PROCEEDINGS, TOUGH Symposium 2006
Lawrence Berkeley National Laboratory, Berkeley, California, May 15–17, 2006

EFFICIENT SCHEMES FOR REDUCING NUMERICAL DISPERSION IN MODELING MULTIPHASE TRANSPORT THROUGH POROUS AND FRACTURED MEDIA

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ABSTRACT

Numerical issues with modeling transport of chemicals or solute in realistic large-scale subsurface systems have been a serious concern, even with the continual progress made in both simulation algorithms and computer hardware in the past few decades. The problem remains and becomes even more difficult when dealing with chemical transport in a multiphase flow system using coarse, multidimensional regular or irregular grids, because of the known effects of numerical dispersion associated with moving plume fronts. We have investigated several total-variation-diminishing (TVD) or flux-limiter schemes by implementing and testing them in the T2R3D code, one of the TOUGH2 family of codes. The objectives of this paper are (1) to investigate the possibility of applying these TVD schemes using multi-dimensional irregular unstructured grids, and (2) to help select more accurate spatial averaging methods for simulating chemical transport given a numerical grid or spatial discretization. We present an application example to show that such TVD schemes are able to effectively reduce numerical dispersion.

INTRODUCTION

Numerical approaches for modeling multiphase flow and tracer or chemical transport in porous media are generally based on methodologies developed for reservoir simulation and groundwater modeling. They involve solving coupled mass-conservation equations that govern the transport processes of all chemical components using finite-difference or finite-element schemes. Since the 1960s, in parallel with rapid advances in multiphase flow simulation and groundwater modeling, significant progress has been made in understanding and modeling solute transport through porous and fractured media (e.g., Scheidegger, 1961; Bear, 1972; Huyakorn et al. 1983; Istok, 1989; Falta et al., 1992; Unger et al. 1996; Forsyth et al. 1998; Wu and Pruess, 2000).

Since the 1970s, transport problems involving solute and contaminant migration in porous and fractured formations have received increasing attention in the groundwater and soil-science literature. As demanded by site characterization, remediation, and other environmental concerns, many quantitative modeling approaches have been developed and applied (e.g., Abriola and Pinder, 1985; Corapcioglu and Baehr, 1987; Forsyth, 1994). More recently, suitability evaluation of underground geological storage of high-level radioactive wastes in unsaturated fractured rocks has generated renewed interest in the investigation of tracer or radionuclide transport in a nonisothermal, multiphase fractured geological system (e.g., Viswanathan et al. 1998; Moridis et al. 2003). In addition, application of tracer tests, including environmental and man-made tracers, has become an important technique in characterizing subsurface porous-medium systems.

Even with the continual progress made in both computational algorithms and computer hardware in the past few decades, modeling coupled processes of multiphase fluid flow and chemical migration in porous and fractured media remains a mathematical challenge. There still exist many unresolved issues and limitations with current numerical approaches. One of the main concerns is that severe numerical dispersion often occurs when using a multidimensional control-volume-type numerical grid in field-scale modeling studies. It becomes even more problematic when dealing with tracer transport when a general 3-D, coarse, irregular grid is used to solve advection-dispersion-type governing equations for handling tracer transport. To overcome these numerical difficulties, scientists have investigated a number of total variation diminishing (TVD) or flux limiter schemes and applied them in transport modeling with varying successes (e.g., Sweby, 1984; Liu et al. 1994; Unger et al. 1996; Forsyth et al. 1998; Oldenburg and Pruess, 1997 and 2000). However, many of these investigations were demonstrated using regular grids. This work continues the effort of reducing numerical dispersion in simulating tracer or chemical plumes as they travel spatially through porous or fractured media. The emphasis in this study is to examine the effectiveness of these TVD schemes in two- or three-dimensional, irregular, and unstructured grids.

The objectives of this paper are (1) to develop a general scheme for implementing different TVD schemes into multidimensional irregular unstructured grids of porous or fractured media, (2) to investigate the applicability of these TVD schemes to such

irregular unstructured grids, and (3) to help select more accurate spatial averaging methods for simulating chemical transport, given a numerical grid or spatial discretization.

In particular, implementation of TVD schemes is carried out using the T2R3D code, one of the TOUGH2 family of codes made up of multidimensional, multiphase, nonisothermal reservoir simulators. In this approach, a subsurface domain is discretized using an unstructured integrated-finite-difference grid, followed by time discretization carried out using a backward, first-order, finite-difference method. The final discrete linear or nonlinear equations are handled fully implicitly, using Newtonian iteration. In addition, the fractured medium is handled using a general multicontinuum modeling approach. Also, we present an application example to demonstrate that TVD schemes are in general able to reduce numerical dispersion effectively.

MODEL FORMULATION

Let us consider a multiphase system consisting of several fluid phases, such as gas, water, and oil (NAPL), with each fluid phase in turn consisting of a number of mass components. To derive a set of generalized governing equations for multiphase fluid flow and multicomponent transport we assume that these processes can be described using a continuum approach within a representative elementary volume in a porous or fractured medium. According to mass conservation principles, a generalized conservation equation of mass components in the porous continuum can be written as follows:

$$\frac{\partial M^k}{\partial t} = G^k + q^k + F^k \qquad (1)$$

where superscript k is the index for the components, k = 1, 2, 3,…, N_c (N_c being the total number of mass components); M is the accumulation term of component k; G^k is the decay or internal generation (reaction) term of mass component k; q^k is an external source/sink term or fracture-matrix exchange term for mass component k and energy; and F^k is the "flow" term of mass movement or net exchange from multiphase flow, or diffusive and dispersive mass transport.

The mass component transport is governed in general by the processes of advection, diffusion, and dispersion. Advective transport of a component or solute is carried by fluid flow, and diffusive and dispersive flux is contributed by molecular diffusion and mechanical dispersion, or hydrodynamic dispersion. These processes are described using a modified Fick's law for the total mass flow term for a component k, by advection and dispersion, written as

$$F^k = -\sum_\beta \nabla \bullet \left(\rho_\beta X_\beta^k \mathbf{v}_\beta\right) + \sum_\beta \nabla \bullet \left(\underline{D}_\beta^k \bullet \nabla\left(\rho_\beta X_\beta^k\right)\right)$$
$$(k = 1, 2, 3,\ldots, N_c) \qquad (2)$$

where ρ_β is the density of phase β; X_β^κ is the mass fraction of component k in fluid β; v_β is a vector of the Darcy's velocity or volumetric flow of fluid phase β; $\underline{D}_\beta^k$ is the hydrodynamic dispersion tensor accounting for both molecular diffusion and mechanical dispersion for component k in phase β, defined by an extended dispersion model (Scheidegger, 1961; Bear, 1972) to include multiphase effects as

$$\underline{D}_\beta^k = \alpha_T^\beta \left|\mathbf{v}_\beta\right| \delta_{ij} + \left(\alpha_L^\beta - \alpha_T^\beta\right) \frac{\mathbf{v}_\beta \mathbf{v}_\beta}{\left|\mathbf{v}_\beta\right|} + \phi S_\beta \tau d_\beta^k \delta_{ij}$$
$$(k = 1, 2, 3,\ldots, N_c) \qquad (3)$$

where α_T^β and α_L^β are transverse and longitudinal dispersivities, respectively, in fluid β of porous media; S_β is the saturation of phase β; τ is tortuosity of the porous medium; d_β^k is the molecular diffusion coefficient of component k within fluid β; and δ_{ij} is the Kronecker delta function ($\delta_{ij} = 1$ for i = j, and $\delta_{ij} = 0$ for $i \neq j$), with i and j being coordinate indices.

NUMERICAL FORMULATION

The methodology for using numerical approaches to simulate multiphase subsurface flow and transport consists in general of the following three steps: (1) spatial discretization of mass conservation Equation (1), (2) time discretization; and (3) iterative approaches to solve the resulting nonlinear, discrete algebraic equations. Among various numerical techniques for simulation studies, a mass-conserving discretization scheme, based on finite volume or integral finite-difference or finite-element methods, is the most commonly used approach, and is discussed here.

Discrete Equations

The component mass-balance Equations (1) are discretized in space using a control-volume, integrated finite difference concept (Narasimhan and Witherspoon, 1976; Pruess, 1991). The control-volume approach provides a general spatial discretization scheme that can represent a one-, two- or three-dimensional domain using a set of discrete meshes. Each mesh has a certain control volume for a proper averaging or interpolation of flow and transport properties or thermodynamic variables.

Time discretization is carried out using a backward, first-order, fully implicit finite-difference scheme. The discrete nonlinear equations for components in the multiphase system at gridblock or node i can be written in a general form:

$$\left\{A_i^{k,n+1} + G_i^{k,n+1}\Delta t - A_i^{k,n}\right\}\frac{V_i}{\Delta t} = \sum_{j\in\eta_i} flow_{ij}^{k,n+1} + Q_i^{k,n+1} \quad (4)$$

(k = 1, 2, 3, …, N_c) and (i=1, 2, 3, …, N)

where superscript k serves also as an equation index for all mass components; superscript n denotes the previous time level, with n+1 the current time level to be solved; subscript i refers to the index of gridblock or node i, with N being the total number of nodes in the grid; Δt is time step size; V_i is the volume of node i; η_i contains the set of direct neighboring nodes (j) of node i; A_i^k, G_i^k, $flow_{ij}^k$, and Q_i^k are the accumulation, decay or generation, the "flow" term (between nodes i and j), and sink/source term at node i for component k.

Equation (4) has the same form regardless of the dimensionality of the system, i.e., it applies to one-, two-, or three-dimensional flow and transport analyses. The accumulation and decay/generation terms for mass components are evaluated at each node i. The "flow" terms in Equation (4) are generic and include mass fluxes by advective and dispersive processes, as described by Equation (5), as well as heat transfer, described by Equation (2). In general, the mass flow term is evaluated as (Wu and Pruess, 2000):

$$flow_{ij}^k = F_{A,ij}^k + F_{D,ij}^k \quad (k = 1, 2 , 3, \ldots, N_c) \quad (5)$$

where $F_{A,ij}^k$ and $F_{D,ij}^k$ are the net mass fluxes by advection and hydrodynamic dispersion along the connection, respectively, with

$$F_{A,ij}^k = A_{ij}\sum_\beta \left(X_\beta^k\right)_{ij+1/2)} F_{\beta,ij} \quad (6)$$

where A_{ij} is the common interface area between the two connected blocks i and j; and the mass flow term ($F_{\beta,ij}$) is the mass flux of fluid phase β along the connection, described by

$$F_{\beta,ij} = \left(\frac{\rho_\beta k_{r\beta}}{\mu_\beta}\right)_{ij+1/2} \gamma_{ij}\left[\psi_{\beta j} - \psi_{\beta i}\right] \quad (7)$$

where γ_{ij} is transmissivity and is defined differently for finite-difference or finite-element discretization. If the integral finite-difference scheme (Pruess, 1991) is used, the transmissivity is calculated as

$$\gamma_{ij} = \frac{A_{ij} k_{ij+1/2}}{D_i + D_j} \quad (8)$$

where D_i is the distance from the center of block i to the interface between blocks i and j. The flow potential term in Equation (7) is defined as

$$\psi_{\beta i} = P_{\beta i} - \rho_{\beta,ij+1/2}\, g\, Z_i \quad (9)$$

where $P_{\beta i}$ is pressure of fluid phase β at node i and Z_i is the depth to the center of block i from a reference datum.

The flow term or the net mass flux by advection and hydrodynamic dispersion of a component along the connection of nodes i and j is determined by

$$F_{D,ij}^k = -\mathbf{n}_{ij} \bullet A_{ij} \sum_\beta \underline{D}_\beta^k \bullet \nabla\left(\rho_\beta X_\beta^k\right) \quad (10)$$

where $\mathbf{n}_{ij}$ is the unit vector along the connection of the two blocks i and j. Wu and Pruess (2000) present a general approach to calculating these flow terms associated with advective and dispersive mass transport in a multiphase system, using a regular or irregular and unstructured multidimensional grid.

Weighting and Flux Limiter Schemes

As shown in Equations (6) and (7), there are in general two types of spatial weighting schemes needed in modeling multiphase transport. The first one is $\left(X_\beta^k\right)_{ij+1/2)}$ in (6) for estimating the averaged mass fraction for calculating advective flux, and the other $\left(\rho_\beta k_{r\beta}/\mu_\beta\right)_{ij+1/2}$ in (7) is used in mobility weighting for the multiphase flow term. In the literature, flux-limiter schemes have been used not only for the first type of weighting, but also for the second type of weighting (e.g., Blunt and Rubin, 1992; and Oldenburg and Pruess, 2000). However, it has been observed in practical simulations that the numerical smearing of saturation fronts is in general much less severe than that with dissolved concentration fronts. Therefore, in this work, we focus our attention on the mass fraction averaging for modeling the concentration plume only, whereas the traditional, full upstream weighting is used in mobility or relative permeability averaging for estimating fluid displacement or saturation fronts.

In addition to spatial weighting schemes, temporal weighting also needs to be addressed in the numerical formulation. Commonly used temporal weighting schemes include fully implicit and Crank-Nicolson methods, while the fully explicit weighting is rarely used because of its strict limitation in time-step size. Among these schemes, the fully implicit method has proven itself to be most effective in handling numerical problems associated with solving highly nonlinear multiphase flow equations. In particular,

the theoretical analysis of advective-dispersive transport through a one-dimensional finite volume grid by Unger et al. (1996) indicates that the fully implicit scheme has no limitations in Courant number under various temporal weighting schemes including flux limiters. They demonstrate how fully implicit temporal weighting leads to unconditionally stable solutions for linear advection-dispersion equations. It should be noted that fully implicit weighting is only a first-order approximation, with numerical errors of the same size as the time step. However, it is our experience (in conducting hundreds and hundreds of large, field-scale simulations of coupled multiphase flow and chemical transport) that fully implicit temporal schemes always result in stable solutions and that temporal discretization errors, caused by a fully implicit scheme, are of secondary importance when compared with the many other unknowns. The key is to have a robust numerical scheme that leads to reliable and stable solutions under different spatial discretization and various physical conditions. Considering that it is impractical to define a Peclet or Courant number for detailed theoretical analyses in most field applications when using multidimensional, irregular, unstructured grids, fully implicit temporal weighting should be selected as a first choice.

Selection of proper spatial-weighting schemes becomes very critical when dealing with coupled processes of multiphase flow and chemical transport in a fractured medium because of the large differences in fracture and matrix characteristics. It is further complicated by the fact that there are no generally applicable weighting schemes or rules applicable to all problems (Wu and Pruess, 2000). The weighting schemes that are used for flux calculation in this work are:

- Upstream weighting for relative permeability and/or mobility
- Matrix permeability and molecular diffusion coefficients for fracture-matrix interaction
- Phase saturation-based weighting functions for determining diffusion coefficients

Consider the schematic of Figure 1, representing a multidimensional irregular, unstructured grid of porous and/or fractured media. To calculate advective flux between nodes i and j, we also need the information from a secondary upstream node (denoted as i2up), which is an upstream node to the upstream one, ups(i, j), between nodes i and j (Unger et al., 1996; Forsyth et al., 1998). As shown in Figure 1, the node i2up is determined by the maximum potential method in terms of maximum fluid influx into ups(i, j), which has been implemented in T2R3D at the Newtonian iteration level for every connection.

Various weighting schemes for spatially averaged mass fraction or concentration for advective flux calculation between nodes i and j are summarized as:

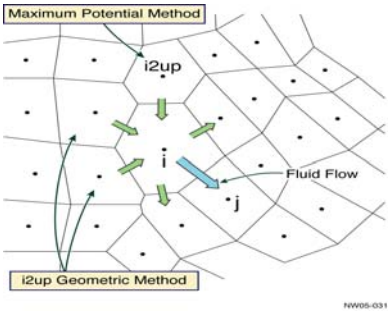

Figure 1. Schematic for determining the second upstream block (i2up) for flow between block i and block j, using the geometric method and the maximum potential method

Upstream:

$$\left(X_\beta^k\right)_{ij+1/2} = \left(X_\beta^k\right)_{ups(i,j)} \tag{11}$$

where subscript ups(i, j) stands for the upstream node for fluid flow between nodes i and j.

Central:

$$\left(X_\beta^k\right)_{ij+1/2} = \left[\left(X_\beta^k\right)_i + \left(X_\beta^k\right)_j\right]/2 \tag{12}$$

Several flux-limiter or TVD schemes tested are as follows:

van Leer limiter:

$$\left(X_\beta^k\right)_{ij+1/2} = \left(X_\beta^k\right)_{ups(i,j)} + \sigma\left(r_{ij}\right)\left[\frac{\left(X_\beta^k\right)_{dwn(i,j)} - \left(X_\beta^k\right)_{ups(i,j)}}{2}\right] \tag{13}$$

where subscript dwn(i, j) is the downstream node of i and j, defined as

$$dwn(i,j) = i + j - ups(i,j) \tag{14}$$

The van Leer weighting factor $\sigma\left(r_{ij}\right)$ is defined as

$$\sigma\left(r_{ij}\right) = 0 \qquad \left(\text{if } r_{ij} \le 0\right)$$
$$= \frac{2r_{ij}}{1+r_{ij}} \qquad \left(\text{if } r_{ij} > 0\right) \tag{15}$$

with the smoothness sensor,

$$r_{ij} = \frac{\left\langle \left(X_\beta^k\right)_{ups(i,j)} - \left(X_\beta^k\right)_{i2ups} \right\rangle \Big/ \left(D_{ups(i,j)} + D_{i2up}\right)}{\left\langle \left(X_\beta^k\right)_{dwn(i,j)} - \left(X_\beta^k\right)_{ups(i,j)} \right\rangle \Big/ \left(D_i + D_j\right)} \tag{16}$$

where $D_{ups(i,\ j)}$ and D_{i2up} are the distances from the center of block ups(i, j) or its upstream block i2up to their common interface along the connection between the blocks.

MUSCL Method:

$$\left(X_\beta^k\right)_{ij+1/2} = \left(X_\beta^k\right)_{ups(i,j)} + \frac{s}{4}\left[\left(1-\frac{s}{3}\right)\Delta_- + \left(1+\frac{s}{3}\right)\Delta_+\right] \quad (17)$$

where

$$s = \frac{2\Delta_+ + \Delta_- + \varepsilon}{\left(\Delta_+\right)^2 + \left(\Delta_-\right)^2 + \varepsilon} \quad (18)$$

$$\Delta_- = \zeta\left\{\left(X_\beta^k\right)_{ups(i,j)} - \left(X_\beta^k\right)_{i2up}\right\} \quad (19)$$

$$\Delta_+ = \left\{\left(X_\beta^k\right)_{ups(i,j)} - \left(X_\beta^k\right)_{dwn}\right\} \quad (20)$$

and

$$\zeta = \frac{D_i + D_j}{D_{ups(i,j)} + D_{i2up}} \quad (21)$$

In (18), ε is a small number, which prevents a zero divide.

Leonard Method:

Leonard flux limiter is also described by (13) with the Leonard weighting factor $\sigma\left(r_{ij}\right)$ is defined as

$$\sigma\left(r_{ij}\right) = \max\left\{0, \min\left(2, 2r_{ij}, (2+r_{ij})/3\right)\right\} \quad (22)$$

with r_{ij} is defined by Equation (16).

The numerical implementation of these TVD schemes is made into the T2R3D code (Wu et al., 1996) for simulation of tracer transport through an isothermal system for this work.

Numerical Solution Scheme

In this section, we discuss a general procedure to solve the discrete nonlinear Equation (4) fully implicitly, using a Newton iteration method. Let us write the discrete nonlinear Equation (4) in a residual form as

$$R_i^{k,n+1} = \left\{A_i^{k,n+1} + G_i^{k,n+1} - A_i^{k,n}\right\}\frac{V_i}{\Delta t} - \sum_{j\in\eta_i} flow_{ij}^{k,n+1} - Q_i^{k,n+1} = 0 \quad (23)$$

k = 1, 2, 3, …, N_c; i = 1, 2, 3, …, N).

Equation (24) defines a set of (N_c × N) coupled nonlinear equations that need to be solved for every balance equation of mass components. In general, (N_c) primary variables per node are needed to use the Newton iteration for the associated (N_c) equations per node. The primary variables are usually selected among fluid pressures, fluid saturations, mass (mole) fractions of components in fluids, and temperatures. In many applications, however, primary variables cannot be fixed and must be allowed to vary dynamically to deal with phase appearance and disappearance (Forsyth et al., 1998). The rest of the dependent variables, such as relative permeability, capillary pressures, viscosity and densities, partitioning coefficients, specific enthalpies, thermal conductivities, dispersion tensor, etc. as well as nonselected pressures, saturations, and mass (mole) fractions, are treated as secondary variables.

In terms of the primary variables, the residual Equation (23) at a node i is regarded as a function of the primary variables at not only node i, but also at all its direct neighboring nodes j. The Newton iteration scheme gives rise to

$$\sum_m \frac{\partial R_i^{k,n+1}\left(x_{m,p}\right)}{\partial x_m}\left(\delta x_{m,p+1}\right) = -R_i^{k,n+1}\left(x_{m,p}\right) \quad (24)$$

where x_m is the primary variable m with m = 1, 2, 3, …, N_c at node i and all its direct neighbors; p is the iteration level; and i =1, 2, 3, …, N.

A numerical method is used to construct the Jacobian matrix for Equation (24) (Forsyth et al., 1995). At each Newton iteration, Equation (24) represents a system of (N_c × N) linearized algebraic equations with sparse matrices, which are solved by a linear equation solver. Note that when using the flux limiter schemes, as discussed in the last subsection, advective mass flux terms in the discrete equation may depend on primary and secondary variables beyond the direct neighboring nodes, such as at node of i2up. In such a situation, the Newton iteration discussed here becomes inexact, because the Jacobian matrix does not include the contributions with respect to the primary variables beyond neighboring nodes. Nevertheless, converged solutions should be correct, because the residuals are exact. This omission in these Jacobian calculations may make solution convergence more problematic. However, many numerical tests have been made for multiphase tracer transport, and no significant numerical problems have been observed.

Fractured Media

The mathematical formulations and flux-limiter schemes discussed above are applicable to both single-continuum and multi-continuum media, as long as the physical processes involved can be described in a continuum sense within either continuum. When handling flow and transport through fractured rock using the numerical formation of this section, fractured media (including explicit

fracture, dual, or multiple continuum models) can be considered as special cases of unstructured grids of Figure 1. Then, a large portion of the work consists of generating a mesh that represents both the fracture and the matrix system under consideration. Several fracture and matrix subgridding schemes exist for designing different meshes for different fracture-matrix conceptual models (e.g., Pruess, 1983).

Once a proper unstructured grid of a fracture-matrix system is generated, fracture and matrix blocks are identified to represent fracture and matrix domains, separately. Formally they are treated identically for the solution in the model. However, physically consistent fracture and matrix properties, parameter weighting schemes, and modeling conditions must be appropriately specified for both fracture and matrix systems.

APPLICATION

One example is presented here to demonstrate application of the TVD schemes, as discussed above, in handling transport through fractured media. The sample problem is based on a two-dimensional site-scale model developed for investigation of the unsaturated zone at Yucca Mountain, Nevada. This example shows transport of one conservative (nonadsorbing) tracer through unsaturated fractured rock using a 2-D, unstructured grid with a dual-permeability conceptualization for handling fracture and matrix interaction.

The 2-D west-east cross-sectional model grid, shown in Figure 2, has a total of 30,000 fracture-matrix gridblocks and 74,000 connections between them in a dual-permeability mesh. The potential repository is located in the middle of the model domain, discretized with locally refined grid (Figure 2), at an elevation of about 1,100 m.

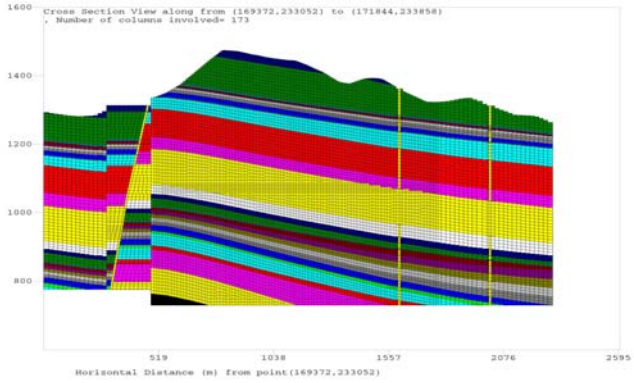

Figure 2. Two-dimensional west-east cross-sectional model domain and grid showing lateral and vertical discretization, hydrogeological layers, repository layout, and several faults incorporated

The 2-D model uses the ground surface as the top model boundary and the water table as the bottom boundary. Both top and bottom boundaries of the model are treated as Dirichlet-type boundaries, i.e., constant (spatially distributed) pressures, liquid saturations and zero initial tracer concentrations are specified along these boundary surfaces. In addition, on the top boundary, a spatially varying, steady-state, present-day infiltration map, as shown in Figure 3, determined by the scientists of the U.S. Geological Survey, is used in this study to describe the net water recharge, with an average infiltration rate of about 5 mm/yr over the model domain. In addition, an isothermal condition is assumed in this study. The properties used for rock matrix and fractures in the dual-permeability model, including two-phase flow parameters of fractures and matrix as well as faults, were estimated from field tests and model calibration efforts (Wu et al., 2002).

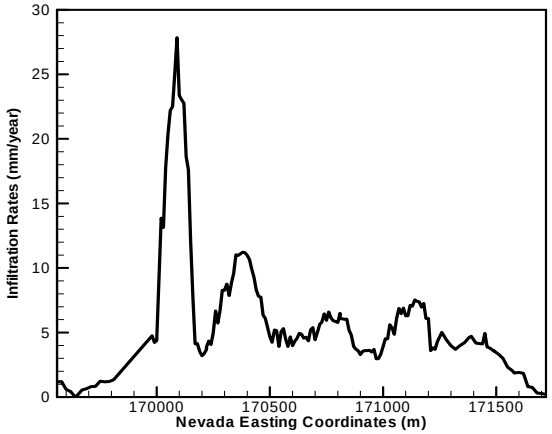

Figure 3. Net infiltration rate along the west-east cross-section model as surface water recharge boundary condition

We consider a conservative liquid tracer migrating from the repository downward by advective and dispersive processes, subject to the ambient steady-state unsaturated flow condition. A constant effective molecular diffusion coefficient of 3.2×10^{-11} (m^2/s) is used for matrix diffusion of the conservative component. Transport starts with a finite amount of the tracer initially released into the fracture elements of the repository blocks. After the simulation starts, no more tracer will be introduced into the system, but the steady-state water recharge from the top boundary continues. Eventually, all the tracer will be flushed out from the 2-D system through the bottom, water table boundary, by advective and diffusive processes.

Figures 4 and 5 show normalized tracer concentration contours in the fracture continuum within the 2-D model at 10 years of tracer release, simulated using various weighting schemes of spatially averaged

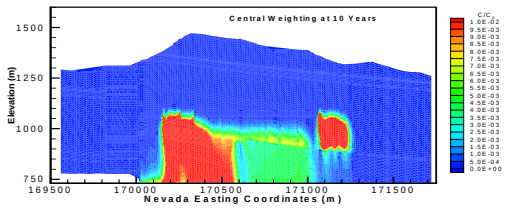

Figure 4. Concentration distributions within the 2-D model at 10 years, simulated using the central weighting scheme mass fraction for advective flux calculation.

Comparisons of simulated concentrations between Figures 4 (central weighting) and 5 (TVD-MUCSL) show a large difference at the time of 10 years. Note that for this problem, all three TVD schemes implemented in this study give similar results, so only the results with MUSCL are shown for the TVD cases in Figure 5. Figure 6 presents fractional cumulative mass breakthrough curves at the water table, also showing some significant difference between the results using the TVD schemes and the central weighting.

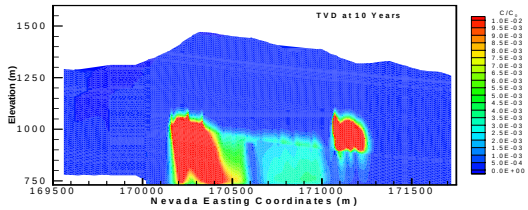

Figure 5. Concentration distributions within the 2-D model at 10 years, simulated using the TVD (MUSCL) scheme

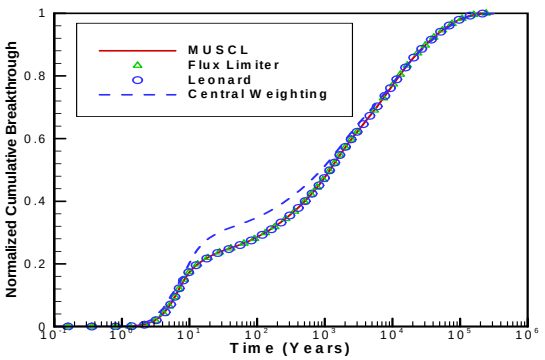

Figure 6. Breakthrough curves of fractional cumulative tracer mass arriving at the water table, since release from the repository, simulated using the different weighting schemes

Overall, the simulation results indicate that at early time, such as in first 10 years (Figure 4), the central weighting scheme underestimates advective transport, while at later time (t > 100 years) it overestimates advective transport, because of selecting too high or too low averaged concentration values. In addition, the TVD schemes are tested and found to have much better numerical performance than the central weighting scheme with respect to taking larger time steps or stability.

SUMMARY AND CONCLUSIONS

We have investigated several TVD schemes by implementing them into the TOUGH2 family of codes, using multidimensional irregular unstructured grids. Our test results show that such TVD schemes are able to reduce numerical dispersion effectively, if used properly. In addition, numerical performance with TVD schemes is significantly improved relative to commonly used central weighting and is comparable to fully upstream weighting. It is encouraging to note that under multiphase conditions using relatively course spatial discretization, these TVD schemes provide more accurate simulation results for modeling large-scale field tracer transport processes through heterogeneous, fractured rock.

ACKNOWLEDGMENTS

The authors would like to thank Lehua Pan for his help with the model grid. Thanks are also due to Guoxiang Zhang, Curt Oldenburg and Dan Hawkes for their review of the paper. This work was supported in part by the U.S. Department of Energy. The support is provided to Berkeley Lab through the U. S. Department of Energy Contract No. DE-AC03-76SF00098.

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