Multicomponent fluid flow by discontinuous Galerkin and mixed methods in unfractured and fractured media

H. Hoteit and A. Firoozabadi
Reservoir Engineering Research Institute, Palo Alto, California, USA

Received 9 June 2005; revised 25 July 2005; accepted 9 August 2005; published 10 November 2005.

A discrete fracture model for the flow of compressible, multicomponent fluids in homogeneous, heterogeneous, and fractured media is presented in single phase. In the numerical model we combine the mixed finite element (MFE) and the discontinuous Galerkin (DG) methods. We use the cross-flow equilibrium concept to approximate the fractured matrix mass transfer. The discrete fracture model is numerically superior to the single-porosity model and overcomes limitations of the dual-porosity models including the use of a shape factor. The MFE method provides a direct and accurate approximation for the velocity field, which is crucial for the convective terms in the flow equations. The DG method associated with a slope limiter is used to approximate the species balance equations. This method can capture the sharp moving fronts. The calculation of the fracture-fracture flux across three and higher intersecting fracture branches is a challenge. In this work, we provide an accurate approximation of these fluxes by using the MFE formulation. Numerical examples in unfractured and fractured media illustrate the efficiency and robustness of the proposed numerical model.


1. Introduction

This paper considers the flow of miscible and compressible multicomponent fluids in unfractured and fractured media. The compositional modeling has broad applications in various disciplines including petroleum engineering (hydrocarbon-gas injection and recycling in gas-condensate reservoirs), hydrology and geochemical engineering (contamination of groundwater aquifers and radioactive waste management in the subsurface). The numerical simulation of the process should overcome many numerical difficulties associated with the unstructured geometry of the fractured field, sharp variations in the rock properties, and high nonlinearity of the multicomponent system due to the compressibility and compositional effects.

The partial differential equations that describe the flow processes are coupled and highly nonlinear. Traditional algorithms that employ the classical finite difference (FD), finite volume (FV) or finite element (FE) methods generally do not provide satisfactory results. These methods may not represent the physics correctly because of two main deficiencies: First, the flow processes are usually convection dominated. These methods combined with first-order upstream techniques produce significant numerical dispersion [Coats, 1980] especially in the neighborhood of shocks in the solution. Second, it is known in the literature [Durlofsky, 1994; Mosé et al., 1994] that for discontinuous and anisotropic permeability these methods may not provide accurate velocity field, because only the pressure is computed as a primary variable and the velocity field has to be approximated from Darcy’s law by a postprocessing step.

The objective of this work is to develop a robust and efficient numerical model that has the following features: (1) the mass is conserved locally at the element level, (2) sharp fronts are predicted without introducing spurious oscillations or excessive numerical dispersion, (3) the velocity field is correctly approximated in anisotropic and in highly heterogeneous media, and should have low mesh dependence, and (4) unstructured grids are used for spatial discretization. To fulfill these requirements, we combined the mixed finite element (MFE) method and the discontinuous Galerkin (DG) method. The MFE method is used to discretize Darcy’s law. The main features for this choice are as follows: the pressure and the fluxes are approximated simultaneously with the same order of convergence, and the method is locally conservative and it can easily accommodate full permeability tensor. This method also produces minimal mesh orientation effect [Darlow et al., 1984]. The fact that the MFE method is more reliable in flux calculation than the FV and FE methods is well known [Durlofsky, 1994; Mosé et al., 1994]. The MFE formulation in our method uses the lowest-order Raviart-Thomas space [Raviart and Thomas, 1977; Thomas, 1977]. The original MFE formulation leads to a saddle point problem for elliptic or parabolic equations i.e., the linear system to solve, that has the cell pressure averages and the interelement fluxes as primary unknowns, is indefinite. The remedy is to use the hybridization technique [Brezzi and Fortin, 1991; Chavent and Roberts, 1991] where new degrees of freedom are appended.
at the element edges. The additional unknowns represent the edge pressure averages (pressure traces). In our method, this approach will not help to make the linear system to become positive definite because of the Newton-Raphson linearization. However, it is still useful since it reduces the size of the linear system which has the traces of the pressure as primary unknowns. The DG method is used to approximate the species balance equations. The state unknown (concentration) is approximated by using linear and bilinear shape functions on triangular and quadrilateral elements, respectively. The use of high-order approximation spaces produces nonphysical oscillations near the shocks. To stabilize the scheme, we use a multidimensional slope limiter [Chavent and Jaffré, 1986; Hoteit et al., 2004b], which reconstructs the solution profile over the grid blocks by imposing some geometrical constraints. Recently, the DG method has received a lot of attention mainly because it can be applied to structured and unstructured grids, it conserves mass locally at the element level and produces low numerical dispersion compared to classical methods. Various versions of DG method have been developed. Cockburn and Shu [1989, 1998] developed the Runge-Kutta discontinuous Galerkin (RKDG) method. The RKDG method is an extension of the DG method to higher temporal and spatial approximation spaces. Recent developments have extended this method to approximate elliptic, diffusion and convection-diffusion problems [Chen et al., 1995; Rivière et al., 1999]. Different problems have been solved by using both the MFE and DG methods. Chavent et al. [1990] used these methods to approximate a two-phase incompressible, immiscible fluid flow. Siegel et al. [1997] and Hoteit et al. [2004a] also combined these methods to solve convection-diffusion equations in porous media. In a similar fashion, our numerical model combines the MFE method to approximate the pressure unknown and the DG method to approximate the flow equations. In this work, however, the compressibility and compositional effects are taken into account. The extension to compressible-compositional systems makes our method distinct from the work of others.

In this work, we also extend the MFE-DG method for fractured media by using the discrete fracture model. Different numerical approaches have been proposed in the literature to model the flow in fractured porous media. The dual-porosity model [Warren and Root, 1963; Kazemi, 1969; Thomas et al., 1983; Arbogast et al., 1990] is widely used in the flow simulators in fractured media. This model represents the fracture network by an equivalent porous medium which generally has the sugar cube configuration. The dual-porosity model is numerically very efficient since computations are only performed in the fracture network. The interaction between the matrix and the fractures is described with empirical transfer functions. Because appropriate transfer functions are not well established especially with gravity, compressibility, and compositional effects, the model is inadequate to describe the compositional effects in fractured media. Another limitation is the modeling of discrete fractures since this model assumes the medium to be described by a dense connected fractured network. One can also use the single-porosity model with explicit grid blocks to describe the fractures in the same way as the matrix is described. In such a model, the geological parameters vary sharply between the matrix and the fractures. The high contrast and different length scales in the matrix and fractures make this approach unpractical. An alternative is the discrete fracture model, which can be considered as a simplification of the single-porosity model. Assuming that the fracture aperture is small compared to the matrix scale, fractures are represented by \((n - 1)\)-dimensional elements in an \(n\)-dimensional domain [Noorishad and Mehran, 1982; Baca et al., 1984; Granet et al., 1998]. This simplification makes the latter much more efficient than the single-porosity model.

Unlike immiscible fluid flow, which has been studied extensively [Kim and Deo, 1999, 2000; Bastian et al., 2000; Karimi-Fard and Firoozabadi, 2003], very few studies are reported in the literature for the compositional modeling in fractured media. Here we intend to demonstrate the possibility of modeling multicomponent compressible flow in discrete fractured media. The reliability and efficiency of this approach are conditional to two essential approximations: the matrix-fracture and the fracture-fracture fluxes. On the basis of the cross-flow equilibrium concept, the pressure in a fracture element is assumed to be equal to the pressure in the surrounding matrix elements. Integrating the flow equations in a control volume that includes the fracture element and the adjacent matrix elements alleviates the computation of the matrix-fracture fluxes. This simplification makes the approach much more efficient than the single-porosity model and overcomes the limitations of the dual-porosity models.

Computing the flux across the intersection of more than two fracture branches is a challenge. Most of the cell-based finite volume schemes that are adapted to a discrete fracture model have the fracture pressure unknowns at the discretized element centers. On structured grids, Slough et al. [1999a, 1999b, 1999c] compute the fluxes between a vertical fracture and a horizontal fracture by assuming a steady state flow in the control volume where the fractures are intersected. However, such technique cannot be applied in unstructured grids with multiintersecting fractures. In our approach, this deficiency is solved definitively due to the MFE formulation.

This paper is organized as follows: First, the differential and algebraic equations describing the displacement of compressible, compositional flow of multicomponent fluids are presented. Second, we describe the numerical model in unfractured media. Different aspects of the numerical approach, the discretization of Darcy’s law by MFE method, the flow equations by the DG method, the linearization technique and the slope limiter are discussed in detail. We then present the extension of the MFE-DG method to fractured media, where we show how to calculate the matrix-fracture and fracture-fracture fluxes. Finally, we present numerical examples in unfractured and fractured media to demonstrate the efficiency and robustness of our numerical approach.

2. Mathematical Model

In a subsurface flow problem, we are interested in the displacement of miscible and compressible fluid of \(n_c\) components. By neglecting the molecular diffusion, the
mass conservation for the $i$th component through the porous medium is expressed by the equations

$$\frac{\partial c_i}{\partial t} + \nabla \cdot (c_i \mathbf{v}) = f_i \quad i = 1, \ldots, n_c \quad \text{in} \quad \Omega \times (0, \tau)$$

$$c_i = z_i c$$

$$\sum_{i=1}^{n_c} z_i = 1 \quad (1)$$

where $\phi$ is the porosity, $c$ is the overall molar density, $c_i$ and $z_i$ are, respectively, the molar density and the mole fraction of component $i$, $f_i$ is a sink/source, $\Omega$ is the 2-D computational domain and $\tau$ denotes the simulation time.

[10] The volumetric velocity field $\vartheta$ appearing in equation (1) is given by the generalized Darcy’s law:

$$\vartheta = -\frac{k}{\mu} (\nabla p - pg) \quad \text{in} \quad \Omega \times (0, \tau) \quad (2)$$

where $k$ is the absolute permeability tensor, $\mu$, $p$, $\rho$ and $g$ are, respectively, the viscosity, pressure, mass density, and the gravitational force field.

[11] Equations (1) and (2) are subject to initial and boundary conditions (BC) of Dirichlet and Neumann type:

$$z_i(x, 0) = z_i^0(x), \quad i = 1, \ldots, n_c \quad \text{in} \quad \Omega$$

$$p(x, 0) = p^0(x) \quad \text{in} \quad \Omega$$

$$p(x, t) = p^0(x), \quad i = 1, \ldots, n_c \quad \text{on} \quad \Gamma^D \times (0, \tau) \quad (3)$$

$$z_i(x, t) \frac{\partial}{\partial n} = q_i^g(x, t), \quad i = 1, \ldots, n_c \quad \text{on} \quad \Gamma^N \times (0, \tau)$$

where $q_i^N$ is the injection rate of component $i$ across the boundary $\Gamma^N$, $p^0$ and $p^D$ are the initial pressure and the imposed pressure on the Dirichlet BC, $n$ denotes the unit-normal outward to the domain boundary $\Gamma^D$. The flow equations (1)–(3) are coupled with an equation of state (EOS) that describes the phase molar density as a function of the composition, temperature and pressure. In this work, the Peng-Robeson EOS is used:

$$\rho = c M$$

$$c = \frac{\rho}{ZRT} Z^2 - \frac{(1 - B)Z^2}{(A - 3B^2 + 2B)}Z - (AB - B^2 - B) = 0 \quad (4)$$

where $M$ is the molecular weight, $T$ the temperature, $R$ the gas constant, $A$ and $B$ are the PR EOS parameters [see, e.g., Firoozabadi, 1999].

3. Numerical Approximation in Unfractured Media

[12] The numerical approach used to solve the coupled system of equations (1)–(4) is based on combining the DG and MFE methods. This system is linearized by using the Newton-Raphson (NR) method. The primary unknown, the pressure, is solved implicitly and the concentration unknowns are computed explicitly in time. The construction of the numerical procedure can be organized in the following steps: (1) discretization of Darcy’s law by the MFE method, (2) discretization of the flow equations by the DG method, (3) combining the MFE and DG discretizations, and (4) data reconstruction by using a slope limiter. Before detailing these steps, we consider a spatial triangulation of the computational domain $\Omega$ consisting of triangles or quadrilaterals. Unlike some other numerical methods, no restrictions are imposed on the element geometrical shape. We also use the notation $K$, discretized block or cell, $E$, edges of the cell $K$, $N_e$, number of edges for each cell ($N_e = 3$ or 4), $N_e$, number of cells in the mesh, and $N_E$, number of edges in the mesh not belonging to $\Gamma^D$.

3.1. Discretization of Darcy’s Law

[13] The essential idea of the MFE method is to approximate simultaneously the pressure and its gradient. The velocity field is approximated in the so-called Raviart-Thomas space of lowest order ($RT_0$) [see, e.g., Chavent and Roberts, 1991; Hoteit et al., 2002]. The main idea is to express the velocity vector for each grid cell with respect to the fluxes across the cell edges. A detailed description of the MFE formulation is presented in appendix A.

[14] On the basis of Raviart-Thomas approximation space, the vectors $\vartheta$ and $g$ in equation (2) can be expressed as

$$\vartheta = \sum_{E \in \partial K} q_K \mathbf{w}_{K,E}$$

$$g = \sum_{E \in \partial K} q_K \mathbf{w}_{K,E}$$

where $w_{K,E}$ is a $RT_0$ basis function, $q_K \mathbf{w}_{K,E}$ is the total flux across an edge $E$ and $q_K \mathbf{w}_{K,E}$ is the flux due to the gravitational force. These vectors are determined by their normal fluxes across the cell edges. Let $K = k/\mu$ be the effective mobility tensor. By inverting $K$, Darcy’s velocity equation becomes

$$K^{-1} \vartheta = -(\nabla p - pg) \quad (6)$$

Multiplying equation (6) by the test function $w_{K,E}$ and integrating by parts, then the total flux $q_K \mathbf{w}_{K,E}$ is expressed through each edge $E$ as a function of the cell pressure average $p_K$ and the edge pressure averages $p_{E,K}$ for each cell $K$, i.e.,

$$q_{K,E} = \alpha_{K,E} \rho p_K - \sum_{E \in \partial K} \beta_{K,E,E'} p_{E,K} - \gamma_{K,E} \quad E \in \partial K \quad (7)$$

where the coefficients $\alpha_{K,E}$, $\beta_{K,E,E'}$ and $\gamma_{K,E}$ depend on the geometrical and rock properties of block $K$.

[15] The continuity of the fluxes across the interelement boundaries provides

$$q_{K,E} = \begin{cases} -q_{K,E} & \text{if } E = K \cap K' \\ q^N_{E} & \text{if } E \in \Gamma^N \end{cases} \quad (8)$$

Equations (7) and (8) lead to the following algebraic linear system with main unknowns; the pressure cell averages in $P$ and the pressure edge averages in $T_P$

$$R^T P - MT_P - V = 0 \quad (9)$$

where

$$R = [R_{K,E}]_{K,K'}; \quad R_{K,E} = \alpha_{K,E} \quad E \in \partial K$$

$$M = [M_{E,E'}]_{E,E'}; \quad M_{E,E'} = \sum_{K \in \partial K} \beta_{K,E,E'} \quad E \notin \Gamma^D$$

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$V$ is a vector of size $N_E$ that describes the boundary conditions.

Equation (9) is valid at any time, so we can write

$$R^T \Delta P - M \Delta T_p = G$$

where $G = -R^T P + M T_p + V$.

3.2. Discretization of the Flow Equations

The DG method is used to discretize the flow equation (1). This method consists of a discontinuous, piecewise, linear (on triangles) or bilinear (on quadrilaterals) approximation of the concentration unknowns $c_i$, $i = 1, \ldots, n_c$. Over each cell $K$, the unknown $c_{i,K}$ is approximated in a discontinuous finite element space, such that,

$$c_{i,K} = \sum_{I=1}^{N_I} \tilde{c}_{i,K,I} \phi_{K,I}$$

where $\phi_{K,I}$ are some finite element shape functions. Multiplying equation (1) by the test functions and integrating by parts yield

$$\int_K \phi \frac{\partial c_{i,K}}{\partial t} \varphi_{K,j} - \int_K c_{i,K} \frac{\partial \varphi_{K,j}}{\partial n} + \int_K \tilde{c}_{i,K,j} \varphi_{K,j} \, dV = \int_{\partial K} f_i \varphi_{K,j} \, ds$$

where $\tilde{c}_{i,K,j}$ denotes the edge concentration in the upstream block. Depending on the influx or efflux with respect to the cell $K$, we have

$$\tilde{c}_{i,K} = \begin{cases} c_{i,K} \text{ if } \partial_n \geq 0 \text{ (efflux)} \\ c_{i,K} \text{ if } \partial_n < 0 \text{ (influx from block } K') \end{cases}$$

Let $\bar{c}_{i,k}, i = 1, \ldots, n_c$, denote the cell average of $c_i$ over $K$. In order to have explicitly the average values $\bar{c}_{i,K}; i = 1, \ldots, n_c$ from the flow equations, it is convenient to sum up equation (12) for $j = 1, \ldots, N_c$. With some simple manipulations, one gets

$$\phi_K \left[ \frac{d\bar{c}_{i,K}}{dt} + \sum_{E \in \partial K} q_{K,E} \bar{c}_{i,E} \right] = |K| \bar{f}_{i,K}$$

where $\bar{f}_{i,K}$ is the cell average of $f_i$ over $K$.

The line integrals in equation (12) are simplified by using the equation

$$\int_E \bar{c}_{i,K,j} \varphi_{K,j} \, dE = q_{K,E} \bar{c}_{i,E}$$

where $\bar{c}_{i,E}$ is the edge average concentration in the upstream block. Replace the flux expression from equation (7) in equation (13) to get

$$\frac{d\bar{c}_{i,K}}{dt} + \bar{c}_{i,K} p_k + \sum_{E \in \partial K} \tilde{\gamma}_{i,E,K} q_{K,E} + \gamma_{i,K} = 0 \quad i = 1, \ldots, n_c$$

where the coefficients $\tilde{\gamma}_{i,K,E}$ and $\gamma_{i,K}$ are functions of $\tilde{\gamma}_{i,K,E}$, $\alpha_K$, $\beta_{i,K,E,E}$, and $\gamma_{i,K}$. The discretization of the time operator in equation (15) by the forward Euler scheme and the linearization by the NR method give

$$\Delta \tau_{i,K} + \Delta t \tilde{\gamma}_{i,K} \Delta p_k + \Delta t \sum_{E \in \partial K} \tilde{\gamma}_{i,E,K} \Delta q_{K,E} = g_{i,K} \quad i = 1, \ldots, n_c$$

where $g_{i,K} i = 1, \ldots, n_c$ denotes the residual functions. The coefficients $\alpha_K$, $\beta_{i,K,E,E}$ in equation (16) are evaluated using edge average concentration $\bar{c}_{i,E}$ from old time level.

3.3. Combining the MFE and DG Discretizations

The PR EOS is applied by using the cell average values of the pressure, molar density, mass density, composition, and the temperature. Define the residual error function $g_K$ as follows:

$$\tilde{G}_K(\tau_{i,K}; i = 1, \ldots, n_c, p_k) = \tau_{K} - \frac{p_k}{RT}$$

The Newton-Raphson linearization of equation (17) yields

$$\tilde{g}_{\tau K} \Delta p_k + \sum_{i=1}^{n_c} \tilde{g}_{\tau_{i,K}} \Delta \tau_{i,K} = -g_K$$

where $\tilde{g}_{\tau K} = \frac{\partial g_K}{\partial p_k}$, $\tilde{g}_{\tau_{i,K}} = \frac{\partial g_K}{\partial \tau_{i,K}} i = 1, \ldots, n_c$.

The derivatives can be calculated by using the PR EOS [see, e.g., Firoozabadi, 1999]. By replacing equation (16) in equation (18) and writing in a matrix notation, we get the system

$$\tilde{D} \Delta P + \tilde{R} \Delta T_p = F$$

where

$$\tilde{D} = [D_{K,K}]_{N_E \times N_E}, \quad \tilde{D}_{K,K} = \Delta \sum_{i=1}^{n_c} \tilde{g}_{\tau_{i,K}} \Delta \tau_{i,K} - \tilde{g}_{\tau K}$$

$$\tilde{R} = [R_{K,E}]_{N_E \times N_c}, \quad \tilde{R}_{K,E} = \Delta \sum_{i=1}^{n_c} \tilde{g}_{\tau_{i,K}} \tilde{\gamma}_{i,E,K}$$

$$F = [F_K]_{N_c}, \quad F_K = \sum_{i=1}^{n_c} \tilde{g}_{\tau_{i,K}} \tilde{c}_{i,E}$$

The system of Equations 10 and 19 can be written together as

$$\begin{pmatrix} \tilde{D} & \tilde{R} \end{pmatrix} \left( \begin{array}{c} \Delta P \\ \Delta T_p \end{array} \right) = \left( \begin{array}{c} F \\ G \end{array} \right)$$

Because $\tilde{D}$ is a diagonal matrix, the Schur complement matrix is readily computed. Thus the numerical procedure leads to the following final system whose primary unknowns are the traces of the pressure on the grid edges.

$$\left( M + \tilde{D}^{-1} \tilde{R} \right) \Delta T_p = \tilde{R} \tilde{T}^{-1} F - G$$

The cell pressure unknowns are then updated by using equation (19). The nodal values for the concentrations
3.4. Slope Limiting

It is known that with a high-order approximation, the DG method becomes unstable. The use of an appropriate slope limiter is essential in order to avoid overshoots and undershoots in the solution. One such slope limiter was introduced by Chavent and Jaffré [1986]. This slope limiter can be interpreted as a generalization of the Van Leer MUSCL 1-D slope limiter [Van Leer, 1974]. The essential idea of this technique is to impose some local constraints in a geometric manner so that the reconstructed solution satisfies an appropriate maximum principle. These constraints state that the value of the state function at a node \( i \), for example, should lie between the minimum and the maximum of the cell averages of all elements containing \( i \) as a vertex. This slope limiter was later modified by Hoteit et al. [2004b]. It is found that limiting the state edge average is more appropriate than limiting the nodal values as Chavent and Jaffré proposed. These modifications improved the capability of the slope limiter in eliminating spurious oscillation and reducing the numerical dispersion as well. More details about the slope limiter used in our method are given in appendix B.

4. Algorithm

The principal steps of the MFE-DG algorithm can be illustrated as follows.

1. Initialize geometry and physical parameters of the problem.
   1.1. For initial pressure, temperature and composition, use the PR EOS to calculate the initial molar and mass densities.
   1.2. For given pressure, temperature and composition, calculate the viscosities.

2. Repeat until the predetermined simulation time is reached.

3. Iterate on the Newton-Raphson linearization steps.
   3.1. Calculate \( \Delta T_P \) by solving the linear system given in equation (21).
   3.2. Calculate \( \Delta P \) locally from equation (19).
   3.3. Calculate the fluxes \( q_{K,E} \) across the edges from equation (7).
   3.4. Calculate the nodal values of the molar densities from equation (12).
   3.5. Reconstruct \( c_i \), \( i = 1, \ldots, n_c \) by applying the slope limiter procedure.
   3.6. Check convergence (\( \| \Delta P \| < \text{TOL}_P \) and \( \| \Delta c_i \| < \text{TOL}_c; \ i = 1, \ldots, n_c \)) if not repeat step 3.

4. For given pressure, temperature and composition update the mass density and the viscosities. Note that, in all the numerical experiments, only one Newton-Raphson iteration step was sufficient to attain convergence.

5. Extension to Fractured Media

In this section, we extend the coupled MFE-DG method to fractured media. The key solution is to correctly approximate the matrix-fracture and fracture-fracture transfers.

5.1. Matrix-Fracture Transfer

Generally, fractures have very small aperture (width) compared to the matrix size. A small aperture places a severe constraint on the time step. The main idea of the discrete fracture model is to use the cross-flow equilibrium concept to account for flow across the fractures [Noorishad and Mehran, 1982; Baca et al., 1984; Granet et al., 1998]. Thus the integrals of the governing equations over the fracture can be simplified by dropping one of the spatial variables through multiplying by the fracture width. Consequently, fractures can be represented by the edges of the control volumes in the grid.

Classical finite element methods can be divided into two categories: the first group includes the methods that use nodal or vertex-based representation for the unknowns, like Galerkin FE and vertex-centered control volume methods and the second group includes the cell-based methods, like cell-centered FV, FD, DG and MFE (see Figure 1). According to the spatial approximation of the unknowns, each method can be adapted to represent the linear representation of the fractures. Unlike the methods of the first category [Bastian et al., 2000; Karimi-Fard and Firoozabadi, 2003; Monteagudo and Firoozabadi, 2004], all methods in the...
second category face difficulties and therefore need special treatments to handle the hybrid spatial approximations [see, e.g., Slough et al., 1999b; Karimi-Fard et al., 2004; Granet et al., 2001]. The cell-based methods require computing the fluxes across the cell edges. Consequently, with a fracture (see Figure 1), some fluxes have to be evaluated across the lateral sides of the fracture. One choice is to add a new degree of freedom representing the edge average of the state unknown (e.g., pressure, concentration or saturation). Such an interface, \( \partial K \), of connected fractures \( (N_I \geq 2) \) of connected fractures \( I \), is shown in Figure 3. In the grid blocks that contain fractures, we assume that the block pressure average and the fracture slice pressure average are equal, that is, \( p_K = p_e \). We impose the flux continuity across the block interfaces, \( \left( q_{K,E} + q_{E,K} \right) = 0; E = K \cap K' \), Similarly, at the intersection point \( o \) of \( N_I (N_I \geq 2) \) of connected fractures \( I \), (see Figure 4), we assume that there is no volumetric accumulation, that is

\[
\sum_{I=1}^{N_I} q_{K,o} = 0
\]  

(24)

By using Equations (23) and (24) in the fracture elements and Equations (7) and (8) in the matrix elements, the flux unknown can then be eliminated and a linear system with the main unknowns; the pressure average and the pressure trace at the extremities of \( I \). The pressure and flux degrees of freedom in the matrix and fracture elements are shown in Figure 3. In the grid blocks that contain fractures, we assume that the block pressure average and the fracture slice pressure average are equal, that is, \( p_K = p_e \). We impose the flux continuity across the block interfaces, \( \left( q_{K,E} + q_{E,K} \right) = 0; E = K \cap K' \), Similarly, at the intersection point \( o \) of \( N_I (N_I \geq 2) \) of connected fractures \( I \), (see Figure 4), we assume that there is no volumetric accumulation, that is

\[
\sum_{I=1}^{N_I} q_{K,o} = 0
\]  

(24)

5.2. Approximation of Darcy’s Law in the Fractures

[25] The same mixed hybrid finite element formulation can be applied to discretize Darcy’s law in the fracture element \( I \). The flux \( q_{I,e} \) across the extremity \( e \) of \( I \) can then be written as

\[
q_{I,e} = \alpha_{I,e} p_I - \sum_{e \in \partial I} \delta_{I,e,a} \nu_{I,e} - \gamma_{I,e} \quad e \in \partial I
\]  

(23)

where \( p_I \) and \( \nu_{I,e} \) are, respectively, the pressure average on \( I \) and the pressure traces at the extremities of \( I \). The pressure and flux degrees of freedom in the matrix and fracture elements are shown in Figure 3. In the grid blocks that contain fractures, we assume that the block pressure average and the fracture slice pressure average are equal, that is, \( p_K = p_e \). We impose the flux continuity across the block interfaces, \( \left( q_{K,E} + q_{E,K} \right) = 0; E = K \cap K' \), Similarly, at the intersection point \( o \) of \( N_I (N_I \geq 2) \) of connected fractures \( I \), (see Figure 4), we assume that there is no volumetric accumulation, that is

\[
\sum_{I=1}^{N_I} q_{K,o} = 0
\]  

(24)

By using Equations (23) and (24) in the fracture elements and Equations (7) and (8) in the matrix elements, the flux unknown can then be eliminated and a linear system with main unknowns; the pressure average and the pressure trace is obtained.

5.3. Approximation of Species Flow Equations

[26] The DG method can be readily extended to fractured media. The only difficulty, here, is the calculation of fracture-fracture flux at the intersection point of the fractures. Let \( K \) be a matrix block that contains a fracture slice \( I \) and \( c_{i,K} \) be the cell average of \( c_i \) over \( K \). The integration of the flow equation (1) over the matrix block and fracture slice is written as

\[
\left( \int_K \phi_k \frac{\partial c_{i,K}}{\partial t} + \int_I \phi_i \frac{\partial c_{i,J}}{\partial t} \right) + \left( \int_K \nabla_i (c_{i,K} \dot{v}) + \int_I \nabla_i (c_{i,J} \dot{v}) \right) = \int_{K,J} f_{i,K} \quad j = 1, \ldots, N_e
\]  

(25)

Table 1. Critical Properties for C1 and C3

<table>
<thead>
<tr>
<th>Properties</th>
<th>C1</th>
<th>C3</th>
</tr>
</thead>
<tbody>
<tr>
<td>Acentric factor</td>
<td>0.01</td>
<td>0.15</td>
</tr>
<tr>
<td>Critical temperature, K</td>
<td>190</td>
<td>370</td>
</tr>
<tr>
<td>Critical pressure, bars</td>
<td>46</td>
<td>42</td>
</tr>
<tr>
<td>Molecular weight, g/mol</td>
<td>16</td>
<td>44</td>
</tr>
</tbody>
</table>
Using the divergence theorem and assuming that the average concentrations in the matrix block and fracture slice are equal, equation (25) is simplified to

$$\frac{d}{dt} \sum_{e} \hat{c}_{K,E} + \sum_{e} \hat{c}_{I,E} = \sum_{e} q_{I,E} = \tilde{f}_{I,K}$$

(26)

where \( \varepsilon \) is the fracture aperture; \( \hat{c}_{K,E} \) and \( \hat{c}_{I,E} \) are the concentrations from the upstream matrix block and fracture slice, respectively. The final linear system, which has the traces of the pressure as primary unknowns, is constructed in a similar way to the algorithm described in unfractured media. The only key step we need to discuss is the calculation of the term in equation (26), which represents the fracture-fracture fluxes.

5.4. Fracture-Fracture Transfer

[27] In discrete fracture models, the approximation of the fluxes at the intersection point of several fracture branches is a challenge. For two intersecting fractures, fluxes along each branch can be easily evaluated by introducing an unknown approximating the pressure at the intersection node. Then, by writing the balance at that node, the pressure unknown can be eliminated and the fluxes can be evaluated. On structured grids, Slough et al. [1999a, 1999b, 1999c] computed the fluxes between a vertical fracture and a horizontal fracture by assuming a steady state flow in the control volume where the fractures intersect. On unstructured grids, Karimi-Fard et al. [2004] used an analogy between flow in fractured porous media and conductance through a network of resistors. They used the so-called star delta rule to calculate the fluxes. Granet et al. [2001] introduced an additional node at the intersection in order to calculate the saturation at an intermediate time. They assumed that the transport between an intersection node and a joint node is twice faster than the transport between two joint nodes.

[28] We have found that the MFE method can naturally solve the problem on structured and unstructured grids without a special treatment. Since the MFE formulation provides the pressure traces, the volumetric fluxes can be computed locally (see equation (23)). The remaining aspect of the problem is to define the material flux or the mobility at the intersection node. In other words, what upstream weighting should be considered in case of multiple upstream fracture branches.

[29] Consider an intersection point \( o \) with \( N_I \) connections, where \( I; i = 1, \ldots, N_I \) are the labels of the connected fracture branches (see Figure 4). In each fracture \( I_i \), we denote by \( m_i \) and \( q_i \) the mobility and the

Table 2. Rock and Fluid Properties

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Injection gas, mole fraction</td>
<td>1.0 C_1, 0.0 C_3</td>
</tr>
<tr>
<td>Initial fluid, mole fraction</td>
<td>0.0 C_1, 1.0 C_3</td>
</tr>
<tr>
<td>Pressure, bars</td>
<td>20</td>
</tr>
<tr>
<td>Temperature, K</td>
<td>394</td>
</tr>
<tr>
<td>Porosity, fraction</td>
<td>0.2</td>
</tr>
<tr>
<td>Permeability, mdarcy</td>
<td>10</td>
</tr>
</tbody>
</table>

Figure 5. Methane composition profile (mole fraction) for various grid refinements by the MFE-DG and FD methods, PV injection = 0.7: Example 1. See color version of this figure in the HTML.
volumetric flux at \( o \). We also classify the influx and efflux at \( o \) such that:

\[
q_i > 0 \quad \text{for} \quad 1 \leq i \leq \ell
\]

\[
q_i \leq 0 \quad \text{for} \quad \ell < i \leq N_f
\]  

(27)

where \( \ell \), \( 1 \leq \ell \leq N_f - 1 \). Note that the effluxes are assumed to have positive sign. The material balance at \( o \) assures the existence of \( \ell \). By writing the total volumetric balance and the total material balance for each component we get,

\[
\sum_{i=1}^{\ell} q_i = - \sum_{i=\ell+1}^{N_f} q_i
\]  

(28)

\[
\sum_{i=1}^{\ell} m_i q_i = - \sum_{i=\ell+1}^{N_f} m_o q_i = -m_o \sum_{i=1}^{N_f} q_i
\]  

(29)

where \( m_o \) refers to the mobility at \( o \); it is the upstream mobility for the effluxes. From Equations 28 and 29, \( m_o \) can be readily calculated:

\[
m_o = \frac{\sum_{i=1}^{\ell} m_i q_i}{\sum_{i=1}^{\ell} q_i}
\]  

(30)

The above expression for the mobility at the intersection \( o \) may be considered as a generalization of the classical upstream technique at the intersection of two fractures. If \( N_f = 2 (\ell = 1) \), for example, equation (30) gives \( m_o = m_1 \) which is the classical upstream solution.

6. Numerical Results

[30] The validity of the model was first checked by comparing the results to a commercial FD-based compositional simulator using the implicit saturation explicit pressure (IMPES) option. The simulator uses the conventional, five-point orthogonal Cartesian grid in 2-D. The linear solver in the commercial simulator is the Orthomin preconditioned by ILU. The numerical experiments given below were performed in order to show the three main objectives of this work: First, the DG method introduces low numerical dispersion compared to the FD-based methods. Even with very refined meshes the FD solution may not be as accurate as the DG solution on a coarse mesh. Further, the FD method in such cases could require orders of magnitude more CPU time compared to the DG method. We also compare the discrete fracture model with the single-porosity model. We then present an example in fractured media by using unstructured grids.

[31] All numerical testes are performed by using a binary mixture of methane (C1) and propane (C3). The properties of these species are given in Table 1. The initial pressure, temperature and matrix porosity are given in Table 2. At the production side, the pressure is kept at \( p_D = p_0 \). Different permeabilities and injection rates are used and viscosities are computed by using the correction of Lohrentz et al. [1964]. The direct solver package UMFPACK of Davis and Duff [1999] is used to solve the linear system in equation (21). A simple adaptive time step algorithm is used. It controls the time step by limiting the maximal local variations in pressure and concentrations. All test runs were performed on a 2 GHz Pentium 4 PC.

6.1. Example 1

[32] We consider a homogeneous 2-D horizontal domain of area 40 m \times 40 m. Methane is injected at one corner to displace propane to the opposite producing corner; the domain is initially saturated with propane (see Table 2).
At the production end, the pressure is kept constant. We compare our code to the FD commercial code. In Figure 5 the composition profile of $C_1$ by the FD and MFE-DG codes are shown at nearly 71% PV displacement. The FD solution has a pronounced numerical dispersion compared to the MFE-DG solution with a $40 \times 40$ grid. Even with more refined grids ($80 \times 80$ and $160 \times 160$), the FD result is still very dispersive; the MFE-DG method for a $40 \times 40$ gridding introduces less numerical dispersion than the FD on a $160 \times 160$ grids (Figure 5). The MFE-DG algorithm is 2–3 orders of magnitude faster than the FD method for the same accuracy (see Table 3).

6.2. Example 2

[33] In this example we consider a 2-D vertical heterogeneous domain of $40 \times 40$ m where the gravity effect is taken into account. The medium has two zones of different permeabilities. One zone is nearly impermeable where its permeability is $10^{-7}$ mdarcy (see Figure 6). Elsewhere the permeability is 10 mdarcy. As shown in Figure 6, the results by the MFE-DG and FD methods for the velocity field are very different. Because of the gravity effect ($C_1$ is lighter than $C_3$), $C_1$ does not propagate in the whole domain as in Example 1. The results for methane composition, which are depicted in Figure 7, show that the FD method has a significant numerical dispersion.

6.3. Example 3

[34] The aim of this example is to show the reliability of the MFE method in approximating the velocity field in heterogeneous media. We consider the same system as in Example 1 with the exception that the porous medium is highly heterogeneous with 6 orders of magnitude for the contrast in permeability. The permeability in each block is chosen at random (Figure 8). The composition distribution of $C_1$ and the velocity filed are depicted in Figure 9.

6.4. Example 4

[35] In this example we compare the accuracy and the efficiency of the discrete fracture model and the single-
Figure 10. Methane composition (mole fraction) from the single-porosity and discrete fracture models, fracture thickness $\varepsilon = 10^{-2}$ m and $\varepsilon = 10^{-3}$ m and PV injection = 0.6: Example 4. See color version of this figure in the HTML.

Figure 11. Methane composition (mole fraction) at different PV injections; one and three fractures with diagonal orientation: Example 5. See color version of this figure in the HTML.
Figure 12. Methane composition (mole fraction) at different PV injections; four connected fractures: Example 5. See color version of this figure in the HTML.

Figure 13. Methane composition (mole fraction) at different PV injections; sugar cube configuration: Example 5. See color version of this figure in the HTML.
porosity model both by the combined MFE-DG method. We consider a rectangular horizontal domain of $40 \text{ m} \times 40 \text{ m}$ containing one fracture (the fracture is shown by the thick solid line in Figure 10). The domain is saturated with propane ($C_3$). Methane ($C_1$) is injected at one corner to displace $C_3$ from the opposite corner. The permeability in the matrix and in the fracture is $10 \text{ mdarcy}$ and $10^4 \text{ mdarcy}$, respectively. For two different fracture thicknesses $10^{-2} \text{ m}$ and $10^{-3} \text{ m}$, Figure 10 shows that methane composition by both models is comparable. The results by the single-porosity model could have more numerical dispersion because of the use of small time steps. The 2-D representation of the fracture with the single-porosity model imposes a sever restriction on the time step size. In the first case where the fracture thickness is $10^{-2} \text{ m}$, the CPU times for the discrete fracture model and single-porosity model are, respectively, 45 and 840 s. The gain in CPU time becomes more significant for thinner fractures. In the second case (fracture thickness is $10^{-3} \text{ m}$), the CPU times is 21 seconds for the former and $1.2 \times 10^4$ seconds for the latter. Thinner fracture relaxes the time step limitation in the discrete fracture model, whereas, this has an opposite effect in the single-porosity model.

### 6.5. Example 5

[36] We present results by the MFE-DG method for fractured media. The computational domain is the unit square with dimension $1 \text{ m} \times 1 \text{ m}$. Methane ($C_1$) is injected at one corner to displace propane ($C_3$) to the opposite corner at a constant pressure of 20 bar. The thickness of the fractures is $10^{-2} \text{ m}$. The permeability in the matrix and in the fractures is, respectively, 10 mdarcy and $10^4$ mdarcy. The injection rate is 0.115 PV/day. Several configurations with one, three, four and a sugar cube configuration for the fractures are considered. Figures 11–13 show the results for $C_1$ composition for the different fracture configurations. All the results presented in Figures 11–13 are based on the runs, which we consider smooth and efficient.

### 7. Concluding Remarks

[37] In this work, a robust and efficient numerical approach has been developed for the solution of compressible flow of multicomponent fluids in homogeneous and in fractured porous media. This numerical approach combines the MFE and DG methods. The hybridized MFE method is used to approximate Darcy’s law where the primary unknowns are the pressure traces on the edges. The DG method is used to approximate the flow equations. The numerical method leads to solve a linear system with the size equal to the number of edges in the mesh. The main features of this work can be summarized in three points.

- **1.** The MFE method provides a highly accurate approximation of the velocity field. This method is less mesh dependent than the FD approximation. Thus constraints, such as the strict Delaunay conditions, are not required on the mesh generation which sometimes could be stiff to satisfy especially on complicated geometries like fractured media. With the MFE method, the flux through multiintersecting fractures is accurately approximated without any special treatment in structured and unstructured grids. It should be noted that this approach is independent of the methods chosen to approximate the flow equations or the fluxes in the matrix. Therefore this approach is also useful for other techniques that are based on finite difference or finite volume methods.

- **2.** This work shows the applicability of the DG method in approximating compressible, multicomponent fluid flow in homogeneous and fractured media. The DG method has superiority to capture shocks or sharp gradients in the solution without creating spurious oscillations or excessive numerical dispersion. Comparisons with a FD-based commercial software showed that the combined MFE-DG method becomes 2–3 orders of magnitude more efficient than the FD method for comparable accuracy in the solution.

- **3.** The discrete fracture concept is a powerful concept for application to connected or disconnected fractures. The geometrical simplification of the fractures significantly reduces the CPU and memory requirements.

### Appendix A

[38] In this appendix we provide details of the MFE approximation, which is based on the Raviart-Thomas space. The hybridized mixed finite element uses as unknowns the cell pressure averages, the edge pressure averages and the interelement fluxes. We use the Raviart-Thomas space of lowest order. The main objective is to express the velocity over each cell with respect to the fluxes across the edges. Consider the reference element $K$ as depicted in Figure A1. The element edges $E$ and the corresponding exterior normals $n$ appear also in Figure A1. The Raviart-Thomas ($RT_0$) basis functions on $K$ are defined by

$$w_{E_1} = \left( \frac{u}{v - 1} \right) ; \quad w_{E_2} = \left( \frac{u - 1}{v} \right) ; \quad w_{E_3} = \left( \frac{u}{v} \right)$$  \hspace{1cm} (A1)
The patterns of these vector fields are shown in Figure A1. One can readily verify that these vector fields are linearly independent and that they satisfy the following properties:

\[ \nabla w_E = \frac{1}{|K|} \]

(A2)

\[ w_{K,n_E} = \begin{cases} 
1/|E| & \text{if } E = E' \\
0 & \text{if } E \neq E'. 
\end{cases} \]

(A3)

The lowest-order Raviart-Thomas space \( RT_{0,K} \) over \( K \) is the functional space generated by \( w_E; i = 1, \ldots, 3 \). Thus any vector \( \chi_K \in RT_{0,K} \) can be written with respect to the basis functions equation (A1) as

\[ \chi_K = \sum_{E \in \partial K} q_{K,E} w_E \]

(A4)

where \( \partial E = \{ E_1, E_2, E_3 \} \).

From Equations A2 and A3, one can readily check that

\[ \int_E \chi_K \cdot n_E = q_{K,E} \]

By inverting the mobility tensor \( K \), Darcy’s equation becomes

\[ K^{-1} \partial = - (\nabla p - \rho g) \]

(A6)

Multiplying equation (A6) by the test function \( w_{K,E} \) and integrating by parts yield

\[ \int_K w_{K,E} K^{-1} \partial = \int_K w_{K,E} (\nabla p - \rho g) \]

\[ = \int_K w_{K,E} \nabla p + \int_K p w_{K,E} g \]

\[ = \int_K p \nabla w_{K,E} - \int_{\partial K} p w_{K,E} n_E \]

\[ + \int_K p w_{K,E} g \quad E \in \partial K \]

(A7)

The integral terms in the right-hand side of equation (A7) are simplified as

\[ \int_K p \nabla \cdot w_{K,E} = \frac{1}{|K|} \int_K p \]

and

\[ \int_{\partial K} p w_{K,E} n_E = \sum_{E \in \partial K} \frac{1}{|E|} \int_E p \]

\[ q_{K,E} = \frac{1}{|E|} \int_E p \]

\[ = \frac{1}{|E|} \int_E p + \int_{\partial K} p w_{K,E} g \quad E \in \partial K \]

(A8)

Replace equation (A1) in equation (A8) to get

\[ \sum_{E \in \partial K} q_{K,E} w_{K,E} = p_K - \eta_{K,E} \]

(A9)

Equation (A9) can be written in matrix form

\[ B_K q_K = p_K - \eta_{K,E} \]

(A10)

where,

\[ B_K = \left[ (B_{E,E'})_{E,E'} \right]_{E \in \partial K} \quad (B_{E,E'})_{E,E'} = \int_K w_{K,E} w_{K,E'} \]

\[ \eta_{K,E} = \left[ \eta_{K,E} \right]_{E \in \partial K} \quad \eta_{K,E} = \int_{\partial K} p w_{K,E} g \]

By inverting \( B_K \), equation (A10) becomes

\[ Q_K = p_K B_K^{-1} - B_K^{-1} \eta_{K,E} \]

(A11)

Thus equation (A11) expresses the fluxes \( q_{K,E} \) through each edge \( E \) as a function of the cell pressure average \( p_K \) and the edge pressure averages \( \eta_{K,E} \), i.e.,

\[ q_{K,E} = \alpha_{K,E} p_K - \sum_{E \in \partial K} (B_{E,E'})_{E,E'} \] \( p_{K,E'} - \beta_{K,E} \]

(E \in \partial K) \]

(A12)

where,

\[ \alpha_{K,E} = \sum_{E \in \partial K} (B_{E,E'})_{E,E'} \quad \text{and} \quad \beta_{K,E} = - \rho_K \sum_{E \in \partial K} (B_{E,E'})_{E,E'} \]

Appendix B

[43] In this appendix, we give details of the slope limiter usually needed to stabilize the DG scheme. We start by the one dimensional space.

B1. Slope Limiter in 1-D Geometry

[44] Let us denote the points and the discretized elements of the 1-D domain by \( \ldots < x_i < x_{i+1} < \ldots \) and by \( K_j = (x_i, x_{i+1}) \). The DG method seeks to approximate the state
variable (say the overall composition \( c \)) in a discontinuous finite element space. Over each element \( K \), \( c \) is approximated by

\[
c(x, t) = c(x, t)|_K = \sum_{j=1}^{i+1} c_{K,j} \varphi_j
\]

where, \( \varphi_j \) are the standard finite element shape functions and \( c_{K,j} \) are the nodal values of \( c \) on the boundaries of \( K \). Note that this approximation allows a discontinuity of \( c \) at the interfaces between elements. The DG method leads sometimes to nonphysical oscillation at the nodal values of \( c \); in this case the slope limiter is essential to stabilize the method.

[45] The basic idea of the slope limiter is to impose some constraints in a geometric manner so that the reconstructed solution satisfies an appropriate maximum principle. This procedure aims to eliminate local maxima or minima from the solution.

[46] Let \( \bar{\tau}_K \) be the cell average over a 1-D element \( K \):

\[
\bar{\tau}_K = \frac{1}{|K|} \int_K c(x) = \frac{1}{2} (c_{K,j} + c_{K,j+1})
\]

The reconstructed nodal values \( (c_{K,j}, c_{K,j+1}) \) of \( (c_{K,j}, c_{K,j+1}) \) should satisfy the following conditions: (1) conservation of mass balance \( c_{K,j} + c_{K,j+1} = c_{K,j} + c_{K,j+1} \), (2) avoidance in creating local extrema

\[
\min\{\bar{\tau}_{K-1}, \bar{\tau}_K\} \leq c_{K,j} \leq \max\{\bar{\tau}_{K-1}, \bar{\tau}_K\}
\]

\[
\min\{\bar{\tau}_K, \bar{\tau}_{K+1}\} \leq c_{K,j+1} \leq \max\{\bar{\tau}_K, \bar{\tau}_{K+1}\}
\]

and (3) minimum modification of \( (c_{K,j}, c_{K,j+1}) \), i.e.,

\[
\| (c_{K,j}, c_{K,j+1}) - (c_{K,j}, c_{K,j+1}) \|_2
\]

is minimal. Therefore the slope limiter process is reduced to a minimization problem. In Figure B1 we see local maximum and minimum at the boundaries of \( K \) (before limiting). The data is reconstructed (after limiting) so that we eliminate these extrema by keeping the same material in the cell. Note that one may use a constant approximation of \( c \) over each cell (i.e., \( \bar{\tau}_K = c_{K,j} = c_{K,j+1} \)). In this case, the scheme is reduced to the first-order upstream finite difference method.

### B2. Slope Limiter in Multidimensional Space

[47] The extension of the slope limiter to the multidimensional space is formulated in such a way that in each cell \( K \), each state variable at a vertex \( j \) lies between the cell averages of all neighboring elements containing \( i \) as a vertex (Figure B2). We define the notation

\[
\bar{\tau}_{\min,i} = \min\{\bar{\tau}_K|i \text{ is a vertex of } K\}
\]

\[
\bar{\tau}_{\max,i} = \max\{\bar{\tau}_K|i \text{ is a vertex of } K\}
\]

Then, the generalization of the slope limiter to multidimensional space seeks to solve the minimization problem:

\[
\min_{\bar{\tau}_K} \| C_K - C_K \|_2,
\]

subject to the linear constraints

**Mass conservation**

\[
\bar{\tau}_K = \frac{1}{|K|} \int_K c_j \ dx
\]

Avoiding local extrema

\[
\bar{\tau}_{\min,i} \leq \bar{\tau}_{\max,i} \leq \bar{\tau}_{\max,i} \quad i = 1, \ldots, N_e.
\]

Note that this minimization problem can be solved readily. For details on this slope limiter, we refer to Hoteit et al. [2004b].

[48] Acknowledgment. This work was supported by the member companies of the Reservoir Engineering Research Institute (RERI) and the U.S. DOE (grant DI-FG26-99BC15177).

**References**


A. Firoozabadi and H. Hoteit, Reservoir Engineering Research Institute, 385 Sherman Avenue, Suite 5, Palo Alto, CA 94306, USA. (af@rerinst.org; hoteiti@rerinst.org)