PDE]). These methods do not suffice to solve the inverse problem; the flow equation becomes a much more difficult hyperbolic PDE to solve when subsurface hydraulic conductivity distributions are sought from given head distributions. In mathematical research, however, adaptive numerical grid methods developed over the past 25 years provide an alternative to solve both forward and inverse flow problems. Until recently, mathematical specialists were required to apply the codes successfully. Breakthroughs in innovative adaptive-grid PDE software for general users have recently been incorporated in commercially available software, such as *PDEase*, leading the way to a new breed of innovative ground water modeling.

We have surveyed, tested, and purchased numerous PDE software packages developed by both the research and commercial industries in the government and private sectors. To date, *PDEase* is the easiest, fastest, and most efficient product for our applications. We continue to seek new, innovative products, and welcome their introduction from any and all arenas.

Background

The LLNL Livermore Site is a designated Superfund site that has been under active remediation since 1988. As required by the Superfund process, estimates of time-to-cleanup, as well as the Baseline Public Health Assessment, were produced by using computational physics models to estimate the flow and transport of contaminants through subsurface porous media. The conceptual models and ground water physics codes were initially simplistic and made broad generalizations for setting parameters and characterizing the Site's subsurface. Subsequent restoration activities, such as defining optimal well placement, required more detailed subsurface characterizations and

modeling with improved spatial resolution. For this reason, a time-dependent, two-dimensional (2-D) version of the CFEST code was employed (Tompson et al., 1991).

As shown in Figure 1, the domain of the region to be modeled was extended far beyond the boundaries of the Livermore Site to minimize the effects of inaccurate estimates of boundary conditions (Tompson et al., 1995). Initial estimated values for hydraulic conductivity

($K_0 = K_0[x,y]$) were chosen to reflect both the measured values from well tests and knowledge of the subsurface gleaned from geophysical data and core analyses. Those values were then subjected to an iterative process that produced, by trial and error, a reasonable fit between measured and CFEST-calculated ground water levels (hydraulic head), which still maintained physically plausible values of K . In this process, the forward CFEST model calculated hydraulic head values ($h = h(x,y)$) using the previously estimated distribution of hydraulic conductivity. If the newly calculated head values did not agree sufficiently with measured values, the K values were adjusted, which is an inverse problem cycle. The process was repeated until the last-calculated CFEST values for hydraulic head agreed suitably with measured values. This time-honored practice of estimating subsurface flow properties is extremely tedious. In addition, there is no assurance that good forward and inverse solutions for h and K , respectively, can be found, much less satisfy the flow equation in both the forward and inverse solutions for both h and K . Serviceable values of K were ultimately found for 2-D flow modeling of the Livermore Site so that, after flow velocities were calculated throughout the domain, contaminant transport was reasonably calculated. The calculations, of course, were subject to the many known caveats of 2-D conceptual and numerical models using estimates of sorption (retardation), porosity, possible abiotic and biotic degradation, and transverse and longitudinal dispersion. These K values were constrained only by flow data; they could possibly be improved by implementing additional constraints from measured contaminant concentrations. However, the input files for executing this process with CFEST were measured in thousands of coding lines, and the preparation of each new problem grid with different property distributions, boundary conditions, etc., was extremely labor-intensive. These factors clearly discouraged extensive sensitivity analyses, as well as frequent updating and improvement of earlier conceptual and numerical models that were needed through the post-Record of Decision to the current compliance monitoring stages of the regulatory process.

PDEase Software

PDEase is a commercially available software product, which is described in the textbook by Backstrom (1994). Developed by SPDE, Inc., of Fremont, California, *PDEase* is a new type of PDE software with flexible code generation features and efficient adaptive grid methods for solving sets of one or more partial differential equations, given initial and boundary conditions. It presently runs on PCs and Sun workstations. It is a language-based system using standard mathematical notation for input and providing numeric and graphic solutions to large classes of steady-state and time-dependent, linear and non-linear systems. *PDEase* solves initial/boundary value problems in up to two spatial dimensions and one time dimension. Extensions to solve transient 3-D applications are planned for future versions.

In short, this new generation of software puts powerful adaptive numeric tools in the hands of everyday scientists and engineers. It enables them to solve problems that in the past would take continuing efforts by teams of scientists, engineers, and computer programmers. *PDEase* is designed to serve scientists and engineers in much the same fashion that spreadsheets and word processors presently serve financial analysts and writers.

For solving both forward and inverse flow models, our testing of *PDEase* showed that it enables ground water professionals, who need not be code specialists, to provide to the software the flow equations, site geometry, sources, sinks, constitutive parameters, and boundary conditions. Its symbolic processors successfully construct the actual numeric solution code and solve it automatically. Grid refinements that conform topologically to evolving flow features are executed dynamically with iterative, finite element solution methods that minimize numerical errors to user-specified limits. Convergence of the numeric solutions can be tested easily with the diagnostic information and interactive graphical displays that appear as the solutions are generated. Internal details of mesh generation, adaptive grid refinement, linear system solution, nonlinear solution techniques, and error estimation are all provided automatically by the software package. Flexible graphical output is also provided and, in most cases, a full model can be specified in a single page of input. When needed for special-purpose applications, additions to the core software package have been made by SPDE, Inc., much as word processing software maintenance and upgrades are provided by their manufacturers.

Results

As shown in Figure 2, the fundamental deterministic flow equation can be solved both as a forward problem for h from given K distributions and as a direct inverse problem for K from given h distributions. (We have not discussed stochastic inverse problems although they have been reviewed briefly by Gelhar [1993].) Indirect inverse solutions of K from uncertain h data are a second type of inverse method, which is usually formulated as a least-squares problem that minimizes differences between calculated and measured head values using methods found in control theory. We present here results of solving: (1) a forward flow problem for baseline conditions in the Livermore basin with both *PDEase* and CFEST, and (2) a direct inverse problem with a known solution. To solve indirect inverse solutions of the flow equation in the least squares sense, extensions of *PDEase* are also quite promising and will be presented in a future article that is now in preparation.

Forward modeling of ground water flow.

Extensive comparisons have been made between *PDEase* and the 2-D CFEST code for ground water flows in the hydrogeologic study area that includes contaminated ground water beneath the Livermore Site. In Figure 1, the conceptual model is depicted on the numerical grid used in the CFEST runs. Municipal water supply wells are located near downtown Livermore. Regions of low hydraulic conductivity (0.1 ft/day) are shown in green or shades of gray in our figures; three higher values of constant conductivity (5.3, 8.0, and 10.0 ft/day) were distributed in the watershed

to calibrate the CFEST flow model with well data under ambient (base line) aquifer conditions at times prior to remediation activities at LLNL. The thickness of the unconfined aquifer is a function of head in the 2-D conceptual model, making the flow system non-linear in h .

Forward solutions of the flow equation by CFEST and *PDEase* are shown in Figure 3. The results agree reasonably well. Both codes are finite element codes; however, the CFEST grid coordinates are fixed whereas the *PDEase* grid is adaptive to minimize PDE solution errors with greater computational efficiency. The CFEST calculation of head isocontours in the ambient state of the aquifer are shown in the right side of Figure 3. In contrast, the *PDEase* solution is presented on the left side of Figure 3, where the hydraulic head is plotted as a 3-D graphic instead of contours, though *PDEase* may do either or both. It is possible that the fixed polygonal grid of CFEST (Figure 1) may require greater resolution to define the boundaries of changes in hydraulic properties, without introducing artifacts in the model results. Similarly, the selected CFEST grid may not fully resolve cones of depression of individual, possibly interfering, wells as is accomplished by the dynamic grid evolution in the *PDEase* solution shown in Figure 4. *PDEase* boundaries can be specified as both arc and line segments. Furthermore, it is very easy to set up or modify the *PDEase* domain descriptions and constitutive parameters so that more analyses can be accomplished rapidly. This process allows the analyst more time to develop better model fits and sensitivity analyses. Most important is the fact that *PDEase* can serve as a verification standard and indicate where additional resolution is needed in fixed grid codes because *PDEase* users can simply request smaller and smaller permissible errors and let the software refine its grid progressively until the requested accuracy is attained. In the author's opinion, compared to CFEST and similar ground water codes, *PDEase* was faster, easier to use and run, and more accurate in this baseline modeling exercise.

Direct Inverse Modeling of Ground Water Aquifer Properties.

If hydraulic head distributions and a small set of K values are available, the flow equation can be solved directly for the entire K distribution. However, hydraulic head distributions can never be known precisely, because they are obtained by interpolating scattered data with experimental error. Nevertheless, the capacity to directly solve the hyperbolic flow equation for K is a major milestone that enables unprecedented solutions of general inverse flow problems by both direct and indirect methods. Figure 4 presents *PDEase* solutions that demonstrate its capacity to directly solve the inverse flow equation with high accuracy relative to existing technology in the MODFLOW/MODINV code currently used in the remediation industry.

For code verification purposes we posed an inverse flow problem with a known solution for K , as shown in Figure 4. The *PDEase* solution for K was nearly exact. It was obtained in approximately 10 minutes on a Sun Sparc 10 work station, and is largely insensitive to initial estimates of K_0 for the hydraulic conductivity. This insensitivity to K_0 is an essential requirement because physical values of K may vary by eight orders of magnitude in heterogeneous subsurfaces like the LLNL Livermore Site. We also posed this problem to the MODINV code (Doherty, 1990), which is perhaps the most successful inverse solution code used in the environmental industry today. Although MODINV is an indirect solution code, it should yield reasonable

solutions of K when run appropriately for well-posed problems with known answers. Our results indicate that MODINV is sensitive to both fixed grid resolution and initial estimates of K_0 . Even when given auspicious initial estimates of K and relatively high grid resolution, MODINV may be 100 times less efficient than the adaptive grid solutions in *PDEase*. The MODINV solutions may also become unstable and fail to converge (Figure 4) when inauspicious estimates of K_0 are used. These difficulties are overcome in a new approach (described in a future article) that solves the inverse least-squares problem by a non-linear solution method that supercedes the Newton-Raphson approach used in many conventional inverse solution codes.

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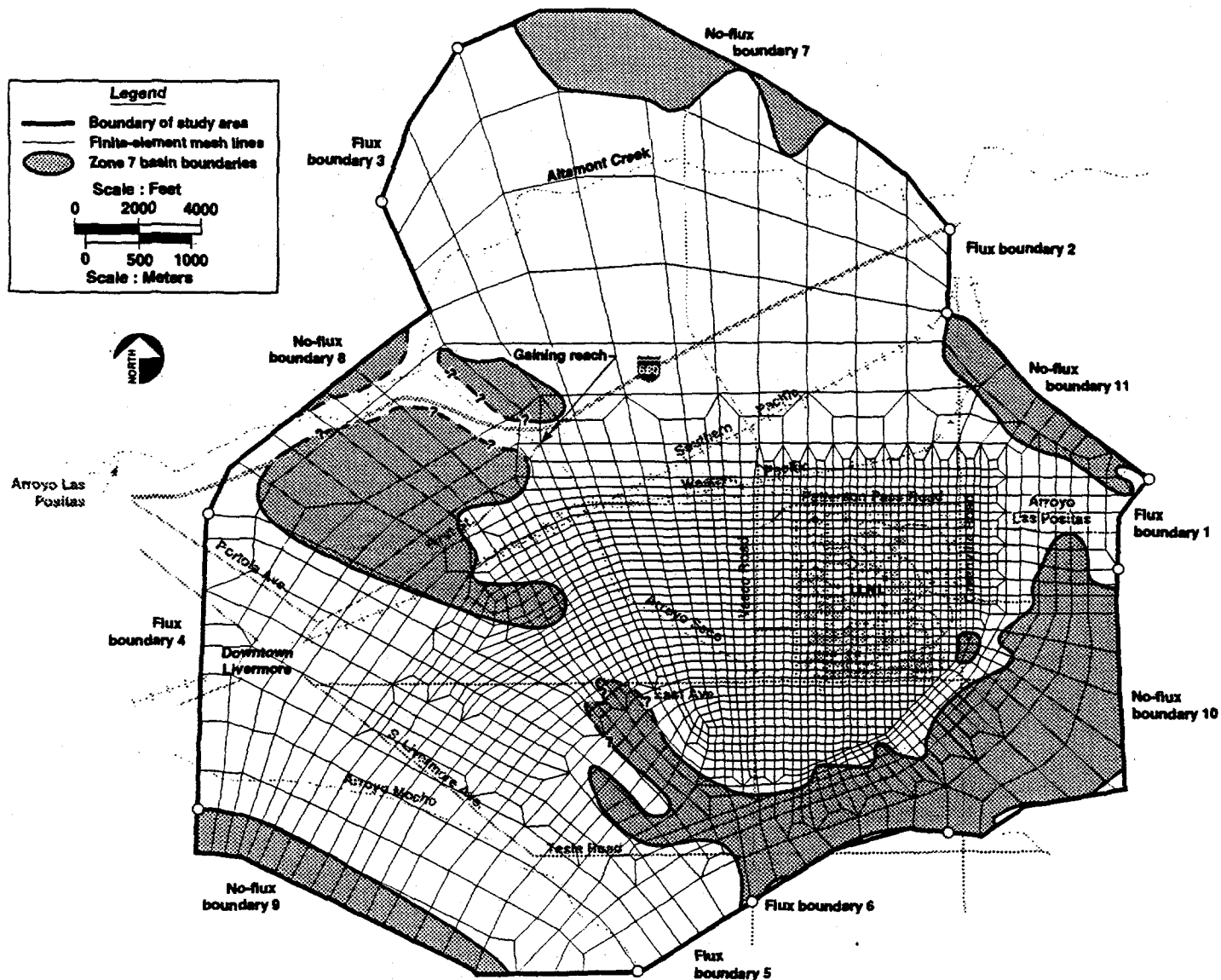


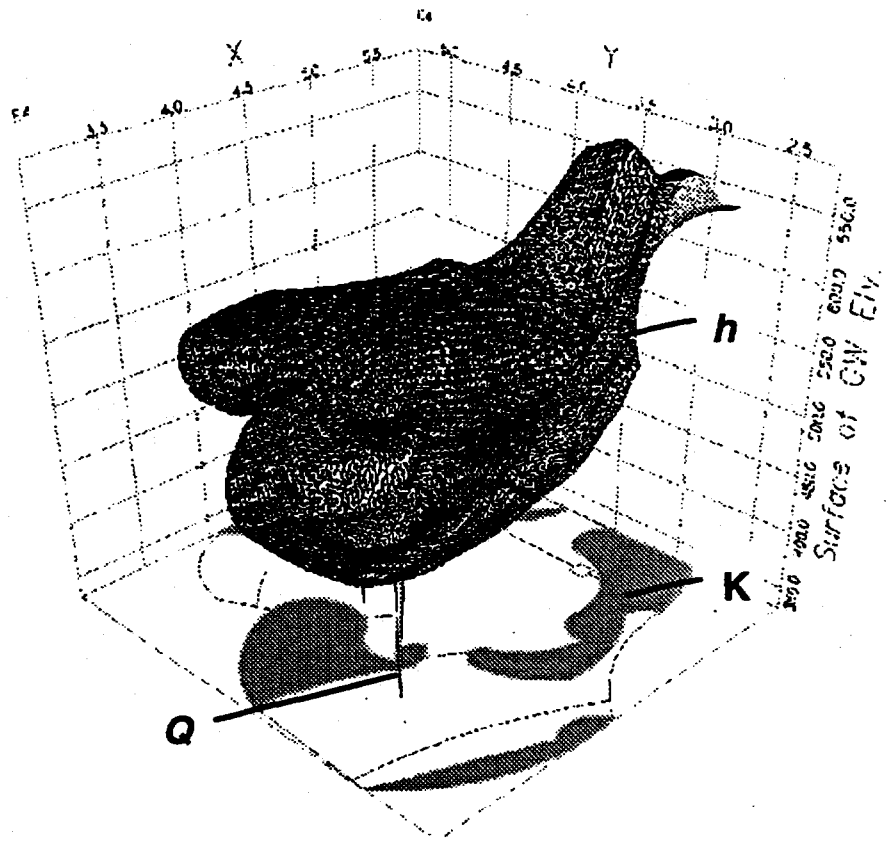
Figure 1. Schematic view of conceptual model for the Livermore regional study with improved computational mesh for CFEST flow and transport simulations.

<u>Forward:</u>	Given: K	$\begin{array}{c} \rightarrow \\ \uparrow \\ \downarrow \\ \leftarrow \end{array}$	Solve: h	(1)
$\nabla \cdot [K(x) \cdot \nabla h(x)] = Q(x)$				
<u>Inverse:</u>	Solve: K	$\begin{array}{c} \leftarrow \\ \uparrow \\ \downarrow \\ \rightarrow \end{array}$	Given: h	

$h \equiv$ hydraulic head
 $K \equiv$ hydraulic conductivity
 $Q \equiv$ sources and sinks (known or postulated)

Figure 2. The fundamental flow equation (1) yields both forward and inverse solutions for deterministic models.

PDEase forward solution for h



CFEST forward solution for h

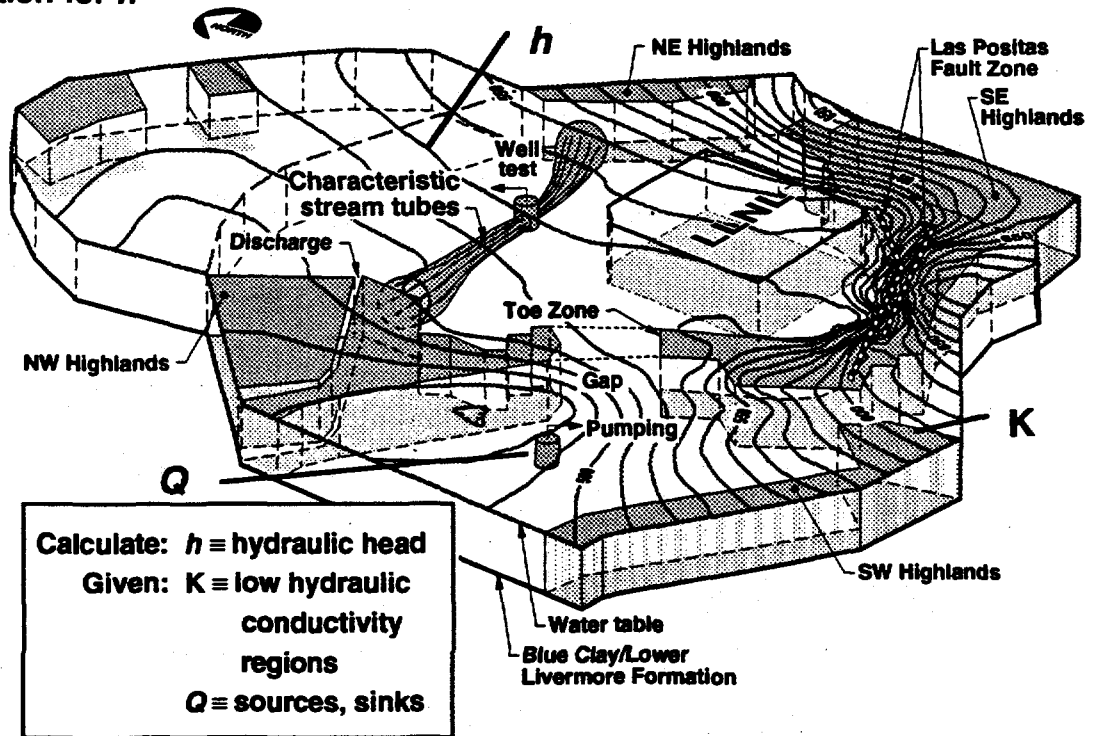


Figure 3. Results of PDEase and CFEST forward modeling of the Livermore region baseline case. Also shown are the PDEase method-of-characteristics solution of ordinary differential equations (ODEs) for stream tubes in a flow net associated with a typical well test in the domain (See Gelhar, Chpt. 6.4).

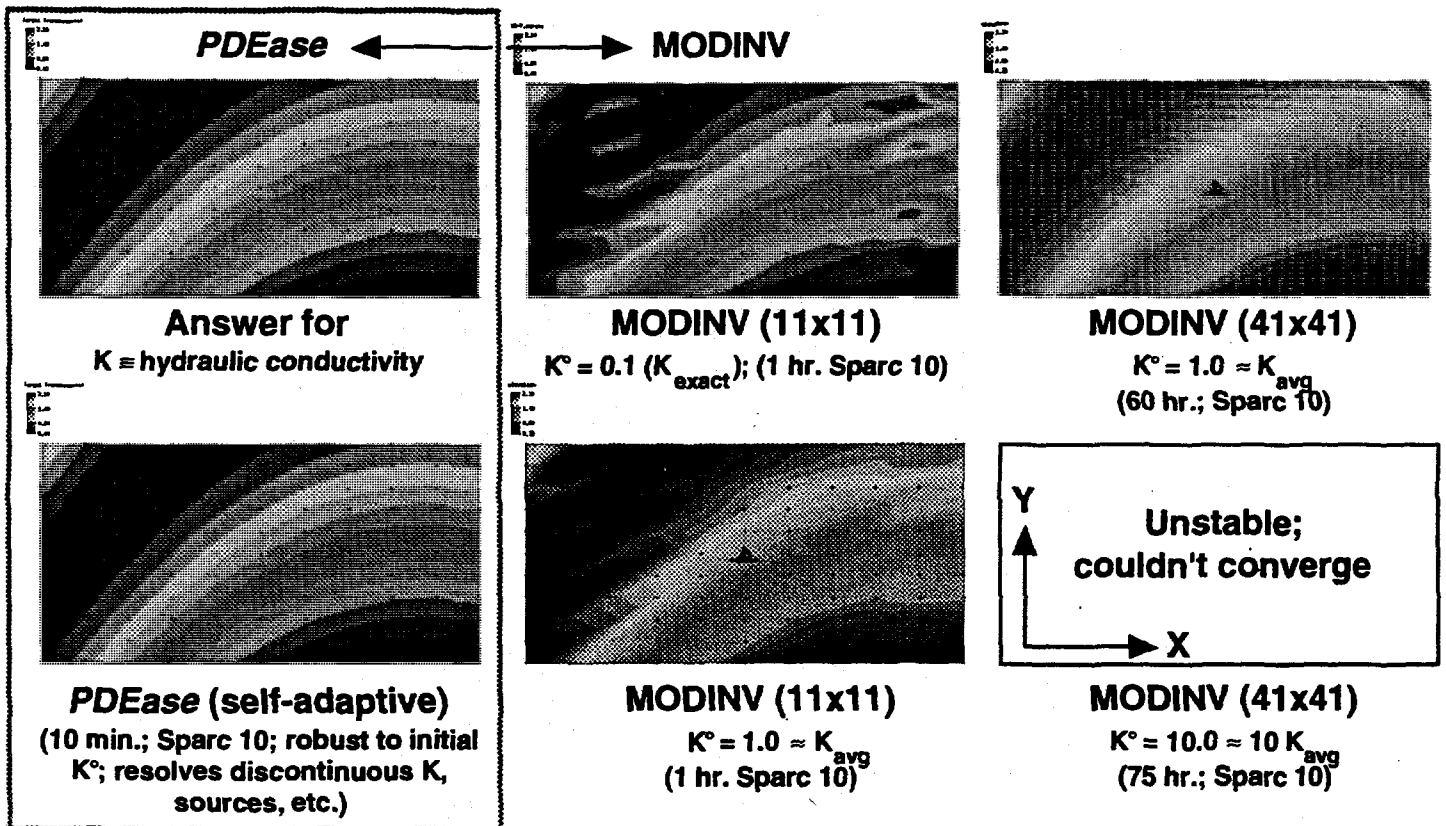


Figure 4. Comparative PDEase and MODFLOW/MODINV results for an inverse flow problem with a known exact solution.