Compositional Modeling by the Combined Discontinuous Galerkin and Mixed Methods

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Summary
In this work, we present a numerical procedure that combines the mixed finite-element (MFE) and the discontinuous Galerkin (DG) methods. This numerical scheme is used to solve the highly nonlinear coupled equations that describe the flow processes in homogeneous and heterogeneous media with mass transfer between the phases. The MFE method is used to approximate the phase velocity based on the pressure (more precisely average pressure) at the interface between the nodes. This approach conserves the mass locally at the element level and guarantees the continuity of the total flux across the interfaces. The DG method is used to solve the mass-balance equations, which are generally convection-dominated. The DG method associated with suitable slope limiters can capture sharp gradients in the solution without creating spurious oscillations. We present several numerical examples in homogeneous and heterogeneous media that demonstrate the superiority of our method to the finite-difference (FD) approach. Our proposed MFE-DG method becomes orders of magnitude faster than the FD method for a desired accuracy in 2D.

Introduction
There has been gradual progress in the development of algorithms for the compositional simulation of hydrocarbon reservoirs in the last 15 years. Before that, there were several major advances in the numerical solution of the combined flow equations and the thermodynamic equilibrium with the equations of state. Despite the advances of the last 25 to 30 years and the enormous progress in the speed of computers in the same period, we cannot yet perform field-scale compositional modeling satisfactorily in heterogeneous reservoirs. The main problem is the continued use of the FD discretization scheme and its inherent limitations. Most of the current compositional simulators use the upstream weighted FD method to approximate the flow equations. Because of the fact that the flow processes are usually convection-dominated, FD methods may produce significant numerical diffusion (Coats 1980). The excessive numerical diffusion requires unrealistic gridding, especially with heterogeneities.

Recently, the DG methods have been successfully implemented to approximate various physical problems, notably hyperbolic systems of conservative laws. One property of these methods is that they conserve mass at the element level in a finite-element framework. Consequently, they enhance the flexibility of finite elements in describing flow in complicated geometries. Furthermore, the choice of the spatial approximation without the continuity across inter-element boundaries allows a simple treatment of combined finite-element cells with different geometries as well as different degrees of approximating polynomials. These methods associated with suitable slope limiters can capture discontinuities or sharp gradients in the solution. The DG method was first implemented for nonlinear scalar conservative laws by Chavent and Salzano (1982). However, these authors noted that a very restrictive timestep should be used to keep stability of the scheme. Later, Chavent and Cockburn (1989) introduced the slope limiter idea following the work of Van Leer (1978). In 1D, the modified scheme proved to be the total variation diminishing (TVD) under a fixed Courant-Friedricks-Levy (CFL) condition. Another class of DG methods such as the Runge-Kutta Discontinuous Galerkin (RKDG) was developed by Cockburn and Shu (1989, 1998). The RKDG method is an extension of the DG method to higher temporal and spatial approximation spaces. Recent developments have extended the DG method to approximate elliptic, diffusion, and convection-diffusion problems (Chen et al. 1995, Riviere et al. 1999, Oden et al. 1998). These methods have also been successfully implemented to approximate physical problems in aerodynamics, Navier-Stokes equations, and flow and transport in porous media.

To the best of our knowledge, the DG method has not been yet implemented in compositional modeling. In this work, we use the DG method to approximate the nonlinear equations describing the species balance. When using constant approximation functions (shape functions), the numerical diffusion caused by upwinding is high enough to keep the scheme stable; in structured grids we get a FD scheme, and in unstructured grids, we get a finite volume (FV) scheme. The use of high-order approximation spaces produces nonphysical oscillations near the shocks. In such a case, the use of an appropriate slope limiter ensures the stability of the method. Our scheme is stabilized by using the multidimensional slope limiter introduced by Hoteit et al. (2004), which is an improved version of that used by Chavent and Jaffré (1986).

Other high-order upwind schemes such as TVD, essentially nonoscillatory (ENO), and weighted-ENO schemes have been used for two-phase multicomponent flow (Mallison et al. 2003, Thiele and Edwards 2001). However, these methods are, generally, limited to 1D space problems. In multidimensional streamline based models, these methods are used to approximate the 1D solution along the streamlines (Douglas et al. 1983). Our proposed algorithm in this work is intended for multidimensional space in both structured and unstructured grids.

The accuracy of the velocity field (that is, the flux calculation) at the interface between the nodes is a key element in the numerical simulation of transport processes. In classical finite-element (FE), FV, and FD methods, the nodal pressures (in FE) and average element pressures (in FD and FV) are approximated first, and then the flux is calculated by local derivatives. This widely used approach for the calculation of the flux in two-phase flow may not be accurate, especially in heterogeneous media, because of pronounced change of pressure gradient across the physical interface. A key solution is to use the MFE method to approximate interface fluxes from Darcy’s law (Raviart and Thomas 1977). The main features for this choice include the fact that the pressure and the fluxes are approximated simultaneously with the same order of convergence; furthermore, the method is locally conservative and can readily accommodate the full permeability tensor. The MFE method is more accurate in flux calculation than the FV and FE methods (Mosé et al. 1994, Durlofsky 1994). In our MFE formulation, we use the lowest-order Raviart-Thomas space (Brezzi and Fortin 1991). The original MFE formulation leads to a saddle-point problem where the primary unknowns are the cell pressure averages and the fluxes across the interfaces. A remedy is to use a hybridization technique (Chavent and Roberts 1991, Ewing and Heinemann 1983) where new degrees of freedom are appended at the element edges. The additional unknowns, which become the
primary unknowns, represent the edge pressure averages (pressure traces). It has been shown that, by using a lumped-mass technique to approximate some integrals, the MFE formulation, on rectangular elements, becomes the same as the classical cell-centered FD method (Russell and Wheeler 1983). However, this approach is limited to structured rectangular gridings and isotropic media. Our formulation is based on analytical calculations of all integrals without restrictions on the discretized elements. In order to use the MFE method in two-phase flow to solve the pressure equation, we introduce the concept of the total velocity following the work of various authors (Durlufsky and Chien 1993, Chen and Ewing 1997a, Chen and Ewing 1997b). This formulation ensures the mass conservation for each component.

The combination of the DG and MFE methods has been implemented by many authors. Chavent et al. (1990) used these methods to solve two-phase, immiscible fluid flow problems. The combined methods were used to solve convection-diffusion equations by Siegel et al. (1997). Bues and Oltean (2000) combined these methods to solve incompressible, single-phase flow in porous media, where they varied the density as a function of concentration. Hoteit and Firoozabadi (2005) combined the DG and MFE methods to approximate single-phase flow of compressible and multicomponent fluid in fractured media. To the best of our knowledge, the combined MEF-DG method has not been implemented in the literature for two-phase, compressible, and multicomponent fluid flow in porous media.

This paper is organized as follows: First, the differential and algebraic equations describing the displacement of two-phase compositional flow are presented. Second, we describe the numerical model that combines the MFE and DG methods. We use the MFE method to approximate Darcy’s law and the pressure equation and the DG method to approximate the species flow equation. In this work, we ignore the capillary pressure and the physical diffusion. Finally, we present numerical examples in homogeneous and heterogeneous media to demonstrate the efficiency and robustness of our numerical approach.

Governing Equations

The governing system describing the two-phase (gas and oil) flow of an $n_c$-component mixture is given by the component balance equations, and the thermodynamic equilibrium between the phases (as stated previously, in this work we neglect capillary pressure and diffusion processes).

The material balance for each component in the two phases can be expressed as

$$\frac{\partial c_{i,c}^e}{\partial t} + \nabla \cdot U_i = 0, \quad i = 1, \ldots, n_c.$$  \hspace{1cm} (1)

where $U_i = (c_{i,x_i} \bar{u}_i + c_{i,x_{io}} \bar{u}_{io})$. The compositions $c_{i}$, $x_{i}$, and $x_{io}$ are constrained by

$$\sum_{i=1}^{n_c} z_i = \sum_{i=1}^{n_c} x_i = \sum_{i=1}^{n_c} x_{io} = 1.$$  \hspace{1cm} (2)

In the previous equations, $\phi$ denotes the porosity, $c$ is the overall molar density, $g$ and $o$ refer to gas and oil phases, $i$ is the component index, $z_i$ is the overall mole fraction of component $i$, $x_{i}$ is the mole fraction of component $i$ in phase $\alpha$ ($\alpha = g, o$), and $c_{i}$ is the molar density of phase $\alpha$. Other variables are $U_i$, the molar flux of component $i$; $\bar{u}_i$ is the phase velocity.

The velocity for each phase is given by the Darcy law

$$\bar{u}_i = \frac{k k_{\alpha}}{\mu_{\alpha}} (\nabla p - \rho_{\alpha} g), \quad \alpha = g, o.$$  \hspace{1cm} (3)

where $k$ is the absolute permeability of the porous medium, $k_{\alpha}$, $\mu_{\alpha}$, and $\rho_{\alpha}$ are the relative permeability, viscosity, and mass density of phase $\alpha$ respectively; $p$ denotes the pressure and $g$ the gravitational vector.

Based on the concept of volume balance, one can obtain the pressure equation (Ács et al. 1985, Watts 1986):

$$\phi \frac{\partial p}{\partial t} + \sum_{i=1}^{n_c} \nabla \cdot U_i = 0, \quad \text{subject to} \quad \nabla \cdot \bar{u}_i = 0.$$  \hspace{1cm} (4)

where $c_j$ is the total fluid compressibility and $\bar{p}_j$ is the total partial molar volume for component $i$.

Neglecting the capillary pressure simplifies the pressure equation and reduces the coupling between the pressure and the species balance equations. We like to mention here that in certain applications such as immiscible gas injection and water injection in heterogeneous and fractured porous media, one has to account for capillary pressure. On the other hand, physical diffusion and dispersion can be much more important than capillary pressure in some applications such as gas injection in fractured reservoirs. Both capillary pressure and physical diffusion will be considered in our future work for the applications in which these mechanisms are important.

Thermodynamic equilibrium is assumed between the fluid phases. The equilibrium implies the equality of the fugacities of each component in the two phases:

$$f_{\alpha}(T, p, x_{\alpha}; i = 1, \ldots, n_c - 1) = f_{\alpha}(T, p, x_{g,i=1}^{\alpha'}, \ldots, n_c) i = 1, \ldots, n_c.$$  \hspace{1cm} (5)

Numerical Model

The numerical procedure proposed in this work is based on the MFE method for the pressure equation and the DG method for the mass-balance equations.

The computational domain is discretized into a grid consisting of triangles and/or quadrilaterals. No restrictions are imposed on the geometrical shape of the elements. In this paper, we present results using rectangles. In works in progress, triangles are being used for the spatial discretization. The following notations are defined: $K$ is the discretized element or cell, $E$ is the edge of cell $K$, $N_e$ is the number of edges for each cell ($N_e = 3$ or $4$), $N_E$ is the number of cells in a mesh, and $N_E$ is the number of edges in a mesh.

Solution of the Pressure Equation.

The basic idea of the MFE method is to approximate simultaneously the pressure and its gradient. In order to apply the MFE method to solve the pressure Eq. 4 and Darcy’s velocities from Eq. 3, we introduce the total velocity term, that is, the sum of gas and oil velocities (Durlufsky and Chien 1993).

Total Velocity. The total velocity, $\bar{u}_t$, is defined as

$$\bar{u}_t = \sum_{\alpha = g, o} \bar{u}_\alpha = \sum_{\alpha = g, o} K_\alpha (\nabla p - \rho_\alpha g),$$  \hspace{1cm} (6)

where $K_\alpha = k_k_k_{\alpha}/\mu_\alpha$ is the mobility of phase $\alpha$.

In a more compact form, Eq. 6 becomes

$$\bar{u}_t = -K (\nabla p - \rho g).$$  \hspace{1cm} (7)

where

$$K = (K_g + K_o)$$

and $\rho = (K_{o,\rho} + K_{g,\rho})/(K_{o,\rho} + K_{g,\rho})$.

Note that $\rho$ is independent of the absolute permeability, $k$.

From Eq. 7, we can write

$$\nabla p = -K^{-1} \bar{u}_t + \rho g.$$  \hspace{1cm} (8)

Substituting Eq. 8 into Eq. 3, we express the phase velocity $\bar{u}_\alpha$ in terms of total velocity $\bar{u}_t$ independent of $\nabla p$.

$$\bar{u}_\alpha = \lambda_\alpha (\bar{u}_t - G_{\alpha}),$$  \hspace{1cm} (9)

where

$$\lambda_\alpha = K_{\alpha}/K,$$

and $G_{\alpha} = \begin{cases} K_{g,\rho}(p - \rho_\alpha)g, & \alpha = g \\ K_{o,\rho}(p - \rho_\alpha)g, & \alpha = o \end{cases}$

Approximation of the Total Velocity.

The total velocity field is approximated in the so-called Raviart-Thomas space of the lowest order ($RT_0$). In each cell $K$, the total velocity can be expressed with respect to the normal flux $q_{K,\alpha}$ across the cell edges $E$:
\[ \vartheta = \sum_{E=K} q_{K,E} w_{K,E} \]  

where \( w_{K,E} \) is the RT basis function with continuous normal component across each cell edge \( E \).

Multiplying Eq. 9 by \( w_{K,E} \) and integrating by parts, then the total flux \( q_{K,E} \) is expressed through each edge \( E \) as a function of the cell pressure average \( p_K \) and the edge pressure average \( p_{K,E} \) for each cell \( K \):

\[ q_{K,E} = \theta_{K,E} p_K = \sum_{E=K} (B_{K,E} \cdot w_{K,E} - \gamma_{K,E}) \quad E \in \delta K, \ldots \]  

where \( \theta_{K,E}, B_{K,E}, \gamma_{K,E} \) are the coefficients that depend on the geometrical shape of the element and the local mobility characteristic. For more details on the formulation of Eq. 9, one may refer to Chavent and Roberts (1991) and Hoteit et al. (2002).

By imposing the flux continuity across the cell interfaces, \( (q_{K,E} = q_{K,E}^{E=E=K'=K}) \), the flux unknown can be eliminated from Eq. 11. As a result, the following linear system with main unknowns; the cell average pressures \( P \) and the edge average pressures \( T_p \) is obtained:

\[ R^TP - MT_P = I, \ldots \]  

where \( M \) is a sparse square matrix of dimension \( N_K \), \( R \) is a sparse \( N_K \times N_E \) rectangular matrix, and \( I \) is a vector of dimension \( N_K \).

**Approximation of the Pressure Equation.** Replacing the phase velocity \( \vartheta \), in Eq. 4 (see also Eq. 1) by its expression given in Eq. 9, the pressure equation becomes

\[ \Phi_{E} \frac{\partial p}{\partial t} + \sum_{i=1}^{n} \nabla_{K} m_i \cdot \delta_{x} = 0, \ldots \]  

where \( m_i = \sum_{a,o,g} c_{a,o,g} x_{a} \lambda_{a} s_i = \sum_{a,o,g} c_{a,o,g} x_{a} \lambda_{a} G_{a,o,g} \).

Integration of Eq. 13 over each cell \( K \) and the use of the divergence theorem yields

\[ \Phi_{K,E} \frac{\partial p_{K,E}}{\partial t} = \sum_{E=K} \nabla_{E} (m_{K} s), \ldots \]  

where \( n \) is the outward unit normal to the cell boundary \( \delta K \), \( \Phi_{K,E} \), and \( p_{K,E} \) are the average values of \( \Phi, \partial_{x}, \) and \( p \) in cell \( K \), respectively. In the scope of this work, the pressure is a smooth function of space and there is no need to consider higher-order spatial approximation of the composition and densities in the pressure equation. The coefficients \( e_{K}, m_{K}, s_{K} \) and \( \nabla \), are, therefore, evaluated at the cell centers. However, using higher-order spatial approximation of the composition is expected to reduce the numerical diffusion in the species balance equations at the expense of simplicity.

Because the total fluid compressibility coefficient \( e_{K} \) in Eq. 14 is outside the time derivative, the local conservation of the method at the cell level is not guaranteed. However, this should not cause a numerical deficiency, because the pressure and velocity calculations have no effect on the material balance in the species flow equations, which is always conserved at the element level thanks to the DG method. Note that other numerical methods such as FV or FD may have a similar conservation problem in solving Eq. 13.

The MFE method of lowest order supports a constant approximation of the flux along each cell interface; for each cell \( K \), the flux \( q_{K,E} \) across edge \( E \) is

\[ q_{K,E} = E| \delta_{K} n_{E} | \]  

Using Eqs. 15 and 11 in Eq. 14, the flux unknown can be eliminated to obtain an expression in terms of the pressures. By applying the Euler backward scheme to discretize the time operator and considering all the coefficients explicitly in time, we obtain a second linear system in terms of the cell average pressures \( P \) and the edge average pressures \( T_p \):

\[ D P - \bar{R}T_p = G, \ldots \]  

In this equation, \( D \) is a square diagonal matrix of dimension \( N_K \), \( \bar{R} \) is a sparse \( N_K \times N_E \) rectangular matrix, and \( G \) is a vector of dimension \( N_K \).

Combining systems in Eqs. 12 and 16, one obtains

\[ \begin{pmatrix} D & \bar{R} \\ -M & I \end{pmatrix} \begin{pmatrix} P \\ T_p \end{pmatrix} = \begin{pmatrix} G \\ I \end{pmatrix}, \ldots \]  

Because \( D \) is a diagonal matrix, the Schur complement matrix is readily computed to have the final linear system in which the pressure traces are the primary unknowns.

\[ (M - RD^{-1}\bar{R}T_p = RD^{-1}G - I, \ldots \]  

After calculating \( T_p \), the cell pressure average, the flux can be computed locally through Eqs. 16 and 11.

**Solution of the Material Balance Equations.** The DG method is used to discretize the species balance equations from Eq. 1. The method consists of a discontinuous, piecewise, linear (on triangles), or bilinear (on quadrilaterals) approximation of the unknowns \( c_{K,E} \). By using constant approximation over the cells, the DG method reduces to the first-order cell-centered finite volume method.

For the sake of simplicity, we only describe the implementation of the DG method to the equation obtained by summing Eq. 1 over the species and using the constraints given by Eq. 2:

\[ \Phi \frac{\partial c}{\partial t} + \nabla \left( \sum_{a,o,g} c_{a,o,g} \partial_{x} n \right) = 0, \ldots \]  

Over each cell \( K \) the unknown \( K \) is approximated in a discontinuous finite element space, so that

\[ c_{K} = \sum_{j=1}^{N} c_{K,j} \varphi_{K,j}, \ldots \]  

where \( \varphi_{K,j} \) is the classical bilinear finite element space function. Multiplying Eq. 19 by the test function \( \varphi_{K,E} \) and integrating by parts yields

\[ \begin{aligned} \Phi_{K} \int_{K} \frac{\partial c_{K}}{\partial t} \varphi_{K,E} = & - \int_{K} \sum_{a,o,g} c_{K,a} \partial_{x} \nabla \varphi_{K,E} \\ & + \int_{K} \sum_{j_{out}} c_{K,a}^{j_{out}} \varphi_{K,E} \partial_{x} n = 0, \ell = 1, \ldots, N_{E}, \end{aligned} \ldots \]  

where the superscript “in/out” denotes the upstream values, which are used to calculate the upstream weighted numerical fluxes. Depending on the incoming or outgoing fluxes with respect to a cell \( K \),

\[ c_{K,\ell}^{j_{in}} = \begin{cases} c_{K,a}^{j_{in}}, & \text{if} \quad \vartheta_{n} n \geq 0, \\ c_{K,a}^{j_{out}}, & \text{otherwise.} \end{cases} \]  

The local system of Eq. 21 allows us to calculate the nodal values \( c_{K,E} \) \( j = 1, \ldots, N_{E} \). Because the solution may have nonphysical oscillations, a reconstruction step is required for the scheme stability.

**Data Reconstruction by Slope Limiter.** It is widely known that with a variable approximation, the DG method becomes unstable. The use of an appropriate slope limiter avoids overshoots and undershoots in the solution. Such a slope limiter is the one introduced by Chavent and Jaffré (1986), which can be interpreted as a generalization of the Van Leer MUSCL 1D slope limiter (1978). The basic idea is to impose 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. The slope limiter from Van Leer was later modified by Hoteit et al. (2004). They found that limiting the state edge average is more appropriate than limiting the nodal values as proposed by Chavent and Jaffrè. This modification improved the slope limiter in eliminating spurious oscillation and reduced the numerical diffusion. Further details on slope limiters are given in the Appendix.

Algorithm. The coupling between the pressure and the mass-balance equations is performed through an implicit pressure and explicit overall compositions procedure. The pressure equation is approximated by the MFE method implicitly in time with the coefficients evaluated from the previous timestep. The mass-balance equations are solved explicitly by the DG method. The principal steps of the combined MFE-DG algorithm are as follows:

1. For a given temperature, pressure, and overall composition, the pressure equation is first performed to determine whether the system is in single phase or in dual phase. If in dual phase, flash calculations are performed. This step provides partial molar volumes in single and in dual phase, phase composition if in dual phase, two-phase compressibility (Wong et al. 1990), and other relevant parameters. We use the Peng-Robinson equation of state (1976) (PR-EOS) in our phase and volumetric calculations.

2. Based on phase composition, pressure, and temperature, mass viscosity is calculated by the methodology of Lohrenz et al. (1964).

3. The pressure equation is solved by the MFE method. In this step, the average pressure across the interfaces (the pressure traces) is calculated globally from Eq. 18.

4. The DG method is used to calculate \( c_{zi,i} = 1, \ldots, n_f \) from the mass balance equations. Then \( c_{zi,i} = 1, \ldots, n_f \) are reconstructed by the slope limiter procedure.

5. The previous steps are repeated until a predetermined time is reached.

Numerical Results

We have extensively tested the algorithm described in the preceding section. In the following, we present some of our results for binary and six-component mixtures for homogeneous and heterogeneous media in 1D and 2D. Linear relative permeabilities are used in all examples except for Example 3, where the relative permeability is a quadratic function of the saturation. The fluid mixtures with only two to three components reveal the essence of the advances in a simple way. All the results are for structured grids. Results for unstructured grids will be presented in a forthcoming publication. Even in a structured grid, the proposed algorithm is far superior to the FD schemes, as we will see shortly. A commercial FD simulator was used to compare with our results from the combined MFE-DG methods. The simulator uses the conventional, five-point orthogonal Cartesian grid in 2D with the implicit pressure explicit saturation (IMPES) option. The linear solver in the commercial simulator is the Orthomin preconditioned by ILU. Because DG formulation is explicit in time, the timestep is restricted to a CFL condition. We used a simple adaptive timestep algorithm that controls the timestep by limiting the maximal local variations in pressure and concentrations. All runs were executed on a 2.4GHz PC-Pentium 4.

1D Problems. The 1D porous medium is 50 m in length for Examples 1 and 2 with a unit sectional area. The length is 1 m in Example 3. The porosity and permeability are 20% and 10 md, respectively. Constant volumetric flow rate is used in the injection end. At the production end, the pressure is kept constant; it is equal to initial pressure. Three examples are presented for two-, three-, and six-component mixtures.

Example 1. In this example, we inject \( C_1 \) at one end in order to displace \( C_3 \) to the other end. Initially, the domain is saturated with \( C_3 \). The data for this example are given in Table 1. In Example 1a, the initial pressure and temperature are \( p = 50 \text{ bar} \) and \( T = 397 \text{ K} \), respectively. The injection rate is \( 0.017 \text{ PV/D} \).

Fig. 1 shows the results in terms of the composition of methane vs. the distance from the injection point. The reference solution is obtained by 500 nodes in the combined MFE-DG methods, where a shock is firmly predicted. Fig. 1 reveals that the combined MFE-DG method has low numerical diffusion compared to the reference solution. The results also show that the FD scheme has a substantial numerical diffusion which decreases as the number of nodes increases. The results with the FD method with 500 nodes and the MFE-DG method with 100 nodes are comparable. The average timesteps used by the FD simulator on the grids of 50, 100, and 500 nodes are approximately 0.30, 0.18, and 0.04 days, respectively. The average timestep used by the MFE-DG method on the grids of 50 and 100 nodes are approximately 0.18 and 0.10 days, respectively. By changing the pressure and temperature to \( p = 69 \text{ bar} \) and \( T = 311 \text{ K} \) (Example 1b), a two-phase region appears. Fig. 2 shows two shocks for the two-phase example. As with Example 1a, the 500-node FD solution and the 100-node MFE-DG solution are comparable. Tables 2 and 3 show the CPU time performance of Examples 1a and 1b. Because the results of the FD scheme with 500 nodes and the MFE-DG method with 100 nodes are comparable, then for this particular example, the latter is four times faster than the former. Note that for the same number of nodes, the MFE-DG method is slower than the FD method, partly because of the additional pressure calculation at the interfaces.

Example 2. We consider the displacement of a binary liquid mixture of \( C_2/C_3 \) by a gas mixture of \( C_1/C_3 \). The injection gas, composed of 90% of \( C_1 \) and 10% of \( C_3 \), is injected at a rate of 0.017 PV/D. The fluid and rock properties for this example are given in Table 1. Fig. 3 shows the phase-behavior data of the ternary mixture \( C_1/C_2/C_3 \) at the initial pressure (also the outlet pressure) and temperature conditions (Table 4). Line AB joins the points of the initial injected gas and domain liquid compositions crossing the two-phase region. A two-phase region is thus expected to appear in the solution after certain injection. The composition profiles of methane and propane in oil and gas phases are depicted in Figs. 4 and 5 after injecting nearly 51% of the pore volume. The reference solution is obtained by the MFE-DG method with 500 nodes. The CPU time is shown in Table 5. It appears that the FD code is two to three times faster than the MFE-DG solution if the same number of nodes is considered. However, the FD solution shows significant numerical diffusion compared to the MFE-DG solution. If comparable accuracy is desired, the MFE-DG method becomes nearly five times more efficient than the DF method.

Example 3. In this six-component problem, \( CO_2 \) is injected to displace the \( C_1/C_2/C_3/C_4/C_{10}/C_{20} \) liquid mixture. The fluid and rock properties for this example are given in Table 4. Two initial pressures, 110 and 191 bar, are considered. With \( n = 110 \text{ bar} \) (Example 3a), the solution is composed of several propagating shocks. These shocks appear in the K-values (Fig. 6), which are plotted at PV injection = 0.66. In Fig. 7, the gas saturation is plotted for various grid refinements by the MFE-DG and FD methods. The reference solution is obtained by the MFE-DG method with 500 nodes. All shocks are captured with 2,000 nodes in the FD method. Results for \( C_{14}, C_{2}, \) and \( C_1 \) are plotted in Fig. 8. By increasing the initial pressure \( (p = 191 \text{ bar}, \text{Example 3b}) \), two shocks appear in the solution. The gas saturation and mole fractions of \( CO_2 \) and \( C_{20} \) are depicted in Fig. 9. Compared with the reference solution that is obtained with 200 nodes by the MFE-DG method, the results by

<table>
<thead>
<tr>
<th>TABLE 1—RELEVANT DATA FOR EXAMPLE 1</th>
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<tbody>
<tr>
<td>Injection gas (mole frac.)</td>
</tr>
<tr>
<td>Initial fluid (mole frac.)</td>
</tr>
<tr>
<td>Pressure (bar)</td>
</tr>
<tr>
<td>Temperature (K)</td>
</tr>
<tr>
<td>Porosity (fraction)</td>
</tr>
<tr>
<td>Permeability (md)</td>
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<tr>
<td>Relative permeability</td>
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the FD method introduce significant numerical diffusion. Thiele and Edwards (2001) have assumed constant K-values and constant velocity using the same composition as we used in this example. These authors used a higher-order Godunov method. Their results are somewhat different from those in Figs. 7 and 8 because of these assumptions.

2D Homogeneous Problem. Example 4. We consider a homogeneous 2D horizontal domain of area 50×50 m². Methane is injected at one corner to displace propane to the opposite producing corner; the domain is initially saturated with propane (see Table 7). At the production well, the pressure is kept constant. As with the 1D examples given previously, we compare our code to the FD commercial code. In Fig. 10, the composition profile of C by the FD and MFE-DG codes are shown at nearly 29, 58, and 73% PV displacements. The gridding is fixed in this example. The FD solution has a pronounced numerical diffusion compared to the MFE-DG solution. Even with more refined grids (80×80, 160×160, and 200×200), the FD result is still very diffusive; the MFE-DG method for a 40×40 gridding introduces less numerical diffusion than the FDM on a 200×200 grid (see Figs. 10 and 11). The MFE-DG algorithm is two to three orders of magnitude faster than the FDM for the same accuracy (see Table 8).

2D Heterogeneous Problem. Example 5. We consider the same mixture as in Example 4. The porous medium, in this example, is
a 2D horizontal domain of area 50×20 m². Two zones of different permeabilities are considered. The permeabilities in Zone 1 (50×10 m²) and Zone 2 (50×10 m²) are 10 md and 0.1 md, respectively (see Fig. 12). Methane is injected with a rate of $3.13 \times 10^{-2}$ PV/D uniformly distributed across the left side of the domain. Pressure is held constant along the right side of the domain. Two examples, Example 5a and Example 5b, are considered with different pressure and temperature conditions (see Table 6). In Example 5a, uniform distribution across the left side of the domain. Pressure is held constant along the right side of the domain. Two examples, Example 5a and Example 5b, are considered with different pressure and temperature conditions (see Table 6). In Example 5a,

**Table 2—CPU Time (Seconds) for Different Number of Nodes for Example 1a: PV Injection = 0.68**

<table>
<thead>
<tr>
<th>No. of nodes</th>
<th>50</th>
<th>100</th>
<th>500</th>
</tr>
</thead>
<tbody>
<tr>
<td>MFE-DG</td>
<td>0.37</td>
<td>1.24</td>
<td>—</td>
</tr>
<tr>
<td>FD</td>
<td>0.14</td>
<td>0.49</td>
<td>4.41</td>
</tr>
</tbody>
</table>

**Table 3—CPU Time (Seconds) for Different Number of Nodes for Example 1b: PV Injection = 0.68**

<table>
<thead>
<tr>
<th>No. of nodes</th>
<th>50</th>
<th>100</th>
<th>500</th>
</tr>
</thead>
<tbody>
<tr>
<td>MFE-DG</td>
<td>0.40</td>
<td>1.33</td>
<td>—</td>
</tr>
<tr>
<td>FD</td>
<td>0.15</td>
<td>0.51</td>
<td>4.62</td>
</tr>
</tbody>
</table>

Fig. 2—Methane composition in gas phase vs. distance at two different PV injections for various refinements in the MFE-DG and FD methods: Example 1b ($p=69$ bar, $T=311$ K).
there is a first-contact miscibility displacement where one shock occurs at the gas/liquid interface. Results for methane composition from the FD and MFE-DG methods are presented in Fig. 13 for four progressively finer grids. The numerical diffusion by the FD method is excessive. We notice that the solution by the MFE-DG method on a 40×20 grid and the FD solution on a 320×160 have nearly the same accuracy. The CPU time given in Table 9 shows that our algorithm is at least three orders of magnitude more efficient than the FD method. In Example 5b, a two-phase region appears. Fig. 14 presents methane composition in a 3D view by the FD and MFE-DG methods on 160×80 and 80×40 grids, respec-

**TABLE 4—RELEVANT DATA FOR EXAMPLE 2**

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Injection gas (mole frac.)</td>
<td>0.90 C₁, 0.10 C₂, 0.00 C₃</td>
</tr>
<tr>
<td>Initial fluid (mole frac.)</td>
<td>0.00 C₁, 0.25 C₂, 0.75 C₃</td>
</tr>
<tr>
<td>Pressure (bar)</td>
<td>69</td>
</tr>
<tr>
<td>Temperature (K)</td>
<td>311</td>
</tr>
<tr>
<td>Porosity (fraction)</td>
<td>0.2</td>
</tr>
<tr>
<td>Permeability (md)</td>
<td>10</td>
</tr>
<tr>
<td>Relative permeability</td>
<td>$k_α = S_α$</td>
</tr>
</tbody>
</table>

---

**Fig. 3**—Methane composition in gas and liquid phases vs. distance for various refinements in the MFE-DG and FD methods: Example 2; PV injection=0.51.
Fig. 15 shows the extract of composition data from Fig. 14 along the line $y=2$ m, parallel to the $x$-axis. In Example 5b, the FD method produces less numerical diffusion than in Example 5a. The FD and MFE-DG methods seem to converge and give similar results on $160\times80$ and $80\times40$ grids, respectively.

**Summary and Conclusions**

An algorithm is developed for two-phase multicomponent fluid flow in homogeneous and heterogeneous porous media with interface mass transfer. Our numerical approach combines the MFE and the DG methods. The MFE method is used to solve implicitly the pressure equation. To reduce the size of the linear system by the classical MFE method, where the cell pressure averages and the fluxes are the primary unknowns, the hybridized MFE method is used. With this technique, the traces of the pressure are the primary unknowns. The cell pressure averages and the fluxes can be calculated locally. The species-balance equations are then solved explicitly using the DG method. In order to avoid spurious oscillations, a slope-limiting operator is used to stabilize the DG method. The slope limiter imposes local monotonicity constraints on the DG solution so that the solution profile is reconstructed free from any local minima or maxima at the edge centers. After solving the pressure and the overall composition, flash calculations are
Fig. 5—Phase diagram of the ternary mixture C₁/C₂/C₃ at ρ=69 bar and T=311 K): Example 2.

Fig. 6—K-values vs. distance: Example 3a; PV injection=0.66.

Fig. 7—Gas saturation for various grid refinements by the MFE-DG and FD methods: Example 3a; PV injection=0.66, ρ=110 bar.

TABLE 5—CPU TIME (SECONDS) FOR DIFFERENT NUMBER OF NODES FOR EXAMPLE 2: PV INJECTION = 0.51

<table>
<thead>
<tr>
<th>No. of nodes</th>
<th>50</th>
<th>100</th>
<th>500</th>
</tr>
</thead>
<tbody>
<tr>
<td>MFE-DG</td>
<td>0.55</td>
<td>1.79</td>
<td>—</td>
</tr>
<tr>
<td>FD</td>
<td>0.17</td>
<td>0.53</td>
<td>5.53</td>
</tr>
</tbody>
</table>

TABLE 6—RELEVANT DATA FOR EXAMPLE 3

<table>
<thead>
<tr>
<th>Injection gas (mole frac.)</th>
<th>1.0 CO₂</th>
</tr>
</thead>
<tbody>
<tr>
<td>Initial fluid (mole frac.)</td>
<td>0.2 C₁, 0.2 C₆, 0.2 C₁₀, 0.2C₁₄, 0.2 C₂₀</td>
</tr>
<tr>
<td>Pressure (bar)</td>
<td>Example 3a: 110, Example 3b: 191</td>
</tr>
<tr>
<td>Temperature (K)</td>
<td>344</td>
</tr>
<tr>
<td>Porosity (fraction)</td>
<td>0.2</td>
</tr>
<tr>
<td>Permeability (md)</td>
<td>10</td>
</tr>
<tr>
<td>Relative permeability</td>
<td>kᵣ = Sᵣ²</td>
</tr>
</tbody>
</table>
performed to obtain the compositions, phase densities, and relevant coefficients.

The main features of this approach are:

1. The MFE method provides a highly accurate approximation of the fluxes, especially in heterogeneous media. This method is naturally adapted to treat a full-permeability tensor. In this paper, the numerical results are performed on structured grids with a scalar permeability.

2. The DG method, combined with an appropriate slope limiter, has superiority to capture shocks or sharp gradients in the solution without creating spurious oscillations or excessive numerical diffusion. This method is also flexible to describe complicated geometries by using unstructured grids.

The numerical results presented in this work, where we compare the accuracy and the performance of our algorithm with an FD-based commercial software, show that the MFE-DG method in

Fig. 8—The composition of $C_{14}$, $CO_2$, and $C_1$ for various grid refinements by the MFE-DG and FD methods: Example 3a, PV injection=0.66, $p=110$ bar.
1D is three to four times faster than the FD method, but in 2D it is at least two to three orders of magnitude more efficient than the FD method for comparable accuracy. The advantage of our algorithm is mainly for 2D problems. It is clear that the gain in 2D is much more than that in 1D. This is mainly because in 2D we may have additional numerical diffusion because of the mesh orientation. In both of the 2D examples presented in the paper, the mesh is anisotropic (that is, the flow is not perpendicular to the mesh interfaces). Unlike the MFE-DG method, the FD method on anisotropic meshes may produce significant numerical diffusion even for fine meshes.

**Nomenclature**

- $c$ = overall molar density, mole/m$^3$
- $c_f$ = total fluid compressibility
- $c_\alpha$ = molar density of the $\alpha$-phase, mole/m$^3$
- $E$ = mesh edge

Fig. 9—Methane composition in gas phase for various grid refinements by the MFE-DG and FD methods: Example 3b; PV injection=0.37, $p$=191 bar.


Thiele, M.R. and Edwards, M.G.: “Physically Based Higher-Order Godunov Schemes for Compositional Simulation,” paper SPE 66403 pre-

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**TABLE 7—RELEVANT DATA FOR EXAMPLES 4 AND 5**

<table>
<thead>
<tr>
<th>Injection gas (mole frac.)</th>
<th>1.0 C1, 0.0 C3</th>
</tr>
</thead>
<tbody>
<tr>
<td>Initial fluid (mole frac.)</td>
<td>0.0 C1, 1.0 C3</td>
</tr>
<tr>
<td>Pressure (bar)</td>
<td>Examples 4 and 5a: 50 Example 5b: 40</td>
</tr>
<tr>
<td>Temperature (K)</td>
<td>Examples 4 and 5a: 397 Example 5b: 311</td>
</tr>
<tr>
<td>Porosity (fraction)</td>
<td>0.2</td>
</tr>
<tr>
<td>Permeability (md)</td>
<td>Example 4: 10 Example 5: 0.1 and 10</td>
</tr>
<tr>
<td>Relative permeability</td>
<td>$k_{ij} = S_{ij}$</td>
</tr>
</tbody>
</table>

---

**Acknowledgments**

This work was supported by the member companies of the Reservoir Engineering Research Inst. (RERI).

**References**


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**NOTES**

$f_{gi}$ = fugacity of component $i$ in gas phase
$f_{oi}$ = fugacity of component $i$ in oil phase
$g$ = acceleration of gravity, m/s^2
$k$ = absolute permeability, m^2
$k_{rel}$ = relative permeability
$K$ = mesh cell
$K_a$ = effective mobility, m.s/kg
$n_i$ = number of components
$N_e$ = number of edges of a cell
$N_K$ = number of cells in a mesh
$p$ = pressure, Pa
$q_{K,E}$ = flux across edge $E$ in $K$
$t$ = time, s
$tp$ = pressure trace, Pa
$U_i$ = molar flux of component $i$
$w_{K,E}$ = $RT_0$ basis function
$\mu$ = viscosity, kg/m.s
$\nu_i$ = total partial molar volume of $i$
$\rho_o$ = mass density of phase $o$, kg/m^3
$\phi$ = porosity, %
$\theta$ = total velocity, m/s
$\theta_{\alpha}$ = velocity of phase $\alpha$, m/s
The DG method may produce nonphysical oscillations near shocks in the solution. This may lead to a numerical stability problem. Slope or flux limiters are a common cure for this problem. The slope limiter used in this work to stabilize the DG method can be applied for unstructured rectangular or triangular meshes. Before outlining the procedure, let us consider a typical gridblock \( P \) with surrounding blocks \( E, W, N, S, \) and \( EN, NW, SE, EN \). Let \( en, nw, ws, \) and \( en \) be the nodes of block \( P \) (see Fig. A-1). The objective
of the slope limiter is to reconstruct the values of the unknown (say, the concentration) at the nodes so that the solution is free from nonphysical oscillations. The procedure is performed in two steps as follows:

1. In the first step, the edge average values of the concentration \( c_e, c_w, c_n, \) and \( c_s \) are reconstructed so that we avoid having local minima or maxima at the edge midpoints without modifying the average material in the block, for example:

\[
\begin{align*}
\min(c_p, c_e) & \leq c_e \leq \max(c_p, c_e) \\
\min(c_p, c_w) & \leq c_w \leq \max(c_p, c_w) \\
\min(c_p, c_n) & \leq c_n \leq \max(c_p, c_n) \\
\min(c_p, c_s) & \leq c_s \leq \max(c_p, c_s)
\end{align*}
\]

(avoid local extrema) 

and 

\[
\begin{align*}
\min(c_p, c_e) & \leq c_e \leq \max(c_p, c_e) \\
\min(c_p, c_w) & \leq c_w \leq \max(c_p, c_w) \\
\min(c_p, c_n) & \leq c_n \leq \max(c_p, c_n) \\
\min(c_p, c_s) & \leq c_s \leq \max(c_p, c_s)
\end{align*}
\]

(avoid local extrema) 

\[
c_e + c_w = 2c_p \quad \text{(conserves the average block material)} \tag{A-1}
\]

\[
c_n + c_s = 2c_p \quad \text{(conserves the average block material)} \tag{A-2}
\]

Eqs. A-1 and A-2 can be solved separately by using a 1D slope limiting procedure, such as minmod, Van Leer, Osher, or other slope limiters.

2. In this step, we reconstruct the concentrations at the nodes \( e_n, n_w, w_s, \) and \( e_r \) of block \( P \). The material conservation leads to the equations
Fig. 13—Methane composition for various grid refinements by the MFE-DG and FD methods: Example 5a; PV injection=0.37 (p=50 bar, T=397 K).

Fig. 14—3D view of methane overall composition by the MFE-DG and FD methods: Example 5b; PV injection=0.37 (p=40 bar, T=311 K).
The nodal concentrations cannot be uniquely calculated from the previously described system of equations. To guarantee a unique solution, we append additional constraints so that the concentration at each node lies between the minimum and the maximum values of concentrations of the blocks that have this node in common, for instance:
\[
\begin{align*}
\min(c_{NW}, c_N, c_P, c_W) & \leq c_m \leq \max(c_{NW}, c_N, c_P, c_W) \\
\min(c_{EN}, c_E, c_P, c_SE) & \leq c_m \leq \max(c_{EN}, c_E, c_P, c_SE) \\
\min(c_{SE}, c_P, c_E, c_WS) & \leq c_m \leq \max(c_{SE}, c_P, c_E, c_WS)
\end{align*}
\]

The problem can then be formulated so that we seek the nodal unknowns to be at minimal distance from the initial nodal concentrations so that the constraints in Eqs. A-3 and A-4 are satisfied. The minimization problem is of rank 3, with 4 unknowns. Thus, it can be reduced to a minimization problem with one variable. The solution can be efficiently obtained with a noniterative procedure. For more details, refer to Hoteit et al. (2004).

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