ANALYSIS OF A COMPOSITIONAL MODEL
FOR FLUID FLOW IN POROUS MEDIA

ZHANGXIN CHEN, GUAN QIN, AND RICHARD E. EWING*

Abstract. In this paper we consider a compositional model for three-phase multicomponent fluid flow in porous media. This model consists of Darcy's law for volumetric flow velocities, mass conservation for hydrocarbon components, thermodynamic equilibrium for mass interchange between phases, and an equation of state for saturations. These differential equations and algebraic constraints are rewritten in terms of various formulations of the pressure and component-conservation equations. Phase, weighted fluid, global, and pseudo-global pressure and component-conservation formulations are analyzed. A numerical scheme based on the mixed finite element method for the pressure equation and the Eulerian-Lagrangian localized adjoint method for the component-conservation equations is developed. Numerical results are reported to show the behavior of the solution to the compositional model and to investigate the performance of the proposed numerical scheme.

Key words. compositional model, porous medium simulation, finite elements

AMS subject classifications. 35K60, 35K65, 76S05, 76T05

1. Introduction. This paper deals with a three-phase multicomponent compositional model often used in petroleum porous medium simulation. This model incorporates compressibility, compositional effects, and mass interchange between phases. It consists of Darcy's law for volumetric flow velocities, mass conservation for hydrocarbon components, thermodynamic equilibrium for mass interchange between phases, and an equation of state for saturations. It models important enhanced oil recovery procedures such as condensing gas drive and miscible gas injection. To understand complex chemical and physical phenomena of fluid flow in petroleum porous media, it has become increasingly important to study such a realistic model.

In this paper we give a qualitative analysis of the compositional model. The mathematical structure of a simplified, one-dimensional multicomponent two-phase compositional model was analyzed in [27], where capillary pressure effects were not considered. Here we analyze multidimensional, three-phase multicomponent fluid flow with the capillary effects. First, we manipulate the differential equations and algebraic constraints of this model to derive a pressure equation and modified component-conservation equations. Various formulations of the pressure equation, including phase, weighted fluid (with saturations as weights), global, and pseudo-global ones,

are described. These formulations have been developed for immiscible fluid flow in [11]; here we extend them to the complex compositional model.

We then analyze the mathematical structure of the differential system of these formulations. This system is of mixed parabolic-hyperbolic type, typical for fluid flow equations in porous media. We prove that the pressure equation is a standard parabolic problem and the modified component-conservation equations are advection-dominated problems in the presence of capillary diffusive forces; they are purely hyperbolic in the absence of these diffusive forces. For simplicity, we neglect hydraulic dispersion and molecular diffusion effects in this paper. We discuss the nonlinearity and coupling of the differential system as well. We show that the pressure equation is weakly nonlinear and less dependent on the conservation equations, these conservation equations are strongly nonlinear and heavily dependent on the pressure, and they are strongly coupled to the thermodynamic equilibrium constraints.

We also develop a numerical scheme for the solution of the compositional model under consideration. Finite difference and finite element methods have been used to solve compositional models under various assumptions on physical data (see, e.g., [1, 2, 14, 28, 29]). The numerical scheme proposed here is based on the mixed finite element method for the pressure equation and the Eulerian-Lagrangian localized adjoint method (ELLAM) for the component-conservation equations. The combination of the mixed and ELLAM methods has been considered for a compositional model in [21, 22, 23], where phase pressure and pseudo total velocity were employed. First, it is known that accurate numerical simulation requires accurate approximations to flow velocities. However, standard finite difference and finite element methods do not lead to accurate velocities. On the other hand, the mixed method has a very satisfactory property in both this aspect and the treatment of the geometrically complex geological structure of porous media (see the references in [12]). Second, due to their advection-dominated features, more suitable methods than the standard finite difference and finite element methods must be exploited for the component-conservation equations. The ELLAM method has been shown to be efficient in handling this type of problems in a mass-conservative manner [8]. Third, to handle the strong coupling of the system of the pressure and component-conservation equations, we utilize a sequential solution procedure in this scheme to decouple it. The sequential procedure has been chosen based on the analysis of the nonlinearity of the compositional system and the choice of primary variables [21, 22, 23]. The numerical scheme considered here utilizes various pressure forms with the usual total velocity.

We finally report numerical experiments to show the behavior of the solution to the compositional model and to investigate the performance of the proposed numerical scheme. The experiments involve a three-phase fluid process.

The rest of the paper is organized as follows. In the next section, we review compositional flow equations. Then in section 3, we analyze an equation of state and thermodynamic equilibrium conditions. In section 4, we derive and analyze the

pressure and modified component-conservation equations. In section 5, we develop our numerical scheme. In section 6, we report numerical experiments. Finally, we give some remarks in section 7.

2. Governing Equations. A compositional flow involves mass interchange between phases and compressibility. In a model for this type of flow, a finite number of hydrocarbon components is used to represent the composition of porous medium fluids. These components associate as phases in the porous medium. In this paper, we describe a compositional model under the assumptions that the flow process is isothermal (i.e., the constant temperature), the components form at most three phases (e.g., gas, oil, and water), and there is no mass interchange between the water phase and the hydrocarbon phases (i.e., the oil and gas phases).

Because of mass interchange between phases, mass is not conserved within each phase; the total mass of each component must be conserved:

$$
(2.1) \quad
\begin{aligned}
&\partial_t(\phi m_w) + \nabla \cdot (\xi_w u_w) = q_w, \\
&\partial_t(\phi m_i) + \nabla \cdot (c_{ig}\xi_g u_g + c_{io}\xi_o u_o) = q_i, \qquad i = 1, \ldots, N,
\end{aligned}
$$

where ∂_t denotes time differentiation, ϕ is the porosity of the porous medium, g, o, and w refer to gas, oil, and water phases, i is the component index, N is the number of hydrocarbon components, m_w and m_i denote the number of overall moles per pore volume of the water and ith hydrocarbon component, c_{ig} and c_{io} are the mole fraction of the ith component in gas and oil phases, ξ_α and u_α are the molar density and volumetric flow velocity of the α phase, and q_w and q_i stand for the molar flow rate of the water and the ith component, respectively, $\alpha = g, o, w$. In (2.1), the volumetric velocity u_α in multiphase flow is given by Darcy's law:

$$
(2.2) \quad u_\alpha = -k\frac{k_{r\alpha}}{\mu_\alpha}(\nabla p_\alpha - \rho_\alpha g_c), \qquad \alpha = g, o, w,
$$

where k is the effective permeability of the porous medium, $k_{r\alpha}$, μ_α, p_α, and ρ_α are the relative permeability, viscosity, pressure, and mass density, respectively, of the α-phase, and g_c is the gravitational constant vector.

In addition to the differential equations (2.1) and (2.2), we also need algebraic constraints for some quantities. The mass balance implies that

$$
(2.3) \quad m_i = m_{ig} + m_{io}, \qquad i = 1, \ldots, N,
$$

where m_{ig} and m_{io} represents the number of moles per pore volume of the ith hydrocarbon component in the oil and gas phases, respectively. Also, the mole fractions c_{ig} and c_{io} are given by

$$
(2.4) \quad c_{i\alpha} = \frac{m_{i\alpha}}{\sum_{j=1}^{N} m_{j\alpha}}, \qquad i = 1, \ldots, N, \quad \alpha = g, o.
$$

In the transport process, the porous medium is fully filled up with fluids:

$$(2.5) \qquad\qquad s_T \equiv s_g + s_o + s_w = 1,$$

where s_α is the saturation of the α-phase, $\alpha = g$, o, w. By their definition, the saturations are expressed in terms of the phase compositions:

$$(2.6) \qquad\qquad s_w = \frac{m_w}{\xi_w}, \quad s_\alpha = \frac{\sum_{i=1}^{N} m_{i\alpha}}{\xi_\alpha}, \qquad \alpha = g, o.$$

The phase pressures are related by capillary pressures:

$$(2.7) \qquad\qquad p_{c\alpha o} = p_\alpha - p_o, \qquad \alpha = g, o, w,$$

where $p_{coo} = 0$, p_{cgo} represents the gas phase capillary pressure, and p_{cwo} is the negative water phase capillary pressure, which are assumed to be known functions of the saturations. The relative permeabilities $k_{r\alpha}$ are also assumed to be known in terms of the saturations. The viscosities μ_α, molar densities ξ_α, and mass densities ρ_α are functions of their respective phase pressure and compositions. Finally, mass interchange between phases is characterized by the variation of mass distribution of each component in the oil and gas phases. As usual, these two phases are assumed to be in the phase equilibrium state at every moment. This is physically reasonable since the mass interchange between phases occurs much faster than the flow of porous medium fluids. Consequently, the distribution of each hydrocarbon component into the two phases is subject to the condition of stable thermodynamic equilibrium, which is given by minimizing the Gibbs free energy of the compositional system (see the discussion in the next section). The closedness of this system in terms of the primary unknowns chosen in this paper will be discussed later in the fourth section. For physical aspects of the compositional flow presented here, consult [2, 3].

3. Thermodynamic Equilibrium. Equations (2.1)–(2.7) form a strongly coupled system of time-dependent, nonlinear differential equations and algebraic constraints. It follows from the Gibbs phase rule that this system can be written in terms of $N + 2$ primary variables and other variables can be expressed as functions of them. The primary variables must be carefully chosen so that main physical properties inherent in the governing equations and constraints are preserved, the nonlinearity and coupling among the equations are weakened, and efficient numerical methods for the solution of the resulting system can be devised. In this paper we choose $(p, m_T, m_1, \cdots, m_N)$ as our primary variables for the reasons to be explained later, where p is some as yet unspecified pressure and $m_T = m_w + \sum_{i=1}^{N} m_i$ (i.e., the total mass per pore volume of the fluids, see [21, 23]). Toward that end, in this section we give a preliminary study on the thermodynamic equilibrium condition on the distribution of hydrocarbon components into phases, which will be needed in the next section.

3.1. The Gibbs-Duhem condition. Though most of the results in Lemmas 3.1 and 3.2 below might be known, we believe that a brief discussion is in order. Also, the arguments used in these two lemmas are different from the usual ones, and the results will be heavily exploited later in this section.

As mentioned before, it is assumed that the oil and gas phases are in the stable phase equilibrium state at every moment, which is expressed in terms of a set of the potential functions $f_{i\alpha}$ of the ith component in the α-phase, $i = 1, \ldots, N$, $\alpha = g, o$. Since the potential functions are derived from thermodynamic principles, they have some important properties. One of these properties is the Gibbs-Duhem condition [25]

$$(3.1) \qquad f_{i\alpha} = \frac{\partial \gamma_\alpha}{\partial m_{i\alpha}}, \qquad i = 1, \ldots, N, \quad \alpha = g, o,$$

where γ_α indicates the total Gibbs free energy of the α-phase. Equation (3.1) says that the potentials are the partial derivatives of the energy with respect to the compositions. From (3.1), we can deduce some other important properties.

Lemma 3.1. *Under* (3.1), *we have*

$$(3.2) \qquad \sum_{i=1}^{N} m_{i\alpha} \frac{\partial f_{i\alpha}}{\partial m_{j\alpha}} = 0, \qquad j = 1, \ldots, N, \quad \alpha = g, o,$$

and

$$(3.3) \qquad \frac{\partial f_{i\alpha}}{\partial m_{j\alpha}} = \frac{\partial f_{j\alpha}}{\partial m_{i\alpha}}, \qquad i, j = 1, \ldots, N, \quad \alpha = g, o.$$

PROOF. Recall that the energy γ_α is defined by

$$\gamma_\alpha = \sum_{i=1}^{N} m_{i\alpha} f_{i\alpha},$$

so

$$\frac{\partial \gamma_\alpha}{\partial m_{j\alpha}} = f_{j\alpha} + \sum_{i=1}^{N} m_{i\alpha} \frac{\partial f_{i\alpha}}{\partial m_{j\alpha}}.$$

This, together with (3.1), implies (3.2). Also, by (3.1), we see that

$$\frac{\partial f_{i\alpha}}{\partial m_{j\alpha}} = \frac{\partial^2 \gamma_\alpha}{\partial m_{j\alpha} \partial m_{i\alpha}} = \frac{\partial^2 \gamma_\alpha}{\partial m_{i\alpha} \partial m_{j\alpha}} = \frac{\partial f_{j\alpha}}{\partial m_{i\alpha}},$$

which implies (3.3). This completes the proof. □

We remark that the consequence of (3.3) is that the matrix $(\partial f_{i\alpha}/\partial m_{j\alpha})_{N \times N}$ is symmetric, $\alpha = g, o$.

3.2. The Kuhn-Tucker conditions. The total Gibbs free energy is defined by

$$(3.4) \qquad\qquad \gamma = \gamma_g + \gamma_o.$$

Now, the constrained minimization problem for the Gibbs free energy of the compositional system under consideration is formulated as follows:

$$(3.5) \qquad
\begin{aligned}
&\text{Given } 0 \leq m_i, \text{ find } (m_{ig}, m_{io}), \; i = 1, \ldots, N, \text{ such that} \\
&\gamma(m_{ig}, m_{io}) = \inf\{\gamma(v_{ig}, v_{io}) : 0 \leq v_{ig}, \; v_{io} \text{ and } v_{ig} + v_{io} = m_i\}.
\end{aligned}$$

From this minimization problem, we easily derive the Kuhn-Tucker conditions [17].

Lemma 3.2. *Let (m_{ig}, m_{io}) be defined as in (3.5). Then*

$$(3.6) \qquad f_{ig}(p, m_{1g}, \ldots, m_{Ng}) = f_{io}(p, m_{1o}, \ldots, m_{No}), \qquad i = 1, \ldots, N,$$

and the Hessian matrix $(\partial f_{ig}/\partial m_{jg} + \partial f_{io}/\partial m_{jo})_{N \times N}$ is symmetric and positive definite at (p, m_{ig}, m_{io}), where p is treated as a parameter.

PROOF. From (2.3), (3.1), and (3.4), we see that

$$\frac{\partial \gamma}{\partial m_{ig}} = \frac{\partial \gamma_g}{\partial m_{ig}} + \sum_{j=1}^{N} \frac{\partial \gamma_o}{\partial m_{jo}} \frac{\partial m_{jo}}{\partial m_{ig}} = \frac{\partial \gamma_g}{\partial m_{ig}} - \frac{\partial \gamma_o}{\partial m_{io}} = f_{ig} - f_{io},$$

so (3.6) follows from (3.5). Similarly, we have that

$$\frac{\partial^2 \gamma}{\partial m_{ig} \partial m_{jg}} = \frac{\partial f_{ig}}{\partial m_{jg}} + \frac{\partial f_{io}}{\partial m_{jo}}.$$

Consequently, we see that $(\partial f_{ig}/\partial m_{jg} + \partial f_{io}/\partial m_{jo})_{N \times N}$ is positive-definite from (3.5) and the theorem of the second-derivative test in calculus; the symmetry is obvious. The proof is complete. []

3.3. Some useful relations. We now exploit Lemmas 3.1 and 3.2 to derive some relations that will be useful in the next section.

Lemma 3.3. *Under the assumption of Lemma 3.2, we have*

$$(3.7) \qquad \sum_{j=1}^{N} m_{j\alpha} \frac{\partial m_{i\beta}}{\partial m_j} = 0, \qquad \alpha, \beta = g, o, \quad \alpha \neq \beta.$$

PROOF. It follows from (3.6) that

$$\frac{\partial f_{io}}{\partial m_j} = \frac{\partial f_{ig}}{\partial m_j};$$

i.e.,

$$\sum_{l=1}^{N} \frac{\partial f_{io}}{\partial m_{lo}} \frac{\partial m_{lo}}{\partial m_j} = \sum_{l=1}^{N} \frac{\partial f_{ig}}{\partial m_{lg}} \frac{\partial m_{lg}}{\partial m_j}.$$

By (2.3) and (3.3), we thus see that

$$(3.8) \qquad \sum_{l=1}^{N} \left(\frac{\partial f_{io}}{\partial m_{lo}} + \frac{\partial f_{ig}}{\partial m_{lg}} \right) \frac{\partial m_{lo}}{\partial m_j} = \frac{\partial f_{ig}}{\partial m_{jg}} = \frac{\partial f_{jg}}{\partial m_{ig}},$$

which, together with (3.2), implies that

$$\sum_{j=1}^{N} \sum_{l=1}^{N} \left(\frac{\partial f_{io}}{\partial m_{lo}} + \frac{\partial f_{ig}}{\partial m_{lg}} \right) \frac{\partial m_{lo}}{\partial m_j} m_{jg} = \sum_{j=1}^{N} \frac{\partial f_{jg}}{\partial m_{ig}} m_{jg} = 0.$$

That is,

$$\sum_{l=1}^{N} \left(\frac{\partial f_{io}}{\partial m_{lo}} + \frac{\partial f_{ig}}{\partial m_{lg}} \right) \sum_{j=1}^{N} \frac{\partial m_{lo}}{\partial m_j} m_{jg} = 0, \qquad i = 1, \ldots, N.$$

Now, by Lemma 3.2 the only solution to this system is the null solution

$$\sum_{j=1}^{N} \frac{\partial m_{lo}}{\partial m_j} m_{jg} = 0, \qquad l = 1, \ldots, N.$$

With the same argument, we can show

$$\sum_{j=1}^{N} \frac{\partial m_{lg}}{\partial m_j} m_{jo} = 0, \qquad l = 1, \ldots, N.$$

Thus the proof is completed. $\square$

Lemma 3.4. *It holds that*

$$(3.9) \qquad \sum_{j=1}^{N} m_{j\alpha} \frac{\partial c_{i\alpha}}{\partial m_{j\alpha}} = 0, \qquad i = 1, \ldots, N, \quad \alpha = g, o.$$

This directly comes from the definition of $c_{i\alpha}$ in (2.4).

Proposition 3.5. *Under the assumption of Lemma 3.2, for α, $\beta = g$, o we have*

$$\sum_{j=1}^{N} m_{j\alpha} \frac{\partial s_\beta}{\partial m_j} = \begin{cases} s_\alpha & \text{if} \quad \alpha = \beta, \\ 0 & \text{if} \quad \alpha \neq \beta. \end{cases}$$

PROOF. It follows from (2.6) that

$$(3.10) \qquad \frac{\partial s_\beta}{\partial m_{j\beta}} = \frac{1}{\xi_\beta} \left(1 - s_\beta \sum_{l=1}^{N} \frac{\partial \xi_\beta}{\partial c_{l\beta}} \frac{\partial c_{l\beta}}{\partial m_{j\beta}} \right),$$

so that

$$\frac{\partial s_\beta}{\partial m_i} = \sum_{j=1}^{N} \frac{\partial s_\beta}{\partial m_{j\beta}} \frac{\partial m_{j\beta}}{\partial m_i} = \frac{1}{\xi_\beta} \left(\sum_{j=1}^{N} \frac{\partial m_{j\beta}}{\partial m_i} - s_\beta \sum_{j=1}^{N} \sum_{l=1}^{N} \frac{\partial \xi_\beta}{\partial c_{l\beta}} \frac{\partial c_{l\beta}}{\partial m_{j\beta}} \frac{\partial m_{j\beta}}{\partial m_i} \right).$$

Hence, we observe that

$$\sum_{i=1}^{N} m_{i\alpha} \frac{\partial s_\beta}{\partial m_i} = \frac{1}{\xi_\beta} \left(\sum_{j=1}^{N} \sum_{i=1}^{N} m_{i\alpha} \frac{\partial m_{j\beta}}{\partial m_i} - s_\beta \sum_{j=1}^{N} \sum_{l=1}^{N} \sum_{i=1}^{N} m_{i\alpha} \frac{\partial \xi_\beta}{\partial c_{l\beta}} \frac{\partial c_{l\beta}}{\partial m_{j\beta}} \frac{\partial m_{j\beta}}{\partial m_i} \right).$$

This, together with (3.7), (3.9), and (2.6), yields the desired result. $\qquad$ []

4. The Compositional System. As mentioned before, the system in (2.1)–(2.7) involves a large number of strongly coupled nonlinear differential equations and algebraic constraints. To alleviate the nonlinearity and coupling, we carefully choose our primary variables and derive a compositional system for them. This system consists of the (various) pressure and modified component-conservation equations. We shall use the usual total flow velocity

$$(4.1) \qquad\qquad u = u_g + u_o + u_w.$$

Several choices for p will be made later. For the time being, let us assume that p has been given.

4.1. The pressure equation. Note that $s_T = s_T(p, m_w, m_1, \ldots, m_N)$, as given in (2.5), is a function of its arguments. Then it follows from the differentiation of (2.5) with respect to time that

$$\frac{\partial s_T}{\partial p} \partial_t p + \frac{\partial s_T}{\partial m_w} \partial_t m_w + \sum_{i=1}^{N} \frac{\partial s_T}{\partial m_i} \partial_t m_i = 0.$$

Apply (2.1) to see that

$$(4.2) \qquad \begin{aligned} c_T \partial_t p + \frac{\partial s_T}{\partial m_w} \nabla \cdot (\xi_w u_w) + \sum_{i=1}^{N} \frac{\partial s_T}{\partial m_i} \nabla \cdot (c_{ig} \xi_g u_g + c_{io} \xi_o u_o) \\ = \frac{\partial s_T}{\partial m_w} q_w + \sum_{i=1}^{N} \frac{\partial s_T}{\partial m_i} q_i, \end{aligned}$$

where c_T is the total fluid and rock compressibility given by

$$(4.3) \qquad c_T = -\phi \frac{\partial s_T}{\partial p} + \left(m_w \frac{\partial s_T}{\partial m_w} + \sum_{i=1}^{N} m_i \frac{\partial s_T}{\partial m_i} \right) \frac{\partial \phi}{\partial p}.$$

By (2.5), we see that

$$(4.4) \qquad \frac{\partial s_T}{\partial m_w} = \frac{\partial s_w}{\partial m_w}, \quad \frac{\partial s_T}{\partial m_i} = \frac{\partial s_g}{\partial m_i} + \frac{\partial s_o}{\partial m_i},$$

and, by (2.4) and (2.6),

$$(4.5) \qquad c_{i\alpha}\xi_\alpha = \frac{m_{i\alpha}}{s_\alpha}, \quad \frac{\partial s_w}{\partial m_w} = \frac{1}{\xi_w}\left(1 - s_w\frac{\partial \xi_w}{\partial m_w}\right).$$

Now, apply (4.1), (4.4), (4.5), and Proposition 3.5 to (4.2) to obtain

$$c_T\partial_t p + \nabla \cdot u - \xi_w\nabla\left(\frac{\partial s_w}{\partial m_w}\right)\cdot u_w - \sum_{i=1}^N \nabla\left(\frac{\partial s_T}{\partial m_i}\right)\cdot(c_{ig}\xi_g u_g + c_{io}\xi_o u_o)$$
$$-\nabla\cdot\left(s_w\frac{\partial \xi_w}{\partial m_w}u_w\right) = \frac{\partial s_w}{\partial m_w}q_w + \sum_{i=1}^N \frac{\partial s_T}{\partial m_i}q_i.$$

Normally, water is assumed to be incompressible or slightly compressible. In this case, we obtain

$$(4.6) \qquad c_T\partial_t p + \nabla \cdot u - \sum_{i=1}^N \nabla\left(\frac{\partial s_T}{\partial m_i}\right)\cdot(c_{ig}\xi_g u_g + c_{io}\xi_o u_o) = \frac{q_w}{\xi_w} + \sum_{i=1}^N \frac{\partial s_T}{\partial m_i}q_i,$$

where, by (2.3) and (2.5),

$$c_T = -\phi\frac{\partial s_T}{\partial p} + \frac{\partial \phi}{\partial p}.$$

In the subsequent analysis, solely for notational convenience we shall utilize the assumption that water is incompressible; then ξ_w is constant. It now remains to express u in terms of p.

4.1.1. Phase pressure. We first review the phase pressure formulation. The oil phase pressure has been often used in petroleum porous medium simulation:

$$(4.7) \qquad p = p_o.$$

For expositional convenience, we introduce the phase mobility functions

$$\lambda_\alpha = \frac{k_{r\alpha}}{\mu_\alpha}, \qquad \alpha = g,\ o,\ w,$$

and the total mobility

$$\lambda = \sum_\alpha \lambda_\alpha,$$

where (and later) $\sum_\alpha = \sum_{\alpha=w,o,g}$. Then it follows from (2.2), (2.7), and (4.7) that

$$(4.8) \qquad u = -k\lambda\left(\nabla p - G_\lambda + \sum_\alpha \frac{\lambda_\alpha}{\lambda}\nabla p_{c\alpha o}\right),$$

where $G_\lambda = g_c\sum_\alpha \rho_\alpha\lambda_\alpha/\lambda$. Substitution of (4.8) into (4.6) yields the equation for the phase pressure p. The analysis of the resulting equation will be described in

subsection 4.1.5 later. The pressure equation as split in (4.6) and (4.8) into a first-order differential system is suitable to the application of the mixed finite element method presented in the next section.

From (2.2) and (2.7), we see that the phase velocity is related to the total velocity by

$$(4.9) \qquad u_\alpha = \frac{\lambda_\alpha}{\lambda} \left(u + k \sum_\beta \lambda_\beta \left\{ \nabla(p_{c\beta o} - p_{c\alpha o}) - (\rho_\beta - \rho_\alpha)g_c \right\} \right), \qquad \alpha = g,\, o,\, w.$$

4.1.2. Weighted fluid pressure. We now define a smoother pressure than the phase pressure given in (4.7). Namely, we define the weighted fluid pressure

$$(4.10) \qquad p = \sum_\alpha s_\alpha p_\alpha.$$

Note that even if some saturation is zero (i.e., some phase disappears), we still have a non-zero smooth variable p. By (2.5) and (2.7), the phase pressures are given by

$$p_\alpha = p + p_{c\alpha o} - \sum_\beta s_\beta p_{c\beta o}, \qquad \alpha = g,\, o,\, w.$$

Then, apply (2.2) and (4.1) to see that

$$(4.11) \qquad u = -k\lambda \left(\nabla p - G_\lambda + \sum_\alpha \frac{\lambda_\alpha}{\lambda} \nabla p_{c\alpha o} - \sum_\alpha \nabla(s_\alpha p_{c\alpha o}) \right).$$

Finally, the relationships between the phase velocities and the total velocity are the same as in (4.9).

Observe that the pressure is strongly coupled to the saturations or to the compositions through the last term on the right-hand side of (4.8) (respectively, the last two terms of (4.11)). To have less coupling, we next introduce the so-called global pressure.

4.1.3. Global pressure. To introduce a global pressure, we assume that three-phase relative permeability and capillary pressure functions satisfy the condition

$$(4.12) \quad \frac{\partial}{\partial s_g}\left(\frac{\lambda_w}{\lambda}\right)\frac{\partial p_{cwo}}{\partial s_w} + \frac{\partial}{\partial s_g}\left(\frac{\lambda_g}{\lambda}\right)\frac{\partial p_{cgo}}{\partial s_w} = \frac{\partial}{\partial s_w}\left(\frac{\lambda_w}{\lambda}\right)\frac{\partial p_{cwo}}{\partial s_g} + \frac{\partial}{\partial s_w}\left(\frac{\lambda_g}{\lambda}\right)\frac{\partial p_{cgo}}{\partial s_g}.$$

This condition is referred to as the total differential condition [9, 11]. When it is satisfied, we can define a pressure

$$p_c(s_w, s_g) = \int_1^{s_w} \left\{ \left(\frac{\lambda_w}{\lambda}\right)(\zeta, 0)\frac{\partial p_{cwo}}{\partial s_w}(\zeta, 0) + \left(\frac{\lambda_g}{\lambda}\right)(\zeta, 0)\frac{\partial p_{cgo}}{\partial s_w}(\zeta, 0) \right\} \mathrm{d}\zeta$$
$$+ \int_0^{s_g} \left\{ \left(\frac{\lambda_w}{\lambda}\right)(s_w, \zeta)\frac{\partial p_{cwo}}{\partial s_g}(s_w, \zeta) + \left(\frac{\lambda_g}{\lambda}\right)(s_w, \zeta)\frac{\partial p_{cgo}}{\partial s_g}(s_w, \zeta) \right\} \mathrm{d}\zeta.$$

We now introduce the global pressure

$$(4.13) \qquad\qquad p = p_o + p_c.$$

Apply (2.2), (2.7), (4.1), (4.12), and (4.13) to see that

$$(4.14) \qquad\qquad u = -k\lambda(\nabla p - G_\lambda).$$

The phase velocity is determined by

$$(4.15) \qquad u_\alpha = \frac{\lambda_\alpha}{\lambda}u + k\lambda_\alpha\Big(\nabla(p_c - p_{c\alpha o}) - \delta_\alpha\Big), \qquad \alpha = g,\, o,\, w,$$

where

$$\delta_\alpha = \sum_\beta \frac{\lambda_\beta}{\lambda}(\rho_\beta - \rho_\alpha)g_c.$$

While condition (4.12) is not satisfied for some of the existing three-phase relative permeability and capillary pressure functions, it has been shown [11] that it is satisfied for some simplified models. Also, a simple numerical procedure for constructing three-phase relative permeability and capillary pressure curves satisfying this condition has been given in [9], some of the numerical examples have been compared with the classical Stone's model [26], which does not satisfy this condition, and similar results have been obtained.

4.1.4. Pseudo-global pressure. The global pressure formulation in the previous subsection requires the total differential condition (4.12) on the shape of three-phase relative permeability and capillary pressure functions. In this subsection, as introduced in [11], we finally consider a pseudo-global pressure formulation, which does not require this condition. For this, assume that the capillary pressures satisfy the usual condition

$$(4.16) \qquad\qquad p_{cwo} = p_{cwo}(s_w), \quad p_{cgo} = p_{cgo}(s_g).$$

We then introduce the mean values

$$(4.17) \qquad \begin{aligned} \left(\widehat{\frac{\lambda_w}{\lambda}}\right)(s_w) &= \frac{1}{1-s_w}\int_0^{1-s_w}\left(\frac{\lambda_w}{\lambda}\right)(s_w,\zeta)\mathrm{d}\zeta, \\ \left(\widehat{\frac{\lambda_g}{\lambda}}\right)(s_g) &= \frac{1}{1-s_g}\int_0^{1-s_g}\left(\frac{\lambda_g}{\lambda}\right)(\zeta,s_g)\mathrm{d}\zeta, \end{aligned}$$

and the pseudo-global pressure

$$p = p_o + \int_{s_{wc}}^{s_w}\left(\widehat{\frac{\lambda_w}{\lambda}}\right)(\zeta)\frac{dp_{cwo}(\zeta)}{ds_w}\mathrm{d}\zeta + \int_{s_{gc}}^{s_g}\left(\widehat{\frac{\lambda_g}{\lambda}}\right)(\zeta)\frac{dp_{cgo}(\zeta)}{ds_g}\mathrm{d}\zeta,$$

where s_{wc} and s_{gc} are such that $p_{cwo}(s_{wc}) = 0$ and $p_{cgo}(s_{gc}) = 0$. Now, apply these definitions to (4.8) to find that

$$(4.18) \qquad u = -k\lambda \left\{ \nabla p - G_\lambda + \sum_\alpha \left(\frac{\lambda_\alpha}{\lambda} - \left(\widehat{\frac{\lambda_\alpha}{\lambda}} \right) \right) \frac{dp_{c\alpha o}}{ds_\alpha} \nabla s_\alpha \right\}.$$

The phase velocities in terms of the total velocity are expressed as in (4.9). A comparison of all these formulations will be mentioned later.

4.1.5. Analysis of the pressure equation. The pressure equation is given by (4.6) and (4.8) (respectively, (4.11), (4.14), or (4.18), depending upon the formulation used). We analyze the global formulation in detail. Substitution of (4.14) into (4.6) yields that

$$(4.19) \qquad \begin{aligned} & c_T \partial_t p - \nabla \cdot \left\{ k\lambda (\nabla p - G_\lambda) \right\} \\ & = \sum_{i=1}^{N} \nabla \left(\frac{\partial s_T}{\partial m_i} \right) \cdot (c_{ig}\xi_g u_g + c_{io}\xi_o u_o) + \frac{q_w}{\xi_w} + \sum_{i=1}^{N} \frac{\partial s_T}{\partial m_i} q_i. \end{aligned}$$

Since the porosity ϕ is a non-decreasing function of pressure, $\partial\phi/\partial p \geq 0$. Also, the fluid compressibility means that $-\phi(\partial s_T/\partial p) > 0$. Hence, the rock and fluid compressibility combines to see that

$$c_T = -\phi \frac{\partial s_T}{\partial p} + \frac{\partial \phi}{\partial p} > 0.$$

Furthermore, although the individual phase mobilities λ_α can be zero ($\alpha = g, o, w$), the total mobility λ is positive. Thus if the absolute permeability k of the porous medium is positive-definite, so is $k\lambda$. Consequently, it follows from (4.19) that the pressure equation is parabolic. Typically, the rock and fluid compressibility is quite small, and the pressure reachs a steady state very rapidly. The analysis for other formulations is exactly the same.

Note that the relative permeabilities $k_{r\alpha}$ ($\alpha = g, o, w$) are strongly nonlinear functions of the saturations and the viscosities μ_α mainly depend on the temperature, which is constant here, and are not so sensitive to the pressure change. Thus it follows from their definitions that the phase mobilities λ_α are the functions of the saturations. However, since the total mobility λ is a much smoother quantity than the phase ones, in general the coefficient in the second term of the left-hand side of (4.19) can be explicitly calculated. Also, the first term on the right-hand side of (4.19) is effectively quadratic in velocities, which is usually small in almost all of the porous medium, and can be explicitly treated. Therefore, according to the rule in [2] that the variables that are functions of the pressure only are considered to be weakly nonlinear and the variables that depend on the saturations are strongly nonlinear, the pressure equation is a weakly nonlinear parabolic equation. It is also less coupled to the mass conservation equations derived in the next subsection.

To analyze other pressure formulations, it suffices to notice that the capillary pressures are usually smaller compared to a porous medium pressure. Consequently, the capillary pressure effects in these pressure equations can be explicitly handled. Hence, the above discussion on the nonlinearity for the global formulation applies to them.

4.1.6. Comparison of formulations. Since the four pressure formulations considered above have the same structure as those developed in [11] for the flow of three immiscible fluids, we just mention a brief comparison of these formulations. For more details on both theoretical and numerical comparisons, consult [11].

The global formulation is far more efficient than the phase and pseudo-global ones from the computational point of view and also more suitable for mathematical analysis since the coupling between the pressure equation and the transport equations derived in the next subsection is much less. The weakness of the global formulation is the need of the satisfaction of the total differential condition (4.12) by the three-phase relative permeability and capillary pressure curves. In general, the phase formulation can be applied. However, if the fractional flow functions of the water and gas phases are close to their respective mean values as defined in (4.17), the pseudo-global formulation is more useful. In the (probably unphysical) case where the capillary pressures p_{cgo} and p_{cwo} are zero, all the formulations are the same.

4.2. The transport system. In this subsection, we derive the system of transport equations, i.e., modified component-conservation equations. Toward that end, first sum the second equation in (2.1) over i, use (2.4), and sum the resulting equation with the first equation in (2.1) to see that

$$(4.20) \qquad \partial_t(\phi m_T) + \nabla \cdot \left(\sum_\alpha \xi_\alpha u_\alpha \right) = q_T,$$

where $q_T = q_w + \sum_{i=1}^N q_i$. By its definition, note that m_T is smoother than m_w. Also, the total molar flux $\sum_\alpha \xi_\alpha u_\alpha$ is a much smoother quantity than the individual flux $\xi_w u_w$. That is why we have chosen m_T instead of m_w as our primary variable.

Next, observe that the second equation in (2.1) for m_i and equation (4.20) for m_T depend on the pressure p explicitly through the phase velocities. Thus we need to utilize (4.9) or (4.15) to eliminate these velocities.

Notice that the relationships between the phase velocities and the total velocity for the phase pressure, weighted fluid pressure, and pseudo-global pressure formulations are all the same. Also, apply (4.12) and the definition of p_c to see that

$$\frac{\partial p_c}{\partial s_w} = \frac{\lambda_w}{\lambda} \frac{\partial p_{cwo}}{\partial s_w} + \frac{\lambda_g}{\lambda} \frac{\partial p_{cgo}}{\partial s_w}, \quad \frac{\partial p_c}{\partial s_g} = \frac{\lambda_w}{\lambda} \frac{\partial p_{cwo}}{\partial s_g} + \frac{\lambda_g}{\lambda} \frac{\partial p_{cgo}}{\partial s_g}.$$

Then it follows from (4.15) that

$$u_\alpha = \frac{\lambda_\alpha}{\lambda} + \lambda_\alpha k \left(\frac{\lambda_w}{\lambda} \nabla p_{cwo} + \frac{\lambda_g}{\lambda} \nabla p_{cgo} - \nabla p_{c\alpha o} - \delta_\alpha \right), \quad \alpha = g,\, o,\, w,$$

which reduces to (4.9). In terms of ∇p_{cwo} and ∇p_{cgo}, the component-conservation equations are thus the same for all pressure formulations. Therefore, it suffices to derive the modified conservation equations for one of them.

Substitution of (4.9) into (4.20) and the use of algebraic manipulations yields

(4.21)
$$\partial_t(\phi m_T) + \nabla \cdot \left(\sum_\alpha \frac{\xi_\alpha \lambda_\alpha}{\lambda} u \right) - \nabla \cdot \left(\sum_\alpha \sum_\beta \frac{\xi_\alpha \lambda_\alpha \lambda_\beta}{\lambda} k(\rho_\beta - \rho_\alpha) g_c \right)$$
$$+ \nabla \cdot \left\{ \left(\sum_\alpha \xi_\alpha \lambda_\alpha - \xi_w \lambda \right) \frac{\lambda_w}{\lambda} k \nabla p_{cwo} + \left(\sum_\alpha \xi_\alpha \lambda_\alpha - \xi_g \lambda \right) \frac{\lambda_g}{\lambda} k \nabla p_{cgo} \right\} = q_T.$$

Similarly, substitute (4.9) into the second equation in (2.1) to have

(4.22)
$$\partial_t(\phi m_i) + \nabla \cdot \left(\sum_{\alpha=g,o} \frac{c_{i\alpha}\xi_\alpha \lambda_\alpha}{\lambda} u \right) - \nabla \cdot \left(\sum_{\alpha=g,o} \sum_\beta \frac{c_{i\alpha}\xi_\alpha \lambda_\alpha \lambda_\beta}{\lambda} k(\rho_\beta - \rho_\alpha) g_c \right)$$
$$+ \nabla \cdot \left\{ -c_{ig}\xi_g \lambda_g k \nabla p_{cgo} + \left(\sum_{\alpha=g,o} c_{i\alpha}\xi_\alpha \lambda_\alpha \right) \left(\sum_{\alpha=g,w} \frac{\lambda_\alpha}{\lambda} k \nabla p_{c\alpha o} \right) \right\} = q_i,$$

for $i = 1, \ldots, N$.

We now write ∇p_{cwo} and ∇p_{cgo} in terms of the overall compositions m_T and m_i. For notational simplicity, let p_{cwo} and p_{cgo} satisfy the usual assumption (4.16). Then it follows from (2.3), (2.6), (4.16), and the definition of m_T that

(4.23)
$$\nabla p_{cwo} = \frac{1}{\xi_w} \frac{dp_{cwo}}{ds_w} \left(\nabla m_T - \sum_{i=1}^N \nabla m_i \right),$$
$$\nabla p_{cgo} = \frac{dp_{cgo}}{ds_g} \left(\frac{\partial s_g}{\partial p} \nabla p + \sum_{i=1}^N \sum_{j=1}^N \frac{\partial s_g}{\partial m_{ig}} \frac{\partial m_{ig}}{\partial m_j} \nabla m_j \right).$$

Finally, substitute them into (4.21) and (4.22) to see that

(4.24)
$$\partial_t(\phi m_T) + \nabla \cdot \left(\sum_\alpha \frac{\xi_\alpha \lambda_\alpha}{\lambda} u \right) - \nabla \cdot \left(\sum_\alpha \sum_\beta \frac{\xi_\alpha \lambda_\alpha \lambda_\beta}{\lambda} k(\rho_\beta - \rho_\alpha) g_c \right)$$
$$- \nabla \cdot \left(d_T \nabla m_T + \sum_{j=1}^N (d_{wj} - d_T) \nabla m_j + d_{wp} \nabla p \right) = q_T,$$

where

$$d_T = - \left(\sum_\alpha \frac{\xi_\alpha}{\xi_w} \lambda_\alpha - \lambda \right) \frac{\lambda_w}{\lambda} \frac{dp_{cwo}}{ds_w} k,$$
$$d_{wj} = - \left(\sum_\alpha \xi_\alpha \lambda_\alpha - \xi_g \lambda \right) \frac{\lambda_g}{\lambda} \frac{dp_{cgo}}{ds_g} \sum_{l=1}^N \frac{\partial s_g}{\partial m_{lg}} \frac{\partial m_{lg}}{\partial m_j} k,$$
$$d_{wp} = - \left(\sum_\alpha \xi_\alpha \lambda_\alpha - \xi_g \lambda \right) \frac{\lambda_g}{\lambda} \frac{dp_{cgo}}{ds_g} \frac{\partial s_g}{\partial p} k,$$

and

(4.25)
$$\partial_t(\phi m_i) + \nabla \cdot \left(\sum_{\alpha=g,o} \frac{c_{i\alpha}\xi_\alpha \lambda_\alpha}{\lambda} u \right) - \nabla \cdot \left(\sum_{\alpha=g,o} \sum_\beta \frac{c_{i\alpha}\xi_\alpha \lambda_\alpha \lambda_\beta}{\lambda} k(\rho_\beta - \rho_\alpha) g_c \right)$$
$$- \nabla \cdot \left(d_{iT} \nabla m_T + \sum_{j=1}^N (d_{ij} - d_{iT}) \nabla m_j + d_{ip} \nabla p \right) = q_i,$$

where, for $i = 1, \ldots, N$,

$$d_{iT} = -\left(c_{ig}\frac{\xi_g}{\xi_w}\lambda_g + c_{io}\frac{\xi_o}{\xi_w}\lambda_o\right)\frac{\lambda_w}{\lambda}\frac{dp_{cwo}}{ds_w}k,$$

$$d_{ij} = -\left(c_{ig}\xi_g[\lambda_g - \lambda] + c_{io}\xi_o\lambda_o\right)\frac{\lambda_g}{\lambda}\frac{dp_{cgo}}{ds_g}\sum_{l=1}^{N}\frac{\partial s_g}{\partial m_{lg}}\frac{\partial m_{lg}}{\partial m_j}k,$$

$$d_{ip} = -\left(c_{ig}\xi_g[\lambda_g - \lambda] + c_{io}\xi_o\lambda_o\right)\frac{\lambda_g}{\lambda}\frac{dp_{cgo}}{ds_g}\frac{\partial s_g}{\partial p}k.$$

The system of transport equations consists of (4.24) and (4.25) for m_T and m_i. Its analysis will be carried out in the next subsection.

4.2.1. The analysis of the transport system. We note that the diffusion terms in (4.24) and (4.25) stem from the phase capillary pressures. From the properties of the capillary pressures $p_{c\alpha o}$ and the phase mobilities λ_α ($\alpha = g, w$) [3], these diffusion terms are quite small compared to the advection terms in these equations, as mentioned before. Thus the transport system is advection-dominated. In the sequential solution procedure presented in the next section, we decouple the diffusion terms in these equations by placing the off-diagonal terms and other non-significant terms to the right-hand side. Also, as in [21, 23] we define the barycentric velocities

$$u_T = \frac{1}{\lambda}\left(\frac{\sum_{i=1}^{N}m_{ig}}{m_T}\frac{\lambda_g}{s_g} + \frac{\sum_{i=1}^{N}m_{io}}{m_T}\frac{\lambda_o}{s_o} + \frac{m_w}{m_T}\frac{\lambda_w}{s_w}\right)u,$$

and

$$u_i = \frac{1}{\lambda}\left(\frac{m_{ig}}{m_i}\frac{\lambda_g}{s_g} + \frac{m_{io}}{m_i}\frac{\lambda_o}{s_o}\right)u.$$

With all these, (2.4), (2.6), and also moving the gravity terms to the right-hand side, it follows from (4.24) and (4.25) that

(4.26) $$\partial_t(\phi m_T) + \nabla \cdot (u_T m_T) - \nabla \cdot (d_T^1\nabla m_T) = F_T,$$

where

$$d_T^1 = \lambda_w\frac{dp_{cwo}}{ds_w}k, \quad d_T^2 = -\sum_\alpha\frac{\xi_\alpha}{\xi_w}\frac{\lambda_\alpha\lambda_w}{\lambda}\frac{dp_{cwo}}{ds_w}k,$$

$$F_T = q_T + \nabla \cdot \left(d_T^2\nabla m_T + \sum_{j=1}^{N}(d_{wj} - d_T)\nabla m_j + d_{wp}\nabla p\right)$$

$$+ \nabla \cdot \left(\sum_\alpha\sum_\beta\frac{\xi_\alpha\lambda_\alpha\lambda_\beta}{\lambda}k(\rho_\beta - \rho_\alpha)g_c\right),$$

and

(4.27) $$\partial_t(\phi m_i) + \nabla \cdot (u_i m_i) - \nabla \cdot (d_i^1\nabla m_i) = F_i,$$

where

$$d_i^1 = c_{ig}\xi_g\lambda_g\frac{dp_{cgo}}{ds_g}\sum_{l=1}^N \frac{\partial s_g}{\partial m_{lg}}\frac{\partial m_{lg}}{\partial m_i}k,$$

$$d_i^2 = -\left(c_{ig}\xi_g\lambda_g + c_{io}\xi_o\lambda_o\right)\frac{\lambda_g}{\lambda}\frac{dp_{cgo}}{ds_g}\sum_{l=1}^N \frac{\partial s_g}{\partial m_{lg}}\frac{\partial m_{lg}}{\partial m_i}k,$$

$$F_i = q_i + \nabla\cdot\left(d_{iT}\nabla m_T + \sum_{j=1}^N(\hat{d}_{ij} - d_{iT})\nabla m_j + d_{ip}\nabla p\right)$$

$$+\nabla\cdot\left(\sum_{\alpha=g,o}\sum_\beta \frac{c_{i\alpha}\xi_\alpha\lambda_\alpha\lambda_\beta}{\lambda}k(\rho_\beta - \rho_\alpha)g_c\right),$$

with $\hat{d}_{ij} = d_{ij}$ for $i \neq j$ and $\hat{d}_{ii} = d_i^2$, $i, j = 1, \ldots, N$.

Note that s_g is less dependent on the pressure p, which, together with the physical properties of λ_g and dp_{cgo}/ds_g, implies that d_{wp} and d_{ip} are small compared to the advection terms and other diffusion terms in (4.26) and (4.27). In this case, the terms involving d_{wp} and d_{ip} in F_T and F_i can be neglected.

Now, the mathematical structure of the transport system is clear. Recall that p_{cwo} is the negative water phase capillary pressure, so $dp_{cwo}/ds_w > 0$ by the property of this capillary pressure. Hence if k is positive-definite, then d_T^1 is nonnegative. The degeneracy of d_T^1 is caused by the fact that λ_w can be zero. Therefore, equation (4.26) is a degenerate parabolic problem. Next, it follows from (3.10) that since the molar densities are less dependent on the phase compositions, we have the approximation

$$\frac{\partial s_g}{\partial m_{lg}} \approx \frac{1}{\xi_g}, \qquad l = 1, \ldots, N.$$

Also, as in (3.8), we see that

$$\sum_{l=1}^N \left(\frac{\partial f_{io}}{\partial m_{lo}} + \frac{\partial f_{ig}}{\partial m_{lg}}\right)\frac{\partial m_{lg}}{\partial m_j} = \frac{\partial f_{io}}{\partial m_{jo}}, \qquad i, j = 1, \ldots, N.$$

This equation physically relates how the phase compositions change with respect to the overall hydrocarbon compositions, at the thermal equilibrium state and fixed pressure. Thus each $\partial m_{ig}/\partial m_i$ should be positive [2, 3]. Consequently, these two facts, together with the positiveness of dp_{cgo}/ds_g, imply that d_i^1 is nonnegative; the degeneracy of d_i^1 is caused now by λ_g. Hence, equation (4.27) is also a degenerate parabolic problem. Finally, we mention that there are $N + 2$ equations for the $N + 2$ primary variables $(p, m_T, m_1, \ldots, m_N)$; the equations consist of the pressure equation in (4.6) and (4.8) (respectively, (4.11), (4.14), or (4.18)) and the transport equations in (4.26) and (4.27) (or (4.24) and (4.25) if desired). Other variables can be calculated by them via the algebraic constraints described in section two. With appropriate boundary and initial conditions, the whole compositional system is solvable (see section 5).

From the definition of u_T and u_i and the previous nonlinearity analysis for the pressure equation, we see that the nonlinearity of the transport equations (4.26) and (4.27) is primarily caused by the phase mobilities (i.e., the relative permeabilities)

and the minimization problem (3.5) (equivalently (3.6)). The coupling between (4.26) and (4.27) is due to the volumetric constraint (2.5), and the coupling among the modified mass conservation equations for the hydrocarbon components comes from (3.5) or (3.6). Finally, through the barycentric velocities, the transport system heavily depends on the total velocity u.

We close this section with a remark. In the case where the capillary pressure effects are fully ignored, equations (4.26) and (4.27) become

$$(4.28) \qquad \partial_t(\phi m_T) + \nabla \cdot (u_T m_T) = \hat{F}_T,$$

where

$$\hat{F}_T = q_T + \nabla \cdot \left(\sum_\alpha \sum_\beta \frac{\xi_\alpha \lambda_\alpha \lambda_\beta}{\lambda} k(\rho_\beta - \rho_\alpha) g_c \right),$$

and

$$(4.29) \qquad \partial_t(\phi m_i) + \nabla \cdot (u_i m_i) = \hat{F}_i, \qquad i = 1, \ldots, N,$$

where

$$\hat{F}_i = q_i + \nabla \cdot \left(\sum_{\alpha=g,o} \sum_\beta \frac{c_{i\alpha} \xi_\alpha \lambda_\alpha \lambda_\beta}{\lambda} k(\rho_\beta - \rho_\alpha) g_c \right).$$

In the sequential solution procedure below, we compute the barycentric velocities from the previous time level to linearize and decouple the advection terms in (4.26) and (4.27). This is reasonable since the barycentric velocities are smoother than the phase velocities due to the introduction of the total velocity and the scaling factors in the definition of u_T and u_i. Then it is obvious that equations (4.28) and (4.29) are purely hyperbolic since they are single equations. This is in striking contrast to the long characteristic analysis presented in [27], where the phase velocities were used.

5. Numerical Scheme. In this section we develop a numerical scheme for solving the compositional system derived in the last section. The sequential solution procedure considered below to decouple this system is similar to that in [21, 23].

5.1. A sequential procedure. As mentioned before, the phase compositions of the porous medium fluid are calculated at the thermodynamic phase equilibrium state when a pressure and the overall compositions of the fluid are prescribed. This solution technique for the phase compositions is called a flash calculation in mechanics and is characterized by the minimization problem (3.5) (or equivalently (3.6)). We now state our sequential solution procedure as follows:

  1. At time $t = 0$, the primary variables $(p, m_T, m_1, \ldots, m_N)$ are computed from the initial data.

2. Use the flash calculation to determine the phase compositions $m_{i\alpha}$, $i = 1, \ldots, N$, $\alpha = g$, o.

3. Evaluate the phase viscosities μ_α by empirical correlations [18] and molar and mass densities $(\xi_\alpha, \rho_\alpha)$ by the equation of state [20], and then the mole fractions $c_{i\alpha}$ and saturations s_α by (2.4) and (2.6).

4. Calculate the coefficients of the pressure equation in (4.6) and (4.8) (respectively, (4.11), (4.14), or (4.18)) and some of the coefficients of the transport system in (4.26) and (4.27), and then proceed to the next time level.

5. Apply the mixed finite element method in the next subsection to solve the pressure equation for u (and p if desired).

6. Exploit the total velocity to complete the calculation of the coefficients of the transport system (i.e., to calculate the barycentric velocities u_T and u_i).

7. Utilize the ELLAM method considered below to solve the transport system for $(m_T, m_1, \ldots, m_N)$.

8. Perform a few iterations between the pressure equation, transport system, and constitutive relations at the current time level, if necessary.

9. Go back to step two to update the coefficients at the current time level and repeat the above procedure until a final state $t = \mathcal{T}$ is reached.

In conventional IMPES solution procedures for the simulation of compositional flow in porous media [1, 2, 14, 28, 29], the pressure equation is solved implicitly with its coefficients evaluated explicitly, and the transport system is solved explicitly to obtain the overall mass of each component. Hence, the size of time steps must be restricted to stablize the overall procedure due to the explicit computation of the transport system. Also, in this procedure, initial guesses in the flash calculation are computed in terms of the phase compositions at the previous time level. Consequently, the size of the time steps has to be severely restricted. In contrast, in this paper the sequential procedure is developed to decouple and linearize the compositional system. Instead of calculating the phase velocities, an accurate total velocity is provided by the mixed method for the transport system. The latter is implicitly solved by the ELLAM method, which produces accurate compositions without oscillations and numerical dispersion even if large time steps are taken. Also, for the initial guesses in the flash calculation, the phase compositions are computed from their values at the previous time level by back-tracking through the characteristics used in the ELLAM method. In summary, in our sequential solution procedure the pressure and transport equations are linearized first and then solved implicitly (we call it a sequential semi-implicit method); it fully utilizes the physics of the flow and transport processes, improves the efficiency and accuracy of the flash calculation, and relaxes the time step restrictions. Finally, we mention that there were attempts [13, 14] to solve compositional models in a fully coupled and implicit scheme. This scheme is stable for large time steps, but its application is restricted to very small problems due to limited computational resources.

5.2. Mixed finite element methods. In this subsection we briefly review the mixed finite element method for the pressure equation. For more information on this method for second order problems, see [4].

Recall that the pressure equation can be written in the general form:

$$\begin{aligned}
c\partial_t p + \nabla \cdot u &= q, & (x,t) \in \Omega \times J, \\
u &= -a(\nabla p - b), & (x,t) \in \Omega \times J,
\end{aligned}$$

(5.1)

where $a(x,t)$ is a uniformly positive definite, bounded, symmetric tensor, $b(x,t)$ is a bounded vector, $c(x,t) > 0$ is a bounded function, Ω is the porous medium domain, and $J = (0, \mathcal{T}]$ $(\mathcal{T} > 0)$ is the time interval of interest. Let $\partial\Omega = \bar{\Gamma}_1 \cup \bar{\Gamma}_2$ with $\Gamma_1 \cap \Gamma_2 = \emptyset$. We consider the boundary conditions

$$\begin{aligned}
p &= -g_1, & (x,t) \in \Gamma_1 \times J, \\
u \cdot \nu &= g_2, & (x,t) \in \Gamma_2 \times J,
\end{aligned}$$

(5.2)

where ν is the outer unit normal to Ω, and $q(x,t)$, $g_1(x,t)$, and $g_2(x,t)$ are given functions. Finally, the initial condition is given by

$$p(x,0) = p^0(x), \qquad x \in \Omega.$$

(5.3)

Problem (5.1)–(5.3) is recast in mixed form as follows. Let

$$\begin{aligned}
L^2(\Omega) &= \left\{ w : \int_\Omega |w(x)|^2 \, dx < \infty \right\}, \\
H(\mathrm{div}; \Omega) &= \{ v \in (L^2(\Omega))^d : \nabla \cdot v \in L^2(\Omega) \}, \\
W &= L^2(\Omega), \\
V^\pi &= \{ v \in H(\mathrm{div}; \Omega) : v \cdot \nu = \pi \text{ on } \partial\Gamma_2 \},
\end{aligned}$$

where d is the space dimension of Ω and $\pi(x)$ is a function defined on $\partial\Gamma_2$. Then the mixed form of (5.1) and (5.2) for a pair of maps $(u,p) : J \to V^{g_2} \times W$ is

$$\begin{aligned}
\left(c\partial_t p, w \right) + (\nabla \cdot u, w) &= (q, w), & \forall w \in W, \\
(a^{-1} u, v) - (p, \nabla \cdot v) &= (b, v) + (g, v \cdot \nu)_{\Gamma_1}, & \forall v \in V^0,
\end{aligned}$$

(5.4)

where $(\cdot, \cdot)$ is the $L^2(\Omega)$ or $(L^2(\Omega))^d$ inner product, as appropriate, and $(\cdot, \cdot)_{\Gamma_1}$ denotes the duality paring between $H^{1/2}(\Gamma_1)$ and $H^{-1/2}(\Gamma_1)$. System (5.4) is obtained from (5.1) by Green's formula. This system has a unique solution [4].

To define a finite element method, we need a partition $\mathcal{E}_h$ of Ω into elements E, say, simplexes, rectangular parallelepipeds, and/or prisms, where only faces on the boundary $\Gamma = \partial\Omega$ may be curved. In $\mathcal{E}_h$, we also need that adjacent elements completely share their common face. Finally, each exterior face has imposed either Dirichlet or Neumann conditions on it.

Let $V_h^\pi \times W_h \subset V^\pi \times W$ denote some standard mixed finite element space for second-order elliptic problems defined over $\mathcal{E}_h$ (see [5, 6, 7, 10, 19, 24] for all the mixed spaces). The mixed finite element solution of (5.4) is $(u_h, p_h) : J \to V_h^{g_2} \times W_h$ satisfying

$$(5.5) \qquad \begin{aligned} \left(c\partial_t p_h, w\right) + (\nabla \cdot u_h, w) &= (q, w), & \forall w \in W_h, \\ (a^{-1} u_h, v) - (p_h, \nabla \cdot v) &= (b, v) + (g, v \cdot \nu)_{\Gamma_1}, & \forall v \in V_h^0. \end{aligned}$$

The approximate initial datum is given by

$$(5.6) \qquad\qquad p_h(x, 0) = p_h^0(x), \qquad x \in \Omega,$$

where p_h^0 is an appropriate approximation in W_h of p^0. The system in (5.5) and (5.6) again has a unique solution. The time differentiation term can be discretized by the standard backward Euler scheme or other more accurate time stepping procedures, for example. The linear system arising from (5.5) is a saddle point problem. To see how to solve this saddle point problem, refer to [12]. As remarked before, the mixed method yields accurate approximations to both the pressure and velocity in a mass-conservative manner. Also, it can handle complicated boundary conditions and geological boundaries.
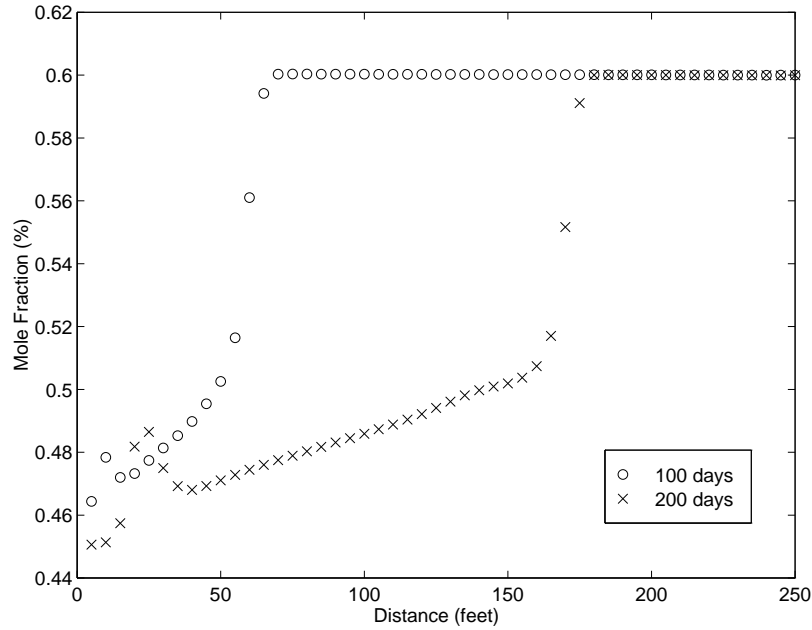
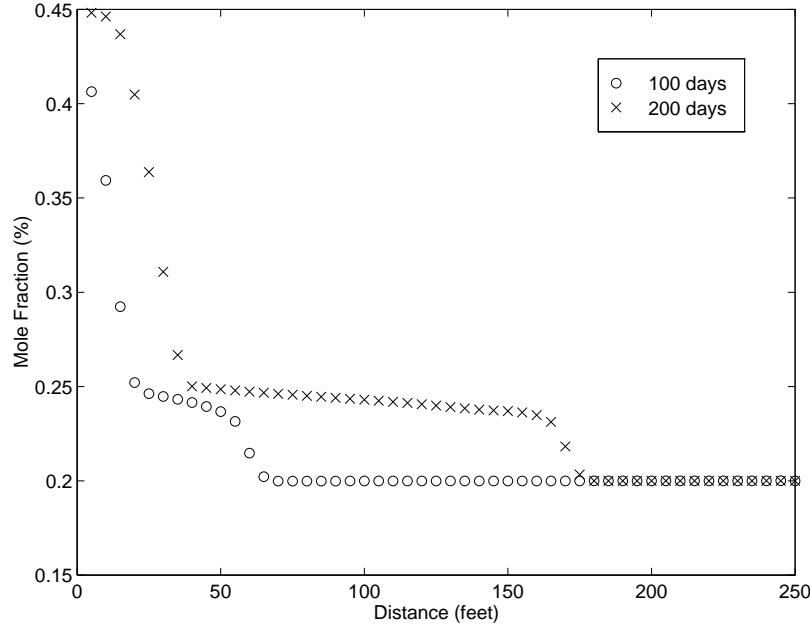FIG. 1. Profile of the mole fraction of methane.

Fig. 2. *Profile of the mole fraction of butane.*

5.3. ELLAM methods. Recall that equations (4.26) and (4.27) are advection-dominated; they are more hyperbolic. Standard finite difference and finite element methods produce numerical solutions with excessive oscillations, while upwinding and stablized versions of these methods tend to generate solutions with nonphysical dispersions. Although conventional Eulerian-Lagrangian methods can overcome these difficulties, they fail to conserve mass. Here we very briefly review the Eulerian-Lagrangian localized adjoint method (ELLAM), which can accurately and efficiently solve advection-dominated problems in a mass-conservative manner.

The transport equations can be written in the form:

$$(5.7) \qquad \partial_t(\phi m) + \nabla \cdot (Vm - D\nabla m) = q, \qquad (x,t) \in \Omega \times J.$$

For each positive integer I, let $0 = t^0 < t^1 < \cdots < t^I = \mathcal{T}$ be a partition of J into subintervals $J^n = (t^{n-1}, t^n]$. With any space-time test function v that vanishes outside $\bar{\Omega} \times J^n$ and is possibly discontinuous in time at t^{n-1}, a space-time weak formulation of (5.7) reads as follows:

$$(5.8) \quad \begin{aligned} &\big(\phi(t^n)m(t^n), v(t^n)\big) + \int_{J^n}(D\nabla m, \nabla v)\mathrm{d}t + \int_{J^n}(Vm - D\nabla m)\cdot \nu, v)_\Gamma \mathrm{d}t \\ &- \int_{J^n}(m, \phi\partial_t v + V\cdot\nabla v)\mathrm{d}t = \Big(\phi(t^{n-1})m(t^{n-1}), v(t^{n-1}_+)\Big) + \int_{J^n}(q,v)\mathrm{d}t, \end{aligned}$$

where $v(x, t_+^{n-1}) = \lim_{t \to t_+^{n-1}} v(x, t)$. In the ELLAM method, the test function v is chosen from the solution space of the adjoint problem of (5.7)

$$(5.9) \qquad -\phi \partial_t v - V \cdot \nabla v - \nabla \cdot (D \nabla v) = 0.$$

This solution space is infinite-dimensional. For a numerical procedure, only a finite number of test functions are needed. Different choices of these functions lead to different classes of approximation methods. In the localized adjoint method used in this paper, the test function v is assumed to satisfy

$$(5.10) \qquad \phi \partial_t v + V \cdot \nabla v = 0 \quad \text{and} \quad \nabla \cdot (D \nabla v) = 0.$$

This implies that v is constant along the characteristics in the direction (ϕ, V). In general, we cannot track the characteristics exactly; the test function should be constant along approximate characteristics. Also, it follows from (5.10) that v can be chosen as standard hat functions in space. Substituting the test functions into (5.8) and carrying out some algebraic manipulations, we can derive the ELLAM method from the resulting weak formulation. For further details on this method, consult [8].
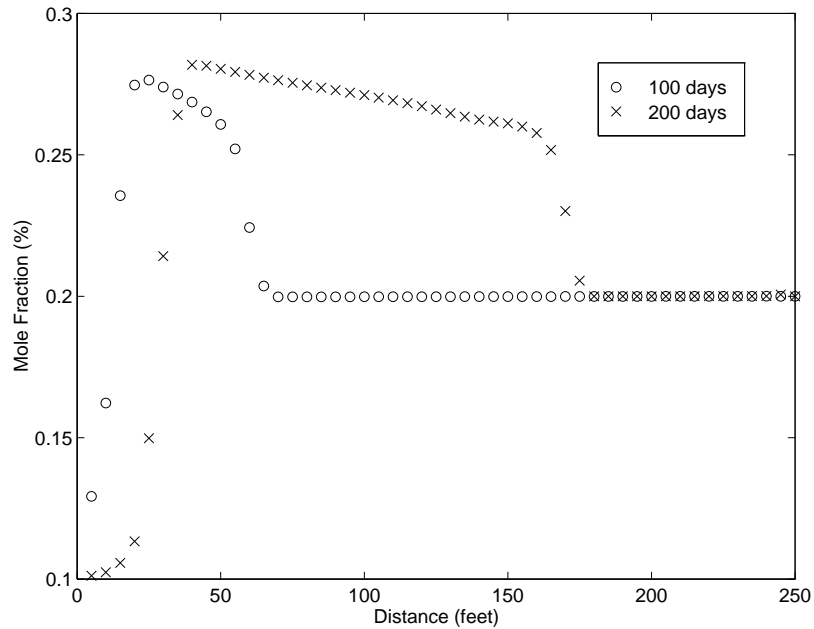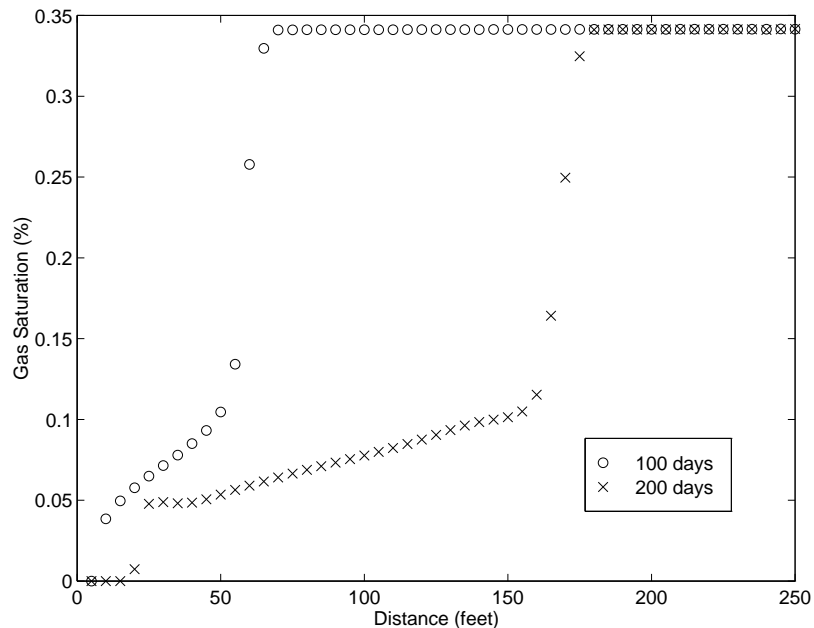

FIG. 3. Profile of the mole fraction of decane.

FIG. 4. *Profile of the gas saturation.*

6. Numerical Tests. The major part of this paper is concerned with the development and analysis of the compositional model and its numerical scheme. In this section we report numerical results for a test example. A comparison of various formulations derived in section 4 has been given in [11] through numerical experiments for the flow of three immiscible fluids in a porous medium. Since the structure of these formulations has the same pattern here, as mentioned before, the test example presented here does not involve the comparison. To have an example applicable to all these formulations, we take the zero capillary pressures

$$p_{cgo} = p_{cwo} = 0.$$

In this case, all the formulations are the same. Also, a comparison of the numerical methods exploited here with other methods such as upwinding finite difference and high-order TVD methods has been described in [23]. We shall not compare our numerical scheme with others. Finally, the main purpose of the test example is to show the behavior of the solution to the compositional system obtained in previous sections, so we shall consider a one-dimensional problem.

The one-dimensional porous medium is 250 ft in length with a sectional area of 50 ft^2. The porosity of the medium is taken to be 20%. The initial pressure is 2000 psi, the temperature is 160° F, and the permeability of the medium is 2 darcy. The
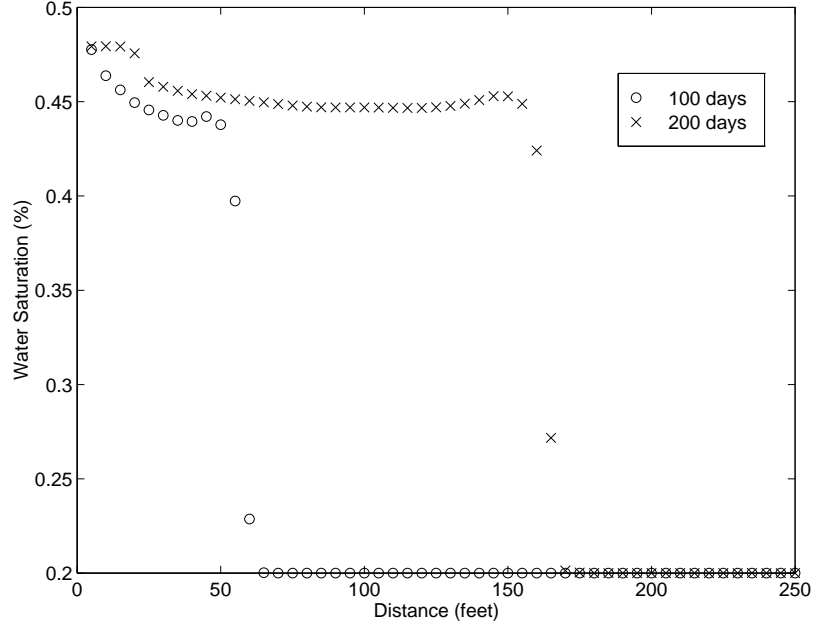
FIG. 5. Profile of the water saturation.

relative permeability functions are defined by the modified Corey's model [15]

$$k_{rg} = \bar{s}_g^{2.5} \left(1 - (1 - \bar{s}_g)^2\right), \quad k_{ro} = \bar{s}_o^{2.5} \left(1 - (1 - \bar{s}_o)^3\right), \quad k_{rw} = 0.1\bar{s}_w^3,$$

where the normalized saturations are given by

$$\bar{s}_g = \frac{s_g - s_{rg}}{1 - s_{rg} - s_{ro} - s_{rw}}, \quad \bar{s}_o = \frac{s_o - s_{ro}}{1 - s_{ro} - s_{rw}}, \quad \bar{s}_w = \frac{s_w - s_{rw}}{1 - s_{ro} - s_{rw}}$$

with the residual saturations

$$s_{rg} = 0, \quad s_{ro} = 0.25, \quad s_{rw} = 0.35.$$

The initial water saturation is 20% and oil saturation is 80%. The molar density of the water phase is 3.467 lb-mole/ft^3 and its viscosity is 0.5 cp. The oil phase is composed of 20% methdane (light hydrocarbon component), 20% butane (medium hydrocarbon component), and 60% decane (heavy hydrocarbon component).

In the test example, we inject 95% water and 5% hydrocarbon mixture (45% methdane, 45% butane, and 5% decane) into the porous medium, and the total injection rate is 1000 lb-mole per day. This example involves a three-phase fluid flow process. The lowest-order Raviart-Thomas space [24] over 40, 50, and 80 elements is
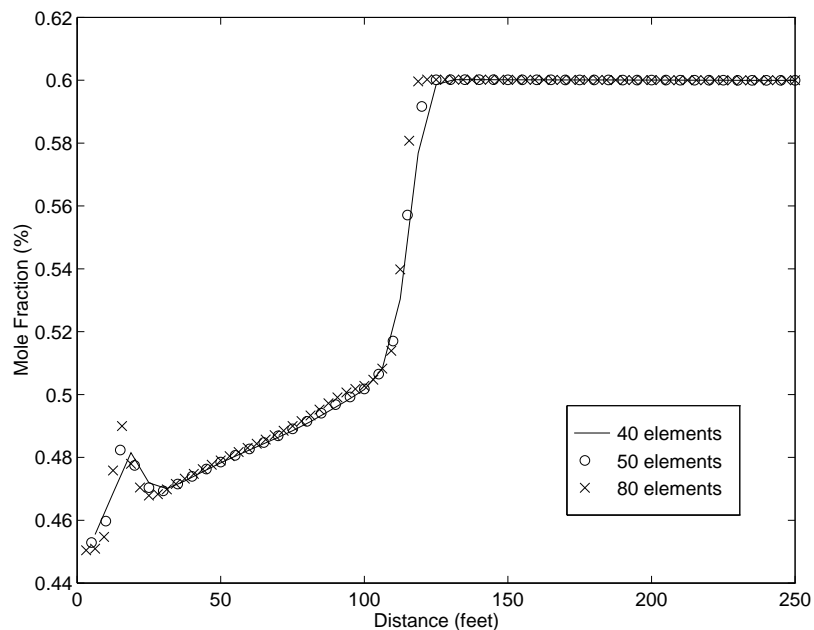
FIG. 6. Profile of the mole fraction of methane.

used, and the sequential solution procedure developed in section five is utilized. The profiles of the mole fractions of methdane, butane, and decane and of the saturations of the gas and phases are displayed in Figures 1–5. The profiles per element vs distance at 100 and 200 days for the experiment of 50 elements are illustrated in these figures. As seen from them, the numerical scheme is stable and captures the sharp front of the solutions. Note that water is the main stream of the injecting fluid, and a water front is formed and propagated as time evolves (at about 55 and 155 ft at 100 and 200 days, respectively, in Figure 5). Also, notice that the porous medium pressure is increased due to the injection, so the resident hydrocarbon fluid is vaporized to form a gas zone, as shown in Figure 4. Figure 3 describes the computed number of the mole fractions of decane, which is the main stream in the oil phase. Note that the transition of the decane corresponds to the intersection of the water and gas fronts. In Figures 6–10, we show the results of varying the grid size; i.e., the profiles of the mole fractions of methdane, butane, and decane and of the saturations of the gas and phases at 150 days for the experiments of 40, 50, and 80 elements are presented. We clearly see the stability and convergence of the numerical scheme proposed here.

7. Conclusions. The compositional flow for multicomponent three-phase fluids in porous media involves a time-dependent, strongly coupled system of an enormous
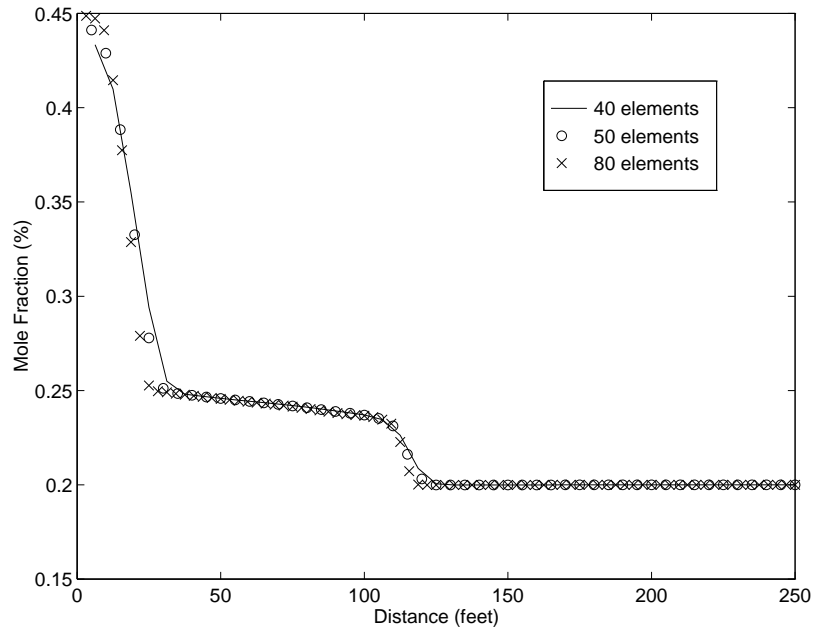
FIG. 7. Profile of the mole fraction of butane.

number of nonlinear partial differential equations and algebraic constraints. For large-scale petroleum fields, this system cannot be solved in a fully coupled and implicit manner. To devise a suitable numerical algorithm for solving it, we have to derive appropriate formulations for these differential equations and algebraic constraints. In this paper, with proper choices of primary variables we have developed a compositional model for multicomponent, multidimensional three-phase fluid flow in porous media. Various pressure formulations have been incorporated in this system to alleviate nonlinearities and couplings. The mathematical analysis carried out here provides a qualitative structure of this compositional model. The analysis is also useful in the design of numerical methods for solving this model. With the mixed finite element method, we can obtain accurate volumetric flow velocities, which are heavily used in the Eulerian-Lagrangian localized adjoint method for the transport system. The latter method is both accurate and efficient for handling advection-dominated problems. The numerical experiments done so far show a strong potential of the numerical scheme proposed in this paper.

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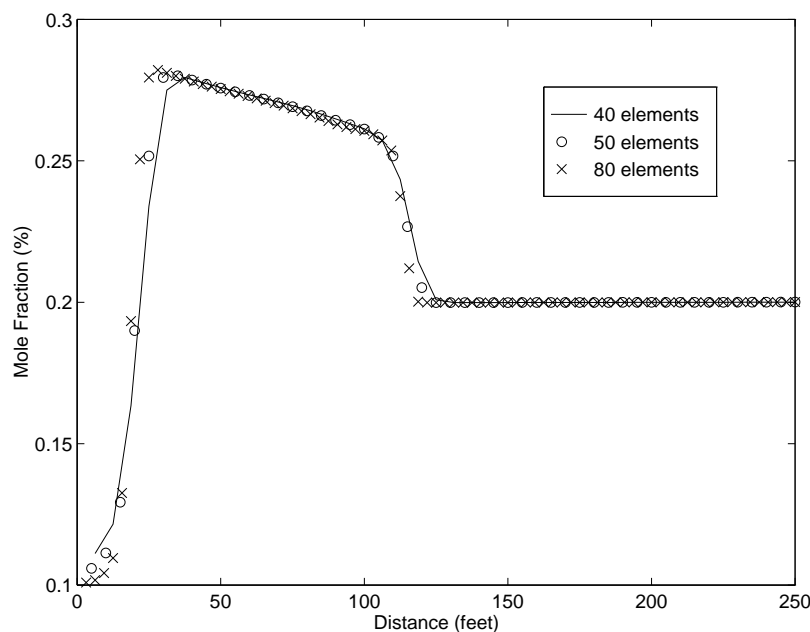
FIG. 8. Profile of the mole fraction of decane.

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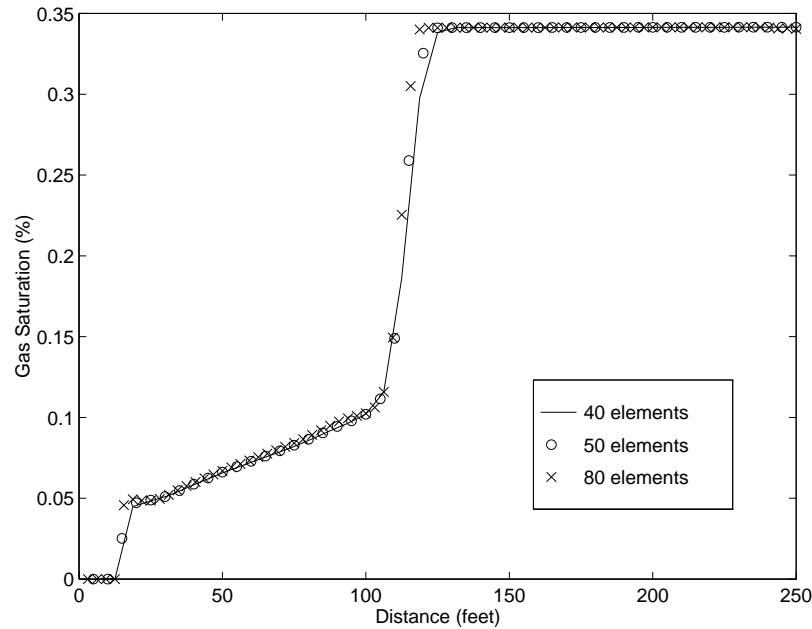
FIG. 9. Profile of the gas saturation.

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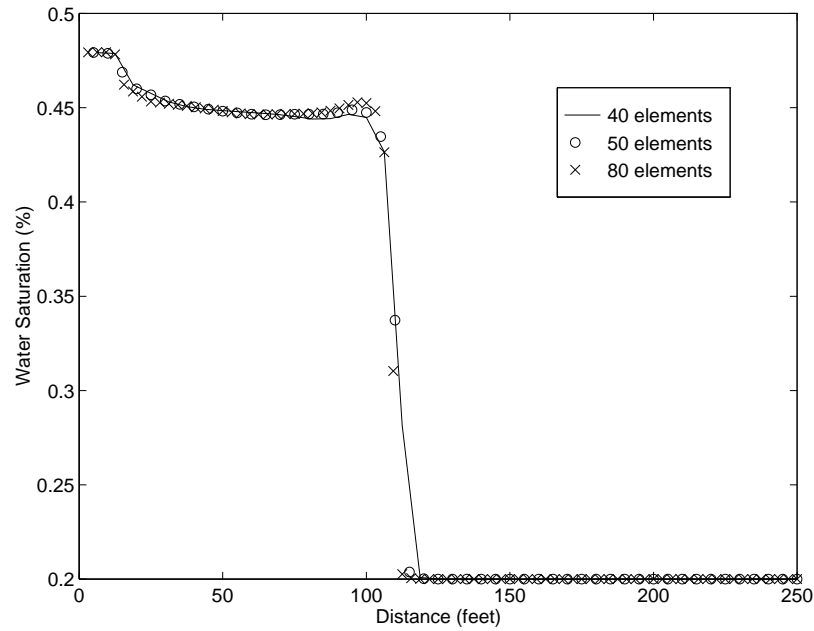
FIG. 10. Profile of the water saturation.

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