

CHAPTER 7

MIXED FINITE ELEMENT APPROXIMATION OF PHASE VELOCITIES IN COMPOSITIONAL RESERVOIR SIMULATION

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Reservoir simulators have traditionally used centered finite differences with upstream weighting to discretize the spatial terms in the partial differential equations describing fluid flow in porous media. These techniques are relatively simple to implement in huge simulation codes, and they produce highly stable results which are sufficiently accurate for black-oil problems. However, as more compositional processes are being studied, it appears that the upstream weighting may degrade the accuracy of the usual discretization schemes to the point that they cannot represent the sharp fronts and rapid velocity fluctuations associated with these more complex problems. We present in this paper a weighting technique based on mixed finite elements which reduces numerical dispersion by lowering the phase velocities and fluid dispersal at the frontal interface. The derivation of this weighting and its implementation into a standard, finite difference compositional model is described in detail, and a method for treating zero permeability grid cells with the mixed method weighting is discussed. We also show that the use of this new weighting technique for both immiscible and miscible processes produces sharper saturation and composition profiles and more rapid frontal advances than standard finite differences with upstream weighting.

1. Introduction

Black-oil reservoir simulators are used to model and predict the results of standard recovery techniques by assuming that the hydrocarbon system consists of only two components, oil and gas, whose compositions are fixed and whose properties depend only upon the pressure and the bubble point pressure. In contrast, compositional simulators account for multiphase flow and interphase mass transfer for each of several components comprising the hydrocarbon phases. In these models, the principles of mass conservation and phase equilibria are used to describe the time evolution of phase pressures and saturations, mole fractions of each component, and the liquid hydrocarbon fraction at each grid point in the reservoir. The multicomponent nature of these models is ideal for simulating a broad range of reservoir processes, such as: (1) miscible flooding by enriched gas or CO₂; (2) cycling of gas-condensate

reservoirs with dry gas; (3) injection of gas into volatile oil reservoirs, and (4) natural depletion of volatile oil or gas condensate reservoirs.

Several different approaches to modeling compositional problems have appeared in the literature. These computational efforts are categorized by their treatment of phase equilibria and by the degree of coupling between the thermodynamics constraints and fluid flow equations. The most frequently used algorithm has been an IMPES (*implicit pressure, explicit saturation*) type scheme where the component material balances are summed to form a pressure equation which is solved by a quasi-Newton scheme. In this procedure, the overall mole fractions and phase saturations are then obtained in an explicit fashion from their respective continuity equations. These compositions and the pressure are next input into a separate phase equilibria routine which yields the mole fractions and densities of each phase. Finally, the algorithm returns to the pressure equation, and the entire procedure is repeated until convergence is achieved. This idea was first proposed in 1969 in a one-dimensional compositional model by Robuck et al. [21] and has been applied to increasingly more complex problems in the works of MacDonald [17], Nolen [19] and Kazemi et al. [14]. These papers are distinct from later sequential formulations since they use K -values and convergence pressures to perform the flash and phase equilibria calculations. The primary disadvantage of these thermodynamic techniques is that the equilibrium predictions may produce thermodynamic functions that are not smooth or continuous, and this often leads to convergence difficulties.

Nghiem et al. [18] have published a model whose formulation is similar to the above except that a cubic equation of state describes the fluid phase properties. The equation of state is used in the phase equilibrium computations to determine the mole fractions of the individual components and is particularly useful for performing these computations near the critical point. The Nghiem formulation produces a pressure equation which can be linearized to give a symmetric, diagonally dominant Jacobian matrix. These desirable matrix features and the equation of state are the only features which differentiate this work from the earlier work of Kazemi et al. [14].

Most commercial simulators utilize IMPES methods, and these formulations appear to have two disadvantages. The high degree of explicit computations in IMPES method should produce a time-step limitation for difficult problems, although such a limitation has not been reported in the literature. Also the pressure equation, which contains a nonlinear function of both pressure and composition, cannot be exactly linearized since the compositions are computed explicitly. Thus, the equation must be solved in a semi-implicit manner, and large numbers of iterations will be required in problems with significant compositional effects.

Coats [5] has addressed these difficulties by developing an equation of state model which couples the thermodynamic and fluid flow equations together in a fully-implicit algorithm. He has shown the applicability of this model by solving both immiscible and multiple contact miscible problems which illustrate the required capabilities of a compositional simulator.

Models which are intermediate between the computational complexity of the fully-implicit simulators and the computational simplicity of the IMPES techniques are those presented by Fussell and Fussell [13] and Young and Stephenson [27]. This method couples the physical phenomena together in a fully-implicit procedure with the important exception that the transmissibilities in the flow equations are treated explicitly. Young and Stephenson also discussed methods of approximating phase behavior with a limited number of components and presented a method of applying their compositional simulator to simpler black-oil problems.

Watts [26] has described another intermediate formulation based on the compositional description of the pressure and saturation equations associated with black-oil simulation. This formulation produces a pressure equation from species continuity equations and thermodynamic identities which contains compositional effects neglected in the IMPES model [1]. The pressure equation and the saturation equation are solved via the sequential, black-oil algorithm [24] using implicit relative permeabilities. This non-Newton procedure is not iterative, and the coupling of the equilibrium constraints to the flow equations and the determination of the phase compositions was not presented. Watts and his colleagues have successfully merged their compositional and traditional black-oil formulations into a single reservoir simulator [15].

Thele et al. [25] recently made an extensive comparison of several different compositional formulations. They compared the fully implicit formulation of Coats [5], the IMPES formulation of Nghiem et al. [18], and the formulation of Young and Stephenson [27] which is intermediate in computational complexity between the other two. Although Coats' formulation seems most capable of solving difficult problems since it is fully implicit, Thele found, as expected, that this method has the largest computer memory requirements and computer times. The immense storage requirements and processing costs for the Coats formulation may be prohibitive for field scale models. Application of this scheme to general field problems also requires an efficient solver for the linearized problem from Newton's method, and this solver must be capable of handling problems with large numbers of unknowns at each grid block.

Thele et al. [25] also reported that the formulation of Nghiem et al. [18] required the least memory, increasing only linearly in the number of components, N_c , while the other algorithms required quadratic growth of memory with N_c . They concluded the Young and Stephenson formulation [27] to be generally the fastest, and, at least at present, under the comparisons made, to be the most preferred method of the three. While the explicit treatment of the transmissibilities in the Young and Stephenson model may create some stability problems, their method produces a much more sparse Jacobian matrix than that of Coats' procedure. This intermediate formulation has more coupling than the sequential algorithms and uses the coupling to form an exact pressure equation through algebraic elimination in the Jacobian matrix, and Young and Stephenson noted that their linearization enabled the Newton iterations to be considerably decreased from the iteration counts reported by Nghiem et al. See [25] for more detailed comparisons of the various formulations.

Thele et al. [25] further noted that each of the three formulations they considered exhibited numerical dispersion problems. In compositional simulation, numerical dispersion can diffuse sharp fluid interfaces yielding erroneous predictions of fluid compositions and corresponding errors in the velocities of the miscible frontal advance. Numerical dispersion can also effect the computed locations of the boundaries of the regions of single-phase and two-phase flow. Coats [5], in one space dimension, and the authors [9], in two space dimensions, have illustrated the effects of numerical dispersion by solving multiple contact miscible problems. These results showed that the location of the miscible front, the concentration profiles, and the hydrocarbon recovery were all affected to some degree by dispersion problems.

Several methods have been proposed in the literature [4, 16] as remedies for numerical dispersion in compositional simulation. These techniques attempt to obtain a cancellation of the temporal and spatial truncation errors via special time-step selections. The methods have been quite successful in one space dimension, but their effectiveness is not clear for multi-

dimensional problems. The method of characteristics and modifications [10, 19, 22] have been somewhat successful in controlling dispersion in reservoir models.

Many aspects of the numerical dispersion and grid-orientation problems are caused by the combination of inaccurate fluid velocities and suboptimal use of upstream weighting of the transport terms in the model flow equations. In this work we shall concentrate on the development of techniques for obtaining more accurate fluid velocities and thus reducing numerical dispersion and grid orientation difficulties for compositional simulation. In such a setting, several species are present, and different phases compete for flow through the reservoir. The total fluid velocity is not sufficient to describe the flow processes, and the phase velocities must be determined separately. Standard finite differences or finite element procedures for determining the phase velocities determine an approximation, P , for the pressure as a set of cell averages, nodal values, or piecewise smooth functions. The resulting P is then differenced or differentiated and then multiplied by the possibly rough function $kk_{r,i}/\mu_i$, to obtain the i th phase velocity, where k is the total permeability, and $k_{r,i}$ and μ_i are the relative permeability and viscosity, respectively, for the i th phase. These processes produce rough and often inaccurate approximations for the various phase velocities which, in turn, reduce the accuracy of the other variables of interest. In this paper, we discuss the use of mixed finite element methods to approximate the important phase velocities in a more accurate fashion. These methods have been used successfully in a first contact miscible displacement setting [6, 10, 11, 23] and for immiscible displacement [2, 3]. Motivated by these preliminary successes, we have begun to extend the techniques to a compositional setting [9]. The mixed method phase velocities are considerably more accurate than those produced by conventional finite difference methods and exhibit a marked effect upon the computed saturation and composition profiles.

Our use of mixed methods for approximating phase velocities is based upon the techniques developed in [7, 8] for approximating the total velocity directly, as a primary variable. Physically, the total fluid velocity is a relatively smooth function of space, changing rapidly in the neighborhoods of wells. This is because local changes in the total fluid pressure compensate for rapid variation in the permeability, resulting in a smooth total fluid velocity. The use of the fluid velocity as a primary variable added both accuracy and robustness to the computations described in [6, 10, 12, 23].

In the methods presented here, a total fluid velocity is first determined and then finite element techniques are used to apportion the velocity to the separate phases without the use of upstream weighting. As the displacement process progresses, and the number of phases present in the reservoir changes in time, the relative permeabilities may vary rapidly with phase saturations. This rapid change in the relative permeabilities enhances the difficulties caused by upstream weighting techniques. Careful treatment of the distribution of the total fluid velocity to the separate phase velocities is thus required and is treated in some detail in this paper.

In the next section we shall present the mathematical formulation which is used for our test simulations. We shall then discuss various computational problems which motivate our use of mixed finite elements. After a description of the mixed method is given, techniques for incorporating the finite element formulation into a finite difference simulator will be described. Finally, sample calculations in both immiscible and multicontact miscible displacement settings will be presented.

2. Mathematical formulation

Mathematical models for fluid flow are obtained from various laws, relations and constitutive equations. The equations which govern multicomponent, multiphase flow in porous media arise from the following sources:

- (1) species continuity equations governing the conservation of mass of each component;
- (2) Darcy's law for the flow of each phase;
- (3) thermodynamic equations describing phase equilibria;
- (4) an equation of state;
- (5) constraint equations which require that the phase saturations sum to unity and the mole fraction in each phase sum to unity.

We shall assume that three phases are present: a liquid phase, a gas phase and an aqueous phase. Let N_c be the number of hydrocarbon components present. For the present discussion, we shall assume that no hydrocarbon components are present in the aqueous phase. We also assume that the mass transfer between hydrocarbon phases is essentially instantaneous compared with the fluid flow. Finally, for simplicity of exposition we shall assume that the porous medium is homogeneous and isotropic and shall neglect dispersion, capillary and gravity forces.

Under the above assumptions, the mass balances in the model are derived from the species continuity equations for each hydrocarbon component and water:

$$\phi \frac{\partial(\rho_o S_o + \rho_g S_g) z_i}{\partial t} = -\nabla \cdot (\rho_o x_i V_o + \rho_g y_i V_g) + q_i, \quad i = 1, 2, \dots, N_c; \quad (2.1)$$

$$\phi \frac{\partial(\rho_w S_w)}{\partial t} = -\nabla \cdot \rho_w V_w + q_w. \quad (2.2)$$

In several compositional formulations, it has been convenient to sum the N_c equations represented in (2.1) to form an overall hydrocarbon balance which is often used to solve for pressure:

$$\phi \frac{\partial \alpha}{\partial t} = -\nabla \cdot (\rho_o V_o + \rho_g V_g) + q, \quad (2.3)$$

where

$$\alpha = \rho_o S_o + \rho_g S_g. \quad (2.4)$$

Any of the other $N_c - 1$ equations from (2.1) can be used with (2.3) to replace the original (2.1).

The phase velocities in (2.1) and (2.3) are related to the reservoir pressure by Darcy's law. Neglecting capillary pressure and gravity forces, the oil velocity is expressed as

$$V_o = -(kk_{ro}/\mu_o)\nabla P. \quad (2.5)$$

Similar expressions hold for the other phase velocities using their respective relative permeabilities and viscosities.

We also assume that thermodynamic equilibrium exists between the hydrocarbon phases,

and this equilibrium is expressed in a set of N_c constraints requiring that the oil and gas fugacities are equal for each component

$$f_{io} = f_{ig}, \quad i = 1, 2, \dots, N_c. \quad (2.6)$$

We have employed the Peng–Robinson [20] equation of state

$$z^3 - (1 - B)z^2 - (A - 3B^2 - 2B)z - (AB - B^2 - B^3) = 0 \quad (2.7)$$

to derive the following equation:

$$\ln \frac{f_i}{x_i P} = \frac{b_i}{b} (z - 1) - \ln(z - B) - \left(\frac{A}{2\sqrt{2}B} \frac{2 \sum_j x_j a_{ij}}{a} - \frac{b_i}{b} \right) \ln \frac{z + 2.414B}{z - 2.414B}, \quad (2.8)$$

from which the fugacity may be computed. The mathematical description is then completed by the following molar and saturation constraints:

$$\sum_{i=1}^{N_c} x_i = 1, \quad \sum_{i=1}^{N_c} y_i = 1, \quad \sum_{i=1}^{N_c} z_i = 1, \quad (2.9)$$

$$S_o + S_g + S_w = 1. \quad (2.10)$$

Also, z_i can be related to x_i and y_i by an overall molar balance

$$z_i = Lx_i + Vy_i, \quad i = 1, 2, \dots, N_c, \quad (2.11)$$

which indicates that only two of three molar constraints are linearly independent.

3. Finite difference discretization

The flow equations in the mathematical model are differenced in the usual industry fashion—backward differences in time and central differences in space. The species balance equations become

$$\begin{aligned} \phi_{i,j} \frac{(\alpha z_k)_{i,j}^{m+1} - (\alpha z_k)_{i,j}^m}{\Delta t} = & \\ = & - \frac{(\rho_o x_k V_o)_{i+1/2,j}^{m+1} - (\rho_o x_k V_o)_{i-1/2,j}^{m+1}}{\Delta x} - \frac{(\rho_o x_k V_o)_{i,j+1/2}^{m+1} - (\rho_o x_k V_o)_{i,j-1/2}^{m+1}}{\Delta y} \\ & - \frac{(\rho_g y_k V_g)_{i+1/2,j}^{m+1} - (\rho_g y_k V_g)_{i-1/2,j}^{m+1}}{\Delta x} - \frac{(\rho_g y_k V_g)_{i,j+1/2} - (\rho_g y_k V_g)_{i,j-1/2}}{\Delta y} \\ & + Q_{k,i,j}, \quad k = 1, \dots, N_c, \end{aligned} \quad (3.1)$$

for $i = 1, \dots, N_x$ and $j = 1, \dots, N_y$. The overall hydrocarbon balance equation becomes

$$\begin{aligned} \phi_{ij} \frac{\alpha_{ij}^{m+1} - \alpha_{ij}^m}{\Delta t} &= \\ &= - \frac{(\rho_o V_o)_{i+1/2,j}^{m+1} - (\rho_o V_o)_{i-1/2,j}^{m+1}}{\Delta x} - \frac{(\rho_o V_o)_{i,j+1/2}^{m+1} - (\rho_o V_o)_{i,j-1/2}^{m+1}}{\Delta y} \\ &\quad - \frac{(\rho_g V_g)_{i+1/2,j}^{m+1} - (\rho_g V_g)_{i-1/2,j}^{m+1}}{\Delta x} - \frac{(\rho_g V_g)_{i,j+1/2}^{m+1} - (\rho_g V_g)_{i,j-1/2}^{m+1}}{\Delta y} + \sum_{k=1}^{N_c} Q_{kij}, \end{aligned} \quad (3.2)$$

for $i = 1, \dots, N_x$ and $j = 1, \dots, N_y$. The water balance equation becomes

$$\begin{aligned} \phi_{ij} \frac{(\rho_w S_w)_{ij}^{m+1} - (\rho_w S_w)_{ij}^m}{\Delta t} &= \\ &= - \frac{(\rho_w V_w)_{i+1/2,j}^{m+1} - (\rho_w V_w)_{i-1/2,j}^{m+1}}{\Delta x} - \frac{(\rho_w V_w)_{i,j+1/2}^{m+1} - (\rho_w V_w)_{i,j-1/2}^{m+1}}{\Delta y} + Q_{w,ij}^{m+1}, \end{aligned} \quad (3.3)$$

for $i = 1, \dots, N_x$ and $j = 1, \dots, N_y$. The production and injection terms, Q_{ij} are either constant (rate specified wells) or functions of pressure (wells with specified bottom hole pressure).

In standard finite difference formulations the transmissibilities

$$T = \rho k k_r / \mu \quad (3.4)$$

are upstream weighted for stability purposes. For example, using Darcy's law, in standard simulators,

$$(\rho_o V_o)_{i+1/2,j} = T_{i+1} \frac{p_{i+1} - p_i}{\Delta x} \quad \text{if } p_{i+1,j} \geq p_{i,j} \quad (3.5)$$

and

$$(\rho_o V_o)_{i+1/2,j} = T_i \frac{p_{i+1} - p_i}{\Delta x} \quad \text{if } p_{i+1,j} \leq p_{i,j}. \quad (3.6)$$

This upstream weighting, although useful for stability, is known to cause numerical dispersion and grid-orientation problems. The aim of this paper is to discuss new techniques which produce stable solutions without resorting so heavily upon upstream weighting.

Normally (3.5), (3.6) and corresponding equations for the other phase velocities are substituted into (3.1)–(3.3) to eliminate the phase velocities and express the flow equations in terms of the pressure. In the mixed method formulation, the phase velocities are approximated directly at these interblock boundaries and these approximations are used in (3.1)–(3.3) without introducing the pressure approximations into (3.1)–(3.3). We shall describe the mixed finite element techniques in the next section.

4. Mixed finite elements

Our use of mixed finite element techniques in a compositional simulation setting is motivated by their success on model problems for less complex physical processes. Mixed finite element methods have been used to study both miscible displacement and immiscible displacement processes. These techniques have been successful in eliminating numerical dispersion and grid-orientation difficulties for first contact miscible displacements in [6, 10, 12, 23] and for problems describing immiscible flow of two fluids by Chavent and coworkers in [2, 3]. In these settings, mixed methods have been used to approximate the Darcy velocity of the total fluid. We will first review the application of these techniques in the miscible displacement setting and then discuss differences and difficulties encountered in extending these ideas to more complex compositional processes.

4.1. Miscible displacement problems

We first review a model problem describing the displacement of one incompressible fluid by another, totally miscible with the first, in a horizontal porous reservoir $\Omega \subset \mathbb{R}^2$ over a time period $J = [t_0, t_1]$. If c is the concentration of the invading fluid, and p and \mathbf{u} are the pressure and Darcy velocity of the total fluid, then a model system of coupled quasilinear partial differential equations relating c , p , and \mathbf{u} is given by [10]

$$-\nabla \cdot \left[\frac{k}{\mu} \nabla p \right] \equiv \nabla \cdot \mathbf{u} = q, \quad x \in \Omega, t \in J, \quad (4.1)$$

$$\phi \frac{\partial c}{\partial t} - \nabla \cdot [D \nabla c - \mathbf{u}c] = q\tilde{c}, \quad x \in \Omega, t \in J. \quad (4.2)$$

The main difference between (4.2) and the continuity equations from Section 2, e.g. (2.2), is the inclusion of the diffusion-dispersion tensor D in (4.2). The form of D can be found in the literature [23]. Also the viscosity μ in (4.1) is determined by some mixing rule, such as

$$\mu(c) = \mu(o)((c^{1/4} - 1)M - 1)^{-4}, \quad (4.3)$$

where M is the mobility ratio between the injected and resident fluids. In addition to (4.1)–(4.2), initial conditions and no-flow boundary conditions are specified.

In the mixed finite element method, (4.1) is solved for both the pressure and the total fluid velocity simultaneously via the following system of first-order partial differential equations:

$$\mathbf{u} = -\frac{k}{\mu} \nabla p, \quad x \in \Omega, t \in J \quad (\text{Darcy's law}), \quad (4.4)$$

$$\nabla \cdot \mathbf{u} = q, \quad x \in \Omega, t \in J \quad (\text{conservation of mass}). \quad (4.5)$$

In more standard finite difference simulations, the k/μ term in (4.4) is upstream weighted for each grid block to obtain the velocities at interblock locations as in (3.5)–(3.6). This upwinding is used for two reasons. First, k/μ is standardly known only at cell block centers, and second, this weighting gives added stability to the resulting linear system.

The finite element methods presented in [7, 8] give a better weighting of the k/μ term due to the ability of its integral formulation to maximize the use of the spatial information on permeability and viscosity. Two distinct formulations can be obtained for the system (4.4)–(4.5). If \mathbf{v} and w are functions, which have similar form and play the same role at the variables \mathbf{u} and p , respectively, we can obtain either the system

$$\iint_{\Omega} \mathbf{u} \cdot \mathbf{v} \, dx = \iint_{\Omega} p \left(\nabla \cdot \frac{k}{\mu} \mathbf{v} \right) \, dx, \quad (4.6)$$

$$\iint_{\Omega} \nabla \cdot \mathbf{u} w \, dx = \iint_{\Omega} q w \, dx, \quad (4.7)$$

or a similar system obtained by replacing (4.6) by

$$\iint_{\Omega} \frac{\mu}{k} \mathbf{u} \cdot \mathbf{v} \, dx = \iint_{\Omega} p \nabla \cdot \mathbf{v} \, dx. \quad (4.8)$$

We note that through the integral formulation of the finite element method, the divergence theorem is applied (essentially integration by parts) to move the derivatives on the pressure p from (4.4) onto the smoother test function \mathbf{v} in (4.6) and (4.8). This is important. Physically, the fluid velocity is a smoothly varying function. If the permeability or the fluid viscosity changes rapidly in a region, the pressure changes rapidly in a compensatory fashion to produce the smooth velocity. Thus, if (k/μ) greatly varies over Ω , so must p , and hence ∇p ; then determining \mathbf{u} from (4.4) by obtaining an approximation of p , and its derivative which is multiplied by $(-k/\mu)$ produces inaccurate results. This is the motivation for removing derivatives from p . Similarly, if (k/μ) changes rapidly in space (4.8) will be a more accurate formulation than (4.6), which involves derivatives of (k/μ) .

The approximations for \mathbf{u} and p are linear combinations of basis functions, defined locally on one or two cell blocks. We first define a particular choice of basis functions. The pressure approximation is a piecewise constant function with, possibly, a different constant value for each grid block. This corresponds exactly to the finite difference interpretation. The corresponding approximation for the Darcy velocity is a two-component vector. The x -component is a continuous piecewise linear function in x with values specified at the grid boundaries and a constant function of y on each cell; the y -component is piecewise linear in y and constant in x . Therefore, the velocity is specified exactly at the locations needed by the finite difference formulation exemplified in (3.2). This will allow the mixing of finite element and finite difference techniques in later discussions. This particular set of basis functions can be interpreted as finite difference approximations, for which asymptotic error estimates and convergence results have been proven [7, 8, 11]. In the computations discussed in [6, 10, 12], a higher-order set of basis functions were used to obtain more accurate approximations at greater computational expense.

If there are N_x grid blocks in the x -direction and N_y in the y -direction, we note that a basis for the space of pressure approximations has $N_x N_y$ elements while, utilizing zero normal velocities for no-flow boundary conditions, we have $(N_x - 1)N_y$ and $N_x(N_y - 1)$ elements in the bases for the x - and y -components, respectively, of the velocity. We replace the test function

w in (4.7) by each different basis function from the pressure space to obtain $N_x N_y$ equations in the $N_x N_y$ unknown pressures. Similarly, using the basis elements for the velocity as test functions we obtain $(N_x - 1)N_y + N_x(N_y + 1)$ equations for the unknown velocity components from (4.8). The special choice of basis functions yields a block system of equations of the form

$$\begin{pmatrix} M_1 & 0 & N_1 \\ 0 & M_2 & N_2 \\ N_1^t & N_2^t & 0 \end{pmatrix} \begin{pmatrix} U_1 \\ U_2 \\ P \end{pmatrix} = \begin{pmatrix} R_1 \\ R_2 \\ R_3 \end{pmatrix}, \quad (4.9)$$

where P , U_1 and U_2 are the unknown vectors for pressure and the x - and y -components of velocity. M_1 and M_2 are tridiagonal matrices of order $(N_x - 1)N_y \times (N_x - 1)N_y$ and $N_x(N_y - 1) \times N_x(N_y - 1)$, respectively; N_1 and N_2 are nonsquare matrices of order $N_x N_y \times (N_x - 1)N_y$ and $N_x N_y \times N_x(N_y - 1)$, and N_1^t and N_2^t are the corresponding transpose matrices.

If (4.6) is used to obtain the velocity equations, M_1 and M_2 have constant coefficients while those of N_1 and N_2 depend upon k/μ , locally. If (4.8) is used, M_1 and M_2 have coefficients depending upon μ/k , while N_1 and N_2 have constant coefficients. The system (4.9) has been shown to be solvable using either (4.6) or (4.8) and asymptotic error estimates have been obtained [6, 7, 11]. Fig. 1, from [10] illustrates typical results of computations using mixed methods on a fairly difficult miscible displacement problem. There is essentially no grid orientation and little apparent numerical dispersion in evidence in Fig. 1. In these results and in all other mixed method investigations it should be noted that k/μ is nonzero over the entire domain Ω .

4.2. Displacement involving compositional effects

In compositional simulation, we must determine phase velocities for each flowing phase. The phase pressures are determined separately in standard finite difference techniques, and the phase velocities are obtained from the corresponding pressures via approximations of Darcy's law. Usually, upstream weighting of the transmissibility terms is used to obtain the

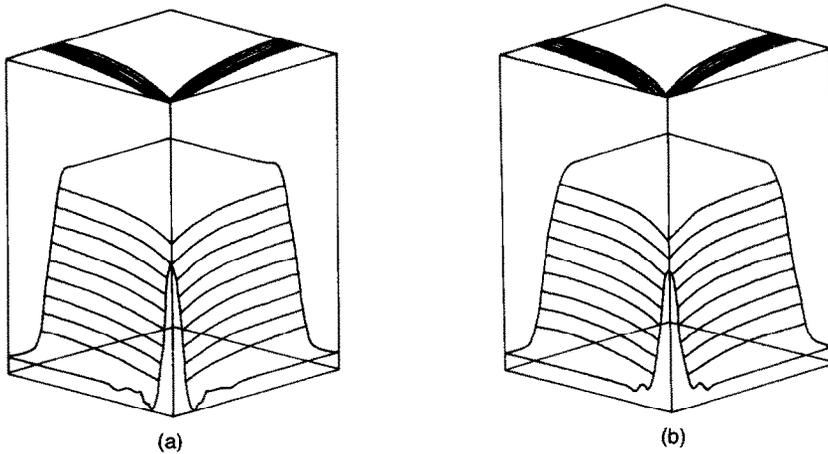


Fig. 1. Concentration profiles—1 PV injected. $M = 10$, $\phi d_m = 0$, $\phi d_1 = 10$, $\phi d_2 = 1$. (a) Diagonal orientation, 20×20 concentration, 15×15 pressure. (b) Parallel orientation, 28×28 concentration, 20×20 pressure.

velocity approximations at the cell boundaries. The high relative permeabilities for the phase behind a fluid interface coupled with upstream weighting causes excessively rapid advance and smearing of the interface. Through the finite element implementation, the values of the transmissibilities are weighted in a manner which more accurately describes the fluid flow, resulting in lower phase velocities at the interface and a better frontal resolution.

We first assume that a fluid pressure approximation has been obtained via a mixed method formulation, finite differences, or some similar method. Then, defining the total fluid mobility as

$$\lambda_T = \frac{kk_{ro}}{\mu_o} + \frac{kk_{rg}}{\mu_g} + \frac{kk_{rw}}{\mu_w}, \quad (4.10)$$

we can describe the total fluid velocity

$$u_T = -\lambda_T \nabla P, \quad (4.11)$$

where the spatial variation of the total mobility, λ_T , is more gradual than the variation of the individual phase mobilities. The approximation for the total velocity can be obtained from P via (4.11) in a variety of ways: upstream weighting, mixed finite element techniques, etc.

Once an approximation to u_T is obtained, the phase velocities can be computed via finite element distributed weighting of the coefficients in an inexpensive manner. The phase velocities are determined by combining (2.5) and (4.11), multiplying the resulting equation by a test function v , and integrating over the reservoir to obtain [9]

$$\iint_{\Omega} \frac{-\lambda_T \mu_i}{kk_{ri}} u_i \cdot v \, dx = \iint_{\Omega} u_T \cdot v \, dx, \quad i = o, g, w. \quad (4.12)$$

We can immediately see a computational difficulty arising from (4.12). In (4.8) we make the assumption that the permeability of the medium k was nonzero. However, in a multiphase flow situation, in regions where the phase saturations are zero or in the residual saturation range, the corresponding relative permeability is also zero. These naturally appearing zeros in the denominator of (4.12) must be treated specially. Zeros of the corresponding analogs for (4.6), while not appearing in the denominator cause severe oscillations on coarse grids if standard finite element techniques are applied.

Using upstream weighted finite differences, flow between adjacent grid blocks with relative permeabilities of one and zero is treated exactly the same as if the relative permeabilities were both one, hence forcing too much fluid to flow and diffusing sharp fluid interfaces. In this situation, the standard formulation of (4.12) cannot be used without modification. Since we are considering a repeated five-spot flow problem, we assume there are no velocity reversals with respect to the wells. Thus, moving along a row of grid blocks, if the relative permeability of the gas phase is zero in one cell, it is zero in all of the remaining cells in that row. When a zero relative gas permeability is encountered, communication between those cells in the matrix is removed, and all the remaining velocities are set to zero. In effect, this reduces the phase velocity to a fraction of the calculated total velocity, thereby lowering the flow at the front in a manner consistent with the finite element weighting of the permeabilities.

In summary, the calculation procedure for the compositional applications is as follows:

- (1) a pressure approximation is obtained via standard finite difference techniques;
- (2) this pressure is used in (4.11) to obtain an approximation to the total fluid velocity, u_T ;
- (3) u_T is apportioned into separate phase velocities via (4.12);
- (4) the approximate phase velocities are used in (3.1)–(3.3) to determine residuals for the flow equations;
- (5) these residuals are used to obtain the next pressure approximation via a finite difference formulation and the process is repeated.

The particular choice of basis functions in the finite element calculations allows easy use of these approximations in a finite difference simulator.

5. Examples

In this section, we review two example problems [9], which have been previously presented to compare the use of finite differences with upstream weighting versus the mixed method weighting. Gas was injected in both problems into a three-component hydrocarbon system which consisted of 44% methane, 12% butane and 44% decane. Gas was initially not present in the reservoir since the pressure was greater than the bubble point pressure; the water saturation was set to its irreducible value of 22%. Both problems were configured as a one quarter, five spot with a porosity of 15%, permeability of 100 md, constant production rate of 22,500 lb moles/day and constant injection rate of 25,000 lb moles/day.

The composition of the injection gas in the first problem was 100% methane which rapidly raised the bubble-point pressure and created an expanding region of two phase, immiscible flow. The results in Fig. 2 illustrate how the gas travels across the reservoir and fingers into the production well at 125 days. While both weighting techniques produce similar $S_g = 0.2$ contours, we see that the upstream weighting contours are quite smeared since this weighting of the relatively high gas permeabilities rapidly disperses this phase into the reservoir. Since the finite element weighting more accurately describes the fluid velocities, the gas dispersal is retarded, producing contours that are much closer together and indicating a much sharper frontal advance. Methane builds up behind the front and actually concentrates along the

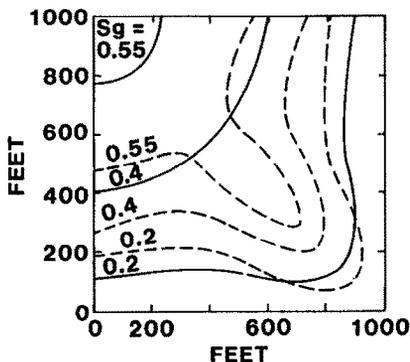


Fig. 2. Gas saturation contours for immiscible displacement at 125 days (5×5 grid).

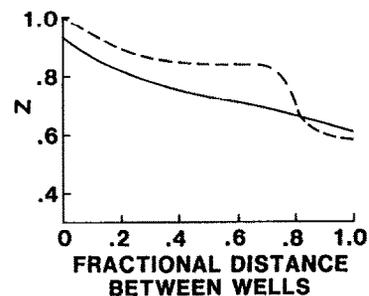


Fig. 3. Methane mole fraction along the diagonal between wells at 125 days.

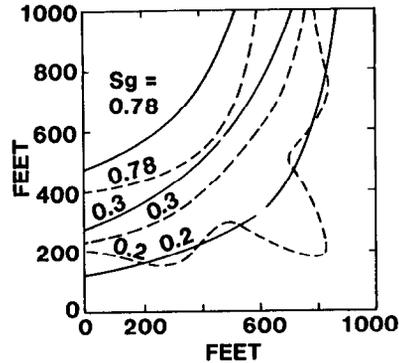


Fig. 4. Gas saturation contours for miscible displacement at 265 days.

diagonal flow path between the wells which leads to the pronounced fingering in Fig. 2. Fig. 3 compares the methane profiles and illustrates the severity of the differences of the two weighting approximations. This figure also shows that the methane fraction at the producer is lower for the finite element computations which accounts for the higher methane concentrations away from the well.

The second example is identical to the first except the composition of the injection gas is changed to 70% methane and 30% butane. This mixture composition enables the injection gas to become miscible with the in-place fluid via a multiple contact mechanism. Fig. 4 compares the results produced by the different weighting schemes at 265 days. We see that the mixed method weighting yields contours which are again closer together and also retards the dispersal of the injection gas so that the miscible front ($S_g = 0.78$) moves further into the reservoir. This figure also illustrates a spatial oscillation in the $S_g = 0.2$ contour, a difficulty which was regularly observed in this problem. This oscillation is due to the coarse grid employed and the resultant grid-orientation problems arising from such a grid. Similar spatial oscillations have been observed for the miscible displacement prototype using standard, higher-order approximations for the pressure and velocity with extremely adverse mobility ratios and an anisotropic dispersion tensor on much finer grids than the one used here [22]. These difficulties lead to inaccurate velocity approximations that cause the nonphysical curvature of the saturation contours.

The results from the mixed method weighting on these immiscible and miscible displacement problems show its potential in compositional simulation. It should be emphasized that the above results were generated from a 5×5 grid. Because of the huge storage requirements of compositional models, grids of this crudeness may remain in reservoir engineering practice for some time. Attempts to reduce grid orientation and numerical dispersion must face this problem at least until full-field capabilities for local grid refinement become operational.

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