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TOUGH Simulations of Updegraff's Set of Fluid and Heat Flow Problems

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Under the sponsorship of the U.S. Nuclear Regulatory Commission, Sandia National Laboratories (SNL) is developing a performance assessment methodology for the analysis of long-term disposal of High-level Radioactive Waste (HRW) in unsaturated welded tuff (the only potential host rock presently under consideration by the U.S. Department of Energy). As part of this effort, a comparison study of three simulation codes modeling strongly coupled mass and heat flow in unsaturated porous media was conducted (Updegraff, 1989).

The three codes evaluated were (1) TOUGH, developed by Pruess (1987) at Lawrence Berkeley Laboratory (LBL); (2) NORIA, developed by Bixler (1985) at SNL; and (3) PETROS, developed by Hadley (1985) at SNL. The capabilities of these codes were tested using 1-D and 2-D problems selected to represent a wide variety of flow systems of different levels of complexity and numerical difficulty, ranging from simple, uncoupled processes (such as 1-D infiltration) to strongly coupled processes (such as 2-D heat-driven flow and vaporization).

The SNL report (Updegraff, 1989) stated that all three codes had serious weaknesses and recommended that a new code be developed. The performance review of TOUGH ranked it as the best of the three codes and concluded that it was capable of solving most of the problems. However, Updegraff (1989) concluded that TOUGH exhibited significant limitations, the most severe of which were difficulty or inability to converge in certain problems, significant numerical dispersion in heat transport problems, and large core storage and execution time requirements.

The purpose of this study was to address the issues raised by Updegraff (1989) in the SNL Report. All the test problems examined in the SNL study were reinvestigated. These included five verification problems (for which either analytical or numerical solutions exist) and three validation problems (for which experimental results are available). In our approach, we first attempted to reproduce Updegraff's (1989) results using the original input data for the eight problems. We then corrected and modified the input data and run TOUGH using the modified inputs. Finally, the new simulation results were discussed.

We demonstrated that (1) the difficulties encountered by Updegraff (1989) can be overcome by careful consideration of the physical processes modeled, (2) TOUGH is capable of handling all the test problems and obtaining correct answers by suitable preparation of input data, without any code modification, and (3) in all test problems TOUGH produces very efficient runs that cover the entire desired simulation periods. A detailed presentation of this study can be found in Moridis and Pruess (1992). In this summary, we discuss two of the test problems: a validation problem of radial heat transport, and a verification problem of a heat convection cell. By analyzing the difficulties encountered by Updegraff (1989), we hope to demonstrate a set of sound simulation principles and practices to be used in the application of TOUGH.

RADIAL HEAT TRANSPORT

The verification test problem of radial heat transport was originally solved analytically by Avdonin (1964), and was later described by Ross et al. (1982). Cold water is injected into a semi-infinite, high-temperature aquifer. The overburden and underburden are impermeable to mass and heat flow, acting as no-flow and adiabatic boundaries. The TOUGH predictions of the temperature distribution were sought after $t = t_{max} = 10^9$ sec (i.e., 32 years) of cold water injection.

Updegraff's Approach and Results

Updegraff (1989) discretized the space domain in 252 unequally sized gridblocks, which included two boundary gridblocks. A very large volume was assigned to the boundary gridblocks, thus ensuring constant boundary pressures and temperatures throughout the simulation. The boundary gridblocks were assigned constant pressures and temperatures. The initial pressure distribution was determined using a logarithmic pressure function (Updegraff, 1989). Instead of a direct injection, the prescribed pressure differential on the boundaries created an influx that resulted in an equivalent system.

Constraining the computation to $\leq$ 3000 time steps, Updegraff (1989) could only simulate the first 1.5×10^6 sec of this problem. He concluded from this that TOUGH was unlikely to simulate the required period of $t_{max} = 10^9$ sec within a reasonable time, and compared the numerical and the analytical solutions at $t = 10^6$ sec. His comparison indicated that the TOUGH solution showed limited numerical dispersion and lagged behind the analytical solution, a discrepancy he assigned to the temperature dependence of the water viscosity and density in TOUGH (unaccounted for in the analytical solution).

Examination of the report and input file revealed the following problems: (1) The correct analytical solution at $t = 10^6$ sec bore no resemblance to the analytical solution shown by Updegraff (1989); (2) incorrect water properties had been used for the computation of the analytical solution, thus producing an incorrect analytical solution and causing conflict with the correct water property data "hardwired" in TOUGH; and (3) an excessively fine discretization had been used immediately next to the well bore. Such a fine discretization can produce severe loss of accuracy when calculating interblock flows from small differences in the pressure of adjacent gridblocks, and it increases the size of the system of linear equations to be solved without resolving additional physics. The inability to reach the desired observation time of $t_{max} = 10^9$ sec was traced to the exceedingly fine space discretization.

Modification and Results

We reduced the number of gridblocks from 252 to 127, which considerably decreased the execution time. In our data set, cold water was injected at the prescribed rate directly into the gridblock next to the wellbore. This approach was more physically correct and significantly reduced the size of the input file. We evaluated the ability of TOUGH to yield an accurate solution at $t = 10^6$ sec (used for comparisons by Updegraff) and $t = t_{max} = 10^9$ sec (specified by the problem). Both upstream and midpoint weighting schemes were considered, for a total of four input files. These produced very efficient runs, which did not suffer from any of the shortcomings reported by Updegraff (1989).

This problem has a "similarity solution" in terms of the variable r^2/t (Doughty and Pruess, 1990; 1992). In Figure 1 we plot the analytical solution, the two TOUGH solutions at $t = 10^6$ sec (with the fine time discretization), and the two TOUGH solutions at $t = 10^9$ sec versus the similarity variable r^2/t. An examination of the results reveals that

1. TOUGH efficiently simulated the radial heat transport problem. The number of time steps to reach 10^6 and 10^9 sec was 27 and 1031.
2. The TOUGH results are consistent with the r^2/t invariance that is known to exist in this problem. At $t_{max} = 10^9$ sec, the two TOUGH solutions virtually coincide with the analytical solution. The midpoint-weighted solution is slightly more accurate, but the difference from the upstream-weighted solution is imperceptible. Similar observations are made for the solutions at $t = 10^6$ sec.

THE CONVECTION CELL EXPERIMENT

The second validation problem is a laboratory convection cell Reda (1984). A porous medium consisting of glass beads with an average diameter of d =0.65 mm fills the annular region between the two vertical concentric cylinders. Application of heat generates a thermal buoyancy force, giving rise to the development of convection cells.

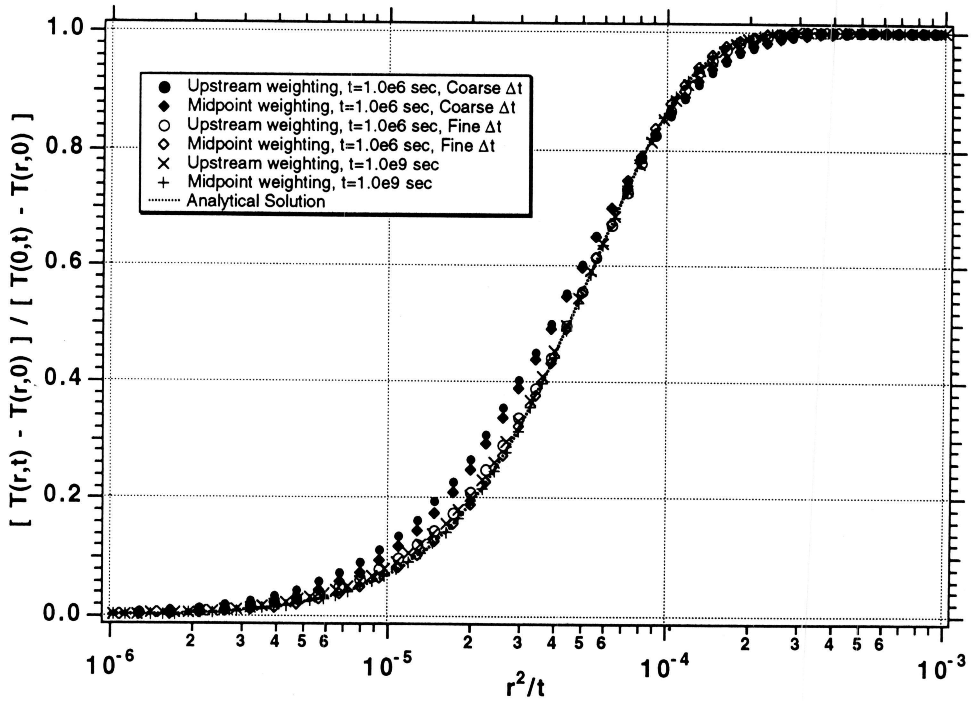

Figure 1. The analytical and numerical similarity solutions to the radial heat flow problem. [XBL 935-784]

Numerical predictions are compared with temperature measurements at the bottom and top of the heating element at a time $t = 10^5$ sec.

Updegraff's Approach and Results

Updegraff's (1989) simulation assigned a very large volume to the gridblocks at the top boundary to maintain a constant temperature and pressure. The outer cylinder boundary gridblocks were assigned a very small volume and a very large specific heat in order to model zero mass flux and constant temperature boundary conditions. Zero mass and heat flux boundaries were assigned along the bottom and the left side of the grid.

Updegraff was unable to simulate this experiment, obtaining results that significantly overpredicted temperatures (by 15 to 30°C) while not exhibiting sufficient temperature differentials between the top and the bottom of the heating elements (less than 10°C, when the observed difference was 30°C). The reasons for Updegraff's failure to successfully simulate this experiment were traced to inadequate and/or inappropriate data inputs. More specifically:

1. The discretization in the radial direction was excessively coarse. Because of cylindrical geometry, large temperature gradients are expected near the heater, and convective effects would be concentrated within a short distance from the heater. The original report on the experiment (Reda, 1984) supported this expectation. Moreover, Reda (1984) stated that the packing of the spherical particles against the heater surface led to important flow channeling effects due to porosity and permeability enhancement. These channeling effects were localized within $5d$ = 3.25 mm. The radial increment Δr used by Updegraff in this region was 20.96 mm; i.e., 6.45 times larger, completely overwhelming its effects, introducing very large discretization errors, and causing the large discrepancies between Updegraff's TOUGH predictions and the experimental data.

2. The assignment of small volumes to the outer boundary gridblocks to approximate the "no-mass-flow" conditions resulted in a boundary with permeable connections to the flow domain, which may have a noticeable impact on predicted convection behavior.

3. Permeability enhancement in the immediate vicinity of the heater was not accounted for

4. The heater domain in Updegraff's simulation was assigned porous medium properties, with nonzero porosity, zero permeability in the r and z directions, and zero medium compressibility. This resulted in enormous pressures because, with the constraint of zero permeability, the gridblocks had no outlet and no compressibility other than that of water. This problem was further exacerbated by the poor selection of the location of the grid points at which the comparisons were made.

Modification and Results

For our simulation, we used a grid with a sufficiently fine discretization in the all-important region near the heater and created two new data sets: the first accounted for permeability-enhancement effects; the second neglected them. A very large volume and specific heat were assigned to the top permeable boundary of the model to maintain constant pressure and temperature. The gridblocks at the outer radial boundary had a very low porosity, zero permeability, and a very high specific heat to force strict "no mass-flow" boundaries while maintaining a constant temperature. The gridblocks assigned to the heater had a very low porosity, a large compressibility, zero permeability to impose a "no-mass-flow" boundary, and the properties of cast iron.

We evaluated the performance of TOUGH by comparing the simulation results (Figure 2) over time to the experimental measurements (Reda, 1984). The maximum simulation time was $t_{max} = 10^5$ sec. The following conclusions were drawn:

1. Both input files produced very efficient runs, covering the simulation period in less than 40 time steps.

2. A very good agreement between experiment and prediction was observed for the period of transient convection, as well as for the steady state. A very strong dependence of temperature on the radial distance was evident.

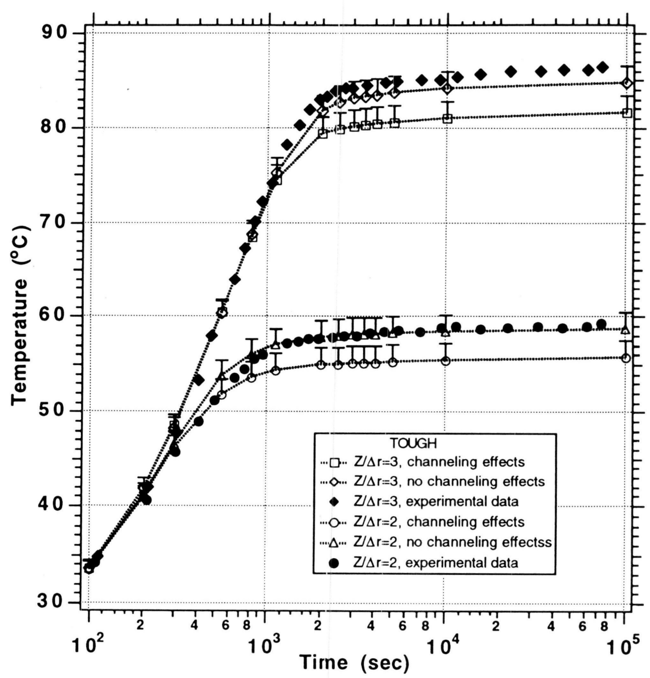

Figure 2. Comparison of TOUGH predictions with experimental data at the heater bottom ($z/\Delta r = 2$) and top ($z/\Delta r = 3$). The bars attached to the TOUGH curves indicate the predicted temperature in the first radial element (i.e., on the surface of the heating element). [XBL 935-785]

3. We found a significant difference between the runs with and without permeability enhancement. Temperatures predicted without permeability enhancement were consistently higher both at the bottom and the top of the heater. Without flow channeling, there was a somewhat slower initiation of convection and a weaker convection process at later times when steady state is approached.

4. Despite its apparent better agreement with measurements (at least near steady state), it is inappropriate to state that neglecting channeling effects produces more accurate results because of the extremely steep temperature gradients in the vicinity of the heater.

5. A significant dependence of temperature on the vertical distance z was noticed (more pronounced near the top than the bottom of the heater), where even minute (i.e., submillimeter) changes in the position of the measuring device can effect sizable temperature differentials. This observation adds further perspective on the comparison between experimental and numerical results.

CONCLUSIONS AND DISCUSSION

TOUGH has performed well on a series of fluid and heat flow problems that involved 1-D and 2-D dimensional flows, with varying degrees of nonlinearity, coupling between fluid and heat flows, and complexity of boundary conditions. These results substantiate the accuracy of the physics model employed in the code and of the mathematical and numerical approaches used. The two-phase two-component fluid and heat flow capability offered by TOUGH, and the flexibility of the space discretization by means of integral finite differences, make possible applications to a great diversity of flow problems on different space and time scales (Pruess, 1990)

Key to successful application of TOUGH is a careful consideration of the physical processes that are involved in a given flow problem. In particular, space discretization, time stepping, and interface weighting procedures need to be carefully selected so that accurate results may be obtained. Application of TOUGH (or, for that matter, of any other two-phase fluid and heat flow code) without due attention to these issues may result in poor (inefficient) performance, inaccurate results, or both. An important aspect of discretization is the interface and time-weighting procedure. TOUGH was designed for robustness and stability in difficult nonlinear problems with phase change and propagating phase fronts. The appropriate weighting procedures for such problems are fully upstream weighting in space and "fully implicit" first-order backward finite differences in time.

Some of the problems and limitations in TOUGH with regard to ease of use and description of physical processes that were noted by Updegraff (1989) were overcome with the recently released successor code, TOUGH2 (Pruess, 1991; ESTSC, 1992). TOUGH2 is upward compatible with TOUGH, with additional capabilities and user-friendly features; these include an internal version control system, more convenient facilities for specifying boundary conditions, and internal mesh processing and generating capabilities (used for mesh generation in Verification Problem 3 and Validation Problems 1 and 2). TOUGH2 offers a multiple interacting continua capability (MINC) for fractured media simulations, a simplified description of Knudsen diffusion by means of a Klinkenberg factor for permeability, and an ability to handle different fluid mixtures.

Further enhancements of process description, such as a capability for multicomponent dispersion and diffusion in multiphase flow, will be included in future releases of TOUGH2. We also expect to release a set of efficient conjugate gradient solvers for use with TOUGH2, which, compared with the presently employed direct solution technique, will drastically shorten execution times for large 3-D problems.

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The Laplace Transform MultiQuadrics (LTMQ) for the Solution of the Groundwater Flow Equation

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MultiQuadrics (MQ) is a true scattered-data grid-free scheme for representing surfaces and bodies in an arbitrary number of dimensions by using approximations given by an expansion in terms of upper hyperboloids. It is continuously differentiable and integrable, and is capable of representing functions with steep gradients with very high accuracy. Hardy (1971) first derived MQ to approximate geographical surfaces and magnetic anomalies, but it was mostly ignored until Franke (1982) showed that MQ outperformed 29 other interpolation methods. Micchelli (1986) and Madych and Nelson (1988) provided the theoretical justification for the performance of MQ.

The extension of MQ to applications in the solution of Partial Differential Equations (PDE) in computational fluid dynamics is credited to Kansa (1990a,b), who employed MQ to solve the advection-diffusion equation, the von Neumann blast wave problem, and Poisson's equation. He showed that MQ (1) yields excellent results with a much coarser distribution of data points, (2) is an excellent estimator of partial derivatives, (3) does not need any special stabilizing treatment for instability and numerical dispersion, (4) is far more efficient and accurate than standard Finite Difference (FD) schemes, and (5) is considerably more flexible and robust than FD in the solution of the traditionally troublesome problem of steep moving fronts.

Laplace transforms are a powerful tool in the solution of PDEs, but their application was limited to simple one-dimensional problems with homogeneous properties. By combining traditional space discretization schemes with Laplace transforms, Moridis and Reddell (1990,1991a,b,c) developed a family of new numerical methods for the solution of parabolic and hyperbolic PDE's. These methods eliminate the need for time discretization of traditional numerical methods while maintaining their flexibility in the simulation of heterogeneous systems with irregular boundaries. The method of Laplace Transform MultiQuadrics (LTMQ) is based on the same concepts but uses MQ as the space approximation scheme.

THE LTMQ METHOD

The governing PDE of transient groundwater flow is

$$\nabla \cdot (K \nabla H) = S_0 \frac{\partial H}{\partial t} + Q \, , \tag{1}$$

where K is the hydraulic conductivity, H is the piezometric head, S_0 is the specific aquifer storativity, $Q = q\, \delta_c(x)\, \delta_c(y)\, \delta_c(z)$, q is the volumetric flow rate of a source or sink per unit volume, and δ_c is the Kronecker delta. The solution of Eq. (1) with the LTMQ method is accomplished in the four steps described in the following sections.

Step 1: The Laplace Transform of the PDE

For a homogeneous and anisotropic 2-D porous medium, the Laplace transform of Eq. (1) expanded in Cartesian coordinates yields

$$K_x \frac{\partial^2 \Psi}{\partial x^2} + K_y \frac{\partial^2 \Psi}{\partial y^2} = S_0 \lambda \Psi - S_0 H(0) + \frac{Q}{\lambda} \, , \tag{2}$$

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