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From Single-Phase to Compositional Flow: Applicability of Mixed Finite Elements

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Abstract. In this paper we discuss the formulation of the governing equations that describe flow of fluids in porous media. Various types of fluid flow, ranging from single-phase flow to compositional flow, are considered. It is shown that all the differential equations governing these types of flow can be effectively rewritten in a fractional flow formulation; i.e., in terms of a global pressure and saturation (or saturations), and that mixed finite element methods can be accurately exploited to solve the pressure equation. Numerical results are presented to see the performance of the mixed methods for the flow equations in three space dimensions.

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1. Introduction

Multiphase flow of fluids in porous media is physically and chemically complex. It involves heterogeneities in the porous media at many different length scales and complicated processes such as diffusion and dispersion. Numerical simulation of these phenomena is a critical step in understanding multicomponent, multiphase flow in porous media (see, e.g., [21] and the bibliography therein).

There are two critical factors that determine the choice of discretization techniques for numerically solving the governing differential equations describing flow of fluids in porous media, the mathematical properties of the differential equations and the geometry of the porous media [21]. It is well known that the transport and diffusion/dispersion terms in the flow and transport equations are governed by fluid velocities [13, 17, 21]. Thus accurate numerical simulation requires accurate approximations for these velocities. Often the flow properties of the porous media change abruptly with sharp changes in lithology. Also, the viscosity changes rapidly in space across fluid interfaces. Consequently, the coefficient in the flow equations is quite rough. In order for fluids to flow smoothly, pressures change

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extremely rapidly. Standard finite difference and finite element methods for solving these flow equations determine a pressure, and then a velocity by differencing or differentiating the resulting pressure and multiplying it by the rough coefficient. This approach generates a rough and inaccurate velocity which then reduces the accuracy of numerical simulation of the fluid flow in porous media [21]. Also, the geologic structure and topography of porous media can have a significant impact on the flow. Finite volume methods with harmonic averaging of the coefficient, which has been very popular in the numerical simulation of flow in porous media, cannot accurately describe the geologic structure and topography.

On the other hand, mixed finite element methods have proven to be very powerful in overcoming the difficulties mentioned above for the standard methods [17, 18]. They can effectively treat the problem of rapidly changing flow properties in porous media, and produce accurate fluid velocities. Further, they conserve mass locally; this property is very important in physics since the flow equations are based on the mass balance law. Finally, the mixed methods can easily handle complicated geometries.

The purpose of this paper is to discuss the applicability of the mixed finite element methods to various types of flow in porous media. These methods have been applied to the solution of the pressure equation in the problem of the single-phase, miscible displacement of one fluid by another [17]. In this paper we show how the mixed methods can be also used to numerically solve two-phase flow, three-phase flow, and compositional flow with mass interchange between phases. We first prove that the governing equations in these types of flow can be written in a fractional flow formulation; i.e., in terms of a global pressure and saturation (or saturations). Then we show that the mixed methods can be applied to solve the pressure equation in the same manner as for the single-phase flow. Finally, extensive numerical results are presented to illustrate the performance of the mixed methods for the flow equations; special attention is paid to a comparison of the mixed methods using different finite elements. Numerical simulation of three-phase flow in a porous medium is also given. Discretization techniques for the solution of the saturation and transport equations are not discussed here; the aim of this paper is to discuss the applicability of the mixed methods to the flow equations.

The rest of the paper is organized as follows. We review the differential problem describing single-phase flow in Section 2. Then, in Section 3 we consider the problem of single-phase, miscible displacement of one (both incompressible and compressible) fluid by another. In Sections 4, 5, and 6, respectively, we derive the differential systems that govern two-phase, three-phase, and compositional flow in a porous medium in a form which very closely resembles that for the single-phase flow. Mixed finite element methods applied to solve the flow equations in all these cases are described in Section 7. Numerical results are presented in Section 8. A concluding remark is given in Section 9. Finally, an appendix is provided with the derivation of various differential equations.

2. Single-Phase Flow

To motivate the later sections, in this section we describe the flow of a fluid in a porous medium $\Omega \subset \Re^3$ with density ρ and pressure p. The usual equations describing single-phase flow in Ω are well understood ([2, 24]):

$$\frac{\partial(\phi\rho)}{\partial t} + \nabla \cdot (\rho u) = \rho q, \quad x \in \Omega, \ \ t > 0, \tag{2.1a}$$

$$u = -\frac{k}{\mu}(\nabla p - \rho\tilde{g}), \quad x \in \Omega, \ \ t > 0, \tag{2.1b}$$

where ϕ and k are the porosity and absolute permeability of the porous medium, u is the volumetric velocity, μ is the viscosity of the fluid, $\tilde{g}$ is the gravitational, downward-pointing, constant vector, and q the source/sink term. We assume that the density satisfies the equation of state

$$\frac{\mathrm{d}\rho}{\rho} = z\,\mathrm{d}p, \tag{2.2}$$

where z is the compressibility factor. Using (2.2), (2.1) becomes

$$\frac{\partial(\phi\rho)}{\partial t} + \nabla \cdot u' = \rho q, \quad x \in \Omega, \ \ t > 0, \tag{2.3a}$$

$$u' = -\frac{k}{z\mu}(\nabla\rho - z\rho^2\tilde{g}), \quad x \in \Omega, \ \ t > 0. \tag{2.3b}$$

As mentioned in the introduction, the fluid velocity u (or the flux u') is of importance in practical situations. Also, the tensor k can be discontinuous. Mixed finite element methods (see the seventh section) can be applied to approximate u (or u') and p (or ρ) simultaneously, via the coupled system of the first-order differential equations in (2.3). This formulation allows the removal of singular terms and accurately treats the problem of rapidly changing flow properties in porous media, as described above. The use of the mixed methods instead of the standard finite difference and finite element methods for the flow equations can be more obviously seen in the next section where we treat the miscible displacement of one fluid by another.

3. Miscible Displacement of One Fluid by Another

In this section we consider the single-phase, miscible displacement of one fluid by another in a porous medium $\Omega \subset \Re^3$. We assume that no volume change results from the mixing of the components. Let c_i denote the (volumetric) concentration of the ith component of the fluid mixture, $i = 1, \ldots, N$, where N is the number

of components. Then, conservation of mass of the ith component in the mixture is given by the expression

$$\frac{\partial(\phi\rho_i c_i)}{\partial t} + \nabla\cdot(\rho_i c_i u) - \nabla\cdot(\rho_i D\nabla c_i) = \rho_i \widetilde{c}_i q, \quad x\in\Omega,\ t>0, \tag{3.1}$$

where the Darcy velocity of the fluid is given again by Darcy's flow

$$u = -\frac{k}{\mu}(\nabla p - \rho\widetilde{g}), \quad x\in\Omega,\ \ t>0, \tag{3.2}$$

$\widetilde{c}_i$ is the concentration of the ith component in the external flow, and D is the diffusion-dispersion coefficient given by

$$D(u) = \phi\{d_m I + |u|(d_l E(u) + d_t E^{\perp}(u))\},$$

where I is the 3×3 identity matrix, $E(u) = \{u_j u_k/|u|^2\}$ is the 3×3 matrix representing orthogonal projection along the velocity vector and $E^{\perp}(u) = I - E(u)$ its orthogonal complement, d_m is the molecular diffusion coefficient, and d_l and d_t are, respectively, the longitudinal and transverse dispersion coefficients. The terms $\widetilde{c}_i$ must be specified at points where injection (i.e., $q>0$) takes place, and $\widetilde{c}_i$ is assumed to be equal to c_i at production points.

We assume that the density ρ_i depends solely on the pressure p and takes the equation of state in the form (2.2); i.e.,

$$\frac{\mathrm{d}\rho_i}{\rho_i} = z_i\,\mathrm{d}p, \tag{3.3}$$

where z_i is the compressibility factor for the ith component. Carrying out the differentiation indicated in (3.1), and using (3.3) and the relations

$$\sum_{i=1}^{N} c_i = \sum_{i=1}^{N}\widetilde{c}_i = 1, \tag{3.4}$$

we obtain the equation for the pressure (see the Appendix)

$$\begin{aligned} &d(c_1,\dots,c_N)\frac{\partial p}{\partial t} + \nabla\cdot u + b(c_1,\dots,c_N,u)\cdot\nabla p = q,\\ &x\in\Omega,\ \ t>0, \end{aligned} \tag{3.5}$$

where

$$d(c_1,\dots,c_N) = \sum_{i=1}^{N}\phi z_i c_i, \qquad b(c_1,\dots,c_N,u) = \sum_{i=1}^{N} z_i(c_i u - D\nabla c_i).$$

Note that the transport and the diffusion–dispersion terms in (3.1) are governed by the velocity u; the mixed finite element methods solve Equations (3.2) and (3.5) simultaneously to produce an accurate approximation for u. The use of these methods for the single-phase, miscible displacement of one incompressible fluid by another was first developed in [17]; then the approach was extended to the case where the components are assumed to be slightly compressible in [18]. We mention that the concentration Equation (3.1) is dominated by the convection term and can be solved, for example, by characteristic based methods [19].

4. Two-Phase Flow

The usual equations describing two-phase immiscible flow in a porous medium $\Omega \subset \Re^3$ are again given by the mass balance Equation and Darcy's law for each of the fluid phases:

$$\frac{\partial(\phi\rho_\alpha s_\alpha)}{\partial t} + \nabla\cdot(\rho_\alpha u_\alpha) = \rho_\alpha q_\alpha, \quad x \in \Omega, \ \ t > 0, \tag{4.1a}$$

$$u_\alpha = -\frac{kk_{r\alpha}}{\mu_\alpha}(\nabla p_\alpha - \rho_\alpha \tilde{g}), \quad x \in \Omega, \ \ t > 0, \tag{4.1b}$$

where $\alpha = w$ denotes the wetting phase (e.g. water), $\alpha = n$ indicates the nonwetting phase (e.g. oil or air), ρ_α, s_α, p_α, u_α, and μ_α are, respectively, the density, (reduced) saturation, pressure, volumetric velocity, and viscosity of the α-phase, q_α is the source/sink term, and $k_{r\alpha}$ is the relative permeability of the α-phase. In addition to (4.1), we also have the customary property for the saturations

$$s_w + s_n = 1. \tag{4.2}$$

The capillary pressure function is defined by

$$p_c(s_w) = p_n - p_w. \tag{4.3}$$

For expositional convenience, we introduce the phase mobility functions

$$\lambda_\alpha = k_{r\alpha}\rho_\alpha/\mu_\alpha, \quad \alpha = w, n,$$

and the total mobility

$$\lambda = \lambda_w + \lambda_n.$$

Finally, we define the fractional flow functions

$$f_\alpha = \lambda_\alpha/\lambda, \quad \alpha = w, n.$$

While the equations in (4.1) formally seem very different from those presented in (3.1), (3.2), and (3.5) in the last section, they can be rearranged in a form which quite closely resembles them. To this end, define the global pressure ([1, 5, 13])

$$p = \tfrac{1}{2}(p_n + p_w) + \frac{1}{2}\int_{s_c}^{s} \frac{\lambda_n - \lambda_w}{\lambda}\frac{\mathrm{d}p_c}{\mathrm{d}\xi}\xi,$$

where $s = s_w$ and s_c is such that $p_c(s_c) = 0$. That is, by (4.3),

$$p = p_n - \int_0^{p_c(s)} f_w(x, p_c^{-1}(\xi))\,\mathrm{d}\xi. \tag{4.4}$$

Also, introduce the weighted total velocity (i.e., the total flux)

$$u = \rho_w u_w + \rho_n u_n. \tag{4.5}$$

Then it follows from (4.2)–(4.5) that the equations in (4.1) can be written as follows (see the Appendix)

$$\frac{\partial}{\partial t}(\phi(\rho_w s_w + \rho_n s_n)) + \nabla \cdot u = \rho_w q_w + \rho_n q_n, \quad x \in \Omega, \ \ t > 0, \tag{4.6a}$$

$$u = -k\lambda(\omega(p, s)\nabla p - G_\lambda), \quad x \in \Omega, \ \ t > 0, \tag{4.6b}$$

and

$$\frac{\partial}{\partial t}(\phi\rho_w s_w) + \nabla \cdot (f_w u + k\lambda f_w f_n \tilde{g}(\rho_w - \rho_n)) + \nabla \cdot (k\lambda f_w f_n \nabla p_c)$$
$$= \rho_w q_w, \quad x \in \Omega, \ \ t > 0, \tag{4.7}$$

where

$$\omega(p, s) = 1 + \int_0^{p_c(s)} \frac{\partial}{\partial p} f_w(p, p_c^{-1}(\xi))\,\mathrm{d}\xi, \qquad G_\lambda = (f_w\rho_w + f_n\rho_n)\tilde{g}.$$

Equations (4.6) and (4.7) are the pressure and saturation equations, respectively. Further, it can be seen that the phase velocity is related to the total velocity by

$$u_w = \rho_w^{-1}(f_w u + k\lambda f_w f_n(\nabla p_c + \tilde{g}(\rho_w - \rho_n))), \tag{4.8a}$$

$$u_n = \rho_n^{-1}(f_n u - k\lambda f_w f_n(\nabla p_c + \tilde{g}(\rho_w - \rho_n))). \tag{4.8b}$$

Now we see that the pressure equations in (4.6) have the same form as those in (3.2) and (3.5), and that the saturation equation (4.7) has the same property as the concentration equation (3.1). Thus, the mixed methods can be used to solve (4.6) for u and p simultaneously, and Equation (4.7) can be dealt with by any methods suitable for convection-dominated problems.

We end this section with two remarks. First, instead of the total flux in (4.5), we could just use the total velocity $u = u_w + u_n$, and derive a similar set of differential equations [10, 11, 13]. However, evidently it follows from (4.5) that the total flux behaves more smoothly. Second, we present a physical explanation for the global pressure p. It follows from (4.3) and (4.4) (also see the Appendix) that

$$\lambda\omega(p, s)\nabla p = \lambda_w \nabla p_w + \lambda_n \nabla p_n.$$

This implies that the global pressure is the pressure that would produce a flow of a fluid (with mobility $\lambda\omega$) equal to the sum of the flows of fluids w and n.

5. Three-Phase Flow

We now extend the approach used for the two-phase flow to the flow of three immiscible fluids in a porous medium $\Omega \subset \Re^3$. The mass balance equation and Darcy's law for each of the fluid phases are expressed by

$$\frac{\partial(\phi\rho_\alpha s_\alpha)}{\partial t} + \nabla \cdot (\rho_\alpha u_\alpha) = \rho_\alpha q_\alpha, \quad x \in \Omega, \ \ t > 0, \tag{5.1a}$$

$$u_\alpha = -\frac{k k_{r\alpha}}{\mu_\alpha}(\nabla p_\alpha - \rho_\alpha \tilde{g}), \quad x \in \Omega, \ \ t > 0, \tag{5.1b}$$

where $\alpha = w$, o, and g denote water, oil, and gas phases, respectively, for example. In addition, we also have

$$\sum_\alpha s_\alpha = 1, \tag{5.2}$$

where (and later) $\Sigma_\alpha = \Sigma_{\alpha=w,o,g}$, and define, for notational convenience, the capillary pressure functions

$$p_{c\alpha o}(s_w, s_g) = p_\alpha - p_o, \quad \alpha = w, o, g, \tag{5.3}$$

where $p_{coo} \equiv 0$, p_{cgo} represents the gas phase capillary pressure, and p_{cwo} is the negative water phase capillary pressure. The phase and total mobility and fractional flow functions are defined in the same way as before; i.e.,

$$\lambda_\alpha = k_{r\alpha}\frac{\rho_\alpha}{\mu_\alpha}, \qquad \lambda = \sum_\alpha \lambda_\alpha, \qquad f_\alpha = \frac{\lambda_\alpha}{\lambda}, \quad \alpha = w, o, g.$$

The case of three-phase flow is quite different from the case of two-phase flow. The three-phase relative permeability and capillary pressure curves are far more complex than the corresponding two-phase curves. It is the complexity of these three-phase curves that complicates the derivation of the global pressure-saturation form for this case. In the two-phase flow, the governing equations can be written in

terms of a global pressure and saturation without any hypothesis, as seen in the last section. However, in the three-phase flow we need a condition on the shape of three-phase relative permeability and capillary pressure curves, which is in fact necessary and sufficient for the governing equations to be written in terms of a global pressure and two saturations. While this condition is not satisfied for all the existing three-phase curves, it has been shown [12] that it is satisfied for some simplified models [15, 16]. Also, a simple numerical procedure for constructing three-phase relative permeability and capillary pressure curves satisfying this condition has been given in [5], some of the numerical examples have been compared with the classical Stone's model [27], which does not satisfy this condition, and similar results have been obtained.

We assume that the fractional flow functions f_α depend on the saturations s_w and s_g and a pressure p (some as yet unspecified pressure), and that there exists a function $p_c(s_w, s_g, p)$ satisfying

$$\nabla p_c = f_w \nabla p_{cwo} + f_g \nabla p_{cgo} + \frac{\partial p_c}{\partial p} \nabla p. \tag{5.4}$$

The assumption on the dependence on the pressure p means that we ignore the error caused by calculating the density and viscosity functions for the α-phase at p instead of p_α. For details on this error, the reader is referred to [13] for a similar treatment for the two-phase flow. It follows [5, 12] that a necessary and sufficient condition for existence of a function p_c satisfying (5.4) is

$$\frac{\partial f_w}{\partial s_g}\frac{\partial p_{cwo}}{\partial s_w} + \frac{\partial f_g}{\partial s_g}\frac{\partial p_{cgo}}{\partial s_w} = \frac{\partial f_w}{\partial s_w}\frac{\partial p_{cwo}}{\partial s_g} + \frac{\partial f_g}{\partial s_w}\frac{\partial p_{cgo}}{\partial s_g}, \tag{5.5}$$

where p is treated as a parameter. Under the condition (5.5), the function p_c is described by

$$\begin{aligned} &p_c(s_w, s_g, p) \\ &= \int_1^{s_w} \left\{ f_w(\xi, 0, p) \frac{\partial p_{cwo}}{\partial s_w}(\xi, 0) + f_g(\xi, 0, p) \frac{\partial p_{cgo}}{\partial s_w}(\xi, 0) \right\} \mathrm{d}\xi + \\ &\quad + \int_0^{s_g} \left\{ f_w(s_w, \xi, p) \frac{\partial p_{cwo}}{\partial s_g}(s_w, \xi) + f_g(s_w, \xi, p) \frac{\partial p_{cgo}}{\partial s_g}(s_w, \xi) \right\} \mathrm{d}\xi. \end{aligned} \tag{5.6}$$

We now define the global pressure by

$$p = p_o + p_c, \tag{5.7}$$

and the total flux by

$$u = \sum_\alpha \rho_\alpha u_\alpha. \tag{5.8}$$

Then, using (5.2)–(5.8), the equations in (5.1) can be rewritten as follows (see the Appendix)

$$\sum_{\alpha} \frac{\partial(\phi\rho_\alpha s_\alpha)}{\partial t} + \nabla \cdot u = \sum_{\alpha} \rho_\alpha q_\alpha, \tag{5.9a}$$

$$u = -k\lambda(\omega\nabla p - G_\lambda), \tag{5.9b}$$

and

$$\frac{\partial(\phi\rho_\alpha s_\alpha)}{\partial t} + \nabla \cdot \left\{\omega^{-1} f_\alpha u + k\lambda_\alpha(\nabla(p_c - p_{c\alpha o}) - \delta_\alpha) - \omega^{-1}\frac{\partial p_c}{\partial p} G_\lambda\right\}$$
$$= \rho_\alpha q_\alpha, \quad \alpha = w, g, \tag{5.10}$$

where

$$\omega(s_w, s_g, p) = 1 - \frac{\partial p_c}{\partial p}, \qquad G_\lambda = \tilde{g}\sum_{\alpha} f_\alpha \rho_\alpha,$$

and

$$\delta_\alpha = \left(f_\beta(\rho_\beta - \rho_\alpha) + f_\gamma(\rho_\gamma - \rho_\alpha)\right)\tilde{g},$$
$$\alpha, \beta, \gamma = w, o, g, \quad \alpha \neq \beta, \quad \beta \neq \gamma, \quad \gamma \neq \alpha.$$

The phase velocity is computed by

$$u_\alpha = \rho_\alpha^{-1}\left\{\omega^{-1} f_\alpha u + k\lambda_\alpha(\nabla(p_c - p_{c\alpha o}) - \delta_\alpha) - \omega^{-1}\frac{\partial p_c}{\partial p} G_\lambda\right\}, \tag{5.11}$$
$$\alpha = w, o, g.$$

The pressure and saturation equations in (5.9) and (5.10) look like those in (4.6) and (4.7), respectively, for the two-phase flow. Thus the approximate methods mentioned earlier can be used to solve Equations (5.9) and (5.10).

Condition (5.5) is referred to as the total differential condition [5, 12]. If we had not assumed this condition, the coupling between the pressure and saturation equations would be much stronger [12]. For other formulations of the governing equations for three-phase fluid flow in a porous medium without this condition, the reader is referred to [12]. The beauty of the global pressure-saturation form is that the three-phase differential system derived via it resembles that for the single-phase flow. Hence, this form is far more efficient than the original phase formulation from the computational point of view. Finally, it can be seen by (5.3) and (5.4) (also see the Appendix) that $\lambda\omega(s_w, s_g, p)\nabla p = \sum_\alpha \lambda_\alpha \nabla p_\alpha$.

Again, as in the case of two-phase flow, the global pressure is the pressure that would produce a flow of a fluid (with mobility $\lambda\omega$) equal to the sum of the flows of the three fluids w, o, and g.

6. Compositional Flow

In this section we consider multiphase flow with mass interchange between phases in a porous medium. We consider the general case where there are N chemical species, or components, each of which may exist in any or all of the three phases: water, oil, and gas. Let $c_{i\alpha}$ be the mass fraction of the ith component in the α-phase, $i = 1, \ldots, N$. The mass of each phase is not conserved because of the possibility of transfer of various components between the phases. Instead, the mass balance equation for the transport of each component can be written as follows:

$$\begin{aligned} &\frac{\partial}{\partial t}(\phi c_{i\alpha}\rho_\alpha s_\alpha) + \nabla\cdot(c_{i\alpha}\rho_\alpha u_\alpha) + \nabla\cdot J_{i\alpha} \\ &\quad = I_{i\alpha} + q_{i\alpha}, \quad i = 1, 2, \ldots, N, \ \ \alpha = w, o, g, \end{aligned} \tag{6.1}$$

subject to the following constraints

$$\sum_{i=1}^{N} c_{i\alpha} = 1, \qquad \sum_{i=1}^{N} J_{i\alpha} = 0, \quad \alpha = w, o, g,$$

$$\sum_{\alpha} s_\alpha = 1, \qquad \sum_{\alpha} I_{i\alpha} = 0, \quad i = 1, 2, \ldots, N,$$

where $J_{i\alpha}$ represents the diffusive unit flux of the ith component in the α-phase, $I_{i\alpha}$ is the interphase exchange term, and $q_{i\alpha}$ is the source/sink term. The Darcy law is repeated by

$$u_\alpha = -\frac{kk_{r\alpha}}{\mu_\alpha}(\nabla p_\alpha - \rho_\alpha \tilde{g}), \quad \alpha = w, o, g. \tag{6.2}$$

Flow equations can be derived by adding (6.1) over species and using the above constraints

$$\frac{\partial(\phi\rho_\alpha s_\alpha)}{\partial t} + \nabla\cdot(\rho_\alpha u_\alpha) = I_\alpha + q_\alpha, \tag{6.3}$$

where

$$I_\alpha = \sum_{i=1}^{N} I_{i\alpha}, \qquad q_\alpha = \sum_{i=1}^{N} q_{i\alpha}.$$

Now we see that the flow equations (6.2) and (6.3) are the same as those in (5.1) for the three-phase immiscible flow. Hence the same fractional flow approach can be adapted here.

We remark that the diffusive unit flux $J_{i\alpha}$ is defined by [9]

$$J_{i\alpha} = -\rho_\alpha D_{i\alpha}\nabla c_{i\alpha}, \quad i = 1, \ldots, N, \ \ \alpha = w, o, g,$$

where $D_{i\alpha}$ is the diffusion coefficient of the ith component in the α-phase, and the interphase mass exchange term for the exchange of mass from the β-phase to the α-phase is given by

$$I_{i\alpha} = \rho_\alpha \kappa_{\beta\alpha}(\overline{c}_{i\alpha} - c_{i\alpha}), \quad \alpha = w, o, g, \ \ \alpha \neq \beta,$$

where $\kappa_{\beta\alpha}$ is the mass transfer rate between the α and β phases and $\overline{c}_{i\alpha}$ is the equilibrium value of the mass fraction of the ith component in the α-phase. Finally, the capillary pressure functions are defined as in (5.3).

7. Mixed Finite Element Methods

From the discussion in the last five sections we see that the (global) pressure equation can be written in the general form

$$c\frac{\partial p}{\partial t} + \nabla \cdot u = q, \quad (x,t) \in \Omega \times J, \tag{7.1a}$$

$$u = -a(\nabla p - b), \quad (x,t) \in \Omega \times J, \tag{7.1b}$$

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, and $J = (0,T]$ ($T > 0$) 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

$$p = -g, \quad (x,t) \in \Gamma_1 \times J, \tag{7.2a}$$

$$u \cdot \nu = \varphi, \quad (x,t) \in \Gamma_2 \times J, \tag{7.2b}$$

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

$$p(x,0) = p^0(x), \quad x \in \Omega. \tag{7.3}$$

Problem (7.1)–(7.3) is recast in mixed form as follows. Let

$$L^2(\Omega) = \left\{ w\colon \int_\Omega |w(x)|^2 \, \mathrm{d}x < \infty \right\},$$
$$H(\mathrm{div};\Omega) = \{v \in (L^2(\Omega))^3 : \nabla \cdot v \in L^2(\Omega)\},$$
$$W = L^2(\Omega),$$
$$V^\pi = \{v \in H(\mathrm{div};\Omega) : v \cdot \nu = \pi \ \text{ on } \ \partial\Gamma_2\},$$

where $\pi(x)$ is a function defined on Γ_2. Then the mixed form of (7.1) and (7.2) for a pair of maps $(u,p)\colon J \to V^\varphi \times W$ is

$$\left(c\frac{\partial p}{\partial t}, w\right) + (\nabla \cdot u, w) = (q, w), \quad \forall w \in W, \tag{7.4a}$$

$$(a^{-1}u, v) - (p, \nabla \cdot v) = (b, v) + (g, v \cdot \nu)_{\Gamma_1}, \quad \forall v \in V^0, \tag{7.4b}$$

where $(\cdot, \cdot)$ is the $L^2(\Omega)$ or $(L^2(\Omega))^3$ inner product, as appropriate, and $(\cdot, \cdot)_{\Gamma_1}$ denotes the duality paring between $H^{1/2}(\Gamma_1)$ and $H^{-1/2}(\Gamma_1)$. (7.4a) is obtained from (7.1a), and (7.4b) from (7.1b) and (7.2a) by integration by parts. 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 $\partial\Omega$ may be curved. In $\mathcal{E}_h$, we also need that adjacent elements completely share their common face. Finally, each exterior face has imposed on it either Dirichlet or Neumann conditions, but not both.

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 [4]). The mixed finite element solution of (7.4) is (u_h, p_h): $J \to V_h^\varphi \times W_h$ satisfying

$$\left(c\frac{\partial p_h}{\partial t}, w\right) + (\nabla \cdot u_h, w) = (q, w), \quad \forall w \in W_h, \tag{7.5a}$$

$$(a^{-1}u_h, v) - (p_h, \nabla \cdot v) = (b, v) + (g, v \cdot \nu)_{\Gamma_1}, \quad \forall v \in V_h^0. \tag{7.5b}$$

The approximate initial datum is given by

$$p_h(x, 0) = p_h^0(x), \quad x \in \Omega, \tag{7.6}$$

where p_h^0 is an appropriate approximation in W_h of p^0. The system in (7.5) and (7.6) again has a unique solution.

The linear system arising from (7.5) is a saddle point problem [4], which can be expensive to solve. One of useful numerical methods for solving this saddle point problem is the inexact Uzawa algorithm (see, e.g., [3, 20]). A more efficient approach was suggested by means of a nonmixed formulation. Namely, it has been shown that mixed finite element methods are equivalent to a modification of nonconforming Galerkin methods (see the references in [8]). The nonconforming methods yield a symmetric and positive definite problem, which can be more easily solved. Finally, when $V_h \times W_h$ is the Raviart–Thomas–Nedelec space [25, 23] of lowest-order over rectangular parallelepipeds, it can be shown that the linear system arising from the mixed formulation can be written as a system generated by a cell-centered finite difference scheme by use of certain quadrature rules [6, 14, 26]. In the nonlinear case where the coefficients a, b, and c depend on the solution p itself, the mixed finite element methods can be defined similarly [7].

8. Numerical Results

In this section we report the results of numerical examples to see the performance of the mixed methods for the flow equations using different finite elements in the

Table I. Convergence of p_h and u_h in Example 1.

$1/h$	L^∞-error of p	L^∞-order of p	L^∞-error of u	L^∞-order of u
10	$0.20217E+00$	—	$0.50276E+00$	—
20	$0.10377E+00$	0.96	$0.26603E+00$	0.92
40	$0.51701E-01$	1.01	$0.14094E+00$	0.92

three-dimensional case. We do some benchmark calculations for a typical second-order problem. Namely, we consider the Laplace equation on the unit cube

$$-\Delta p = q, \quad x \in \Omega = (0,1)^3, \tag{8.1a}$$

$$p = -g, \quad x \in \Gamma_1, \tag{8.1b}$$

$$\partial p/\partial \nu = \varphi, \quad x \in \Gamma_2. \tag{8.1c}$$

The application of these methods to practical problems of flow in porous media will be reported in a forthcoming paper.

EXAMPLE 1. In the first example the data are chosen as follows

$$\begin{aligned} &q = 3\pi^2 \sin(\pi x)\sin(\pi y)\sin(\pi z),\\ &\Gamma_1 = \{x=0\}\cup\{x=1\}\cup\{y=0\}\cup\{y=1\},\\ &\Gamma_2 = \{z=0\}\cup\{z=1\},\\ &g = -1, \qquad \varphi = -\pi\sin(\pi x)\sin(\pi y). \end{aligned}$$

The exact solution of (8.1) is then

$$p(x,y,z) = 1 + \sin(\pi x)\sin(\pi y)\sin(\pi z).$$

Uniform partitions of Ω into simplexes are taken, and the lowest-order Raviart–Thomas–Nedelec mixed space [25, 23] over simplexes is used. In Table I, the errors and convergence orders in the $L^\infty(\Omega)$-norm for the solution p and its gradient $u = -\nabla p$ are shown. From the results in this table, we see that the mixed method is first-order accurate for both the solution and its gradient; i.e., optimal order.

EXAMPLE 2. In this example the same set of data is chosen as in Example 1; but the Raviart–Thomas–Nedelec mixed space [25, 23] of lowest-order over rectangular parallelepipeds is applied here. The numerical results are presented in Table II. From this table, we find that the convergence orders for both the solution and its gradient are almost second-order accurate. This implies that we have superconvergence for both variables, and agrees with theoretical results [22, 28].

Table II. Convergence of p_h and u_h in Example 2.

$1/h$	L^∞-error of p	L^∞-order of p	L^∞-error of u	L^∞-order of u
10	$0.27371E-01$	—	$0.56533E-01$	—
20	$0.72552E-02$	1.92	$0.14669E-01$	1.95
40	$0.18757E-02$	1.95	$0.37151E-02$	1.98

Table III. Convergence of p_h and u_h in Example 3.

$1/h$	L^∞-error of p	L^∞-order of p	L^∞-error of u	L^∞-order of u
10	$0.38712E-02$	—	$0.98421E-02$	—
20	$0.19800E-02$	0.97	$0.51799E-02$	0.93
40	$0.98322E-03$	1.00	$0.27001E-02$	0.94

EXAMPLE 3. We also did a lot of numerical experiments for time-dependent problems. Similar results to those in Examples 1 and 2 are obtained. As example, in this example we consider the model problem

$$\frac{\partial p}{\partial t} - \Delta p = q, \quad x \in \Omega = (0,1)^3, \ \ t > 0, \tag{8.2a}$$

$$p = 0, \quad x \in \partial\Omega, \ \ t > 0, \tag{8.2b}$$

where the right-hand side function is determined by

$$q = x(1-x)y(1-y)z(1-z) \times \left\{1 + 2(1+t)\left(\frac{1}{x(1-x)} + \frac{1}{y(1-y)} + \frac{1}{z(1-z)}\right)\right\}.$$

The initial datum is determined by the following true solution at $t = 0$:

$$p(x,y,z) = (1+t)x(1-x)y(1-y)z(1-z).$$

The same partitions and space as in Example 1 are used here, and the backward Euler discretization scheme for the time differentiation term is used. The time step is taken to be proportional to the space step $\Delta t = \mathcal{K}h$ where $h = \Delta x = \Delta y = \Delta z$ and $\mathcal{K}$ is the proportionality constant. The numerical results at $t = 1$ are displayed in Table III. They coincide with the theoretical results $O(\Delta t + h)$.

9. Concluding Remark

We have shown that the governing differential equations describing multiphase flow of fluids in a porous medium can be written in a fractional flow formulation;

i.e., in terms of a global pressure and saturation (or saturations), and that the mixed finite element methods can be accurately and efficiently applied to solve the pressure equation. The numerical experiments carried out in this paper agree with theoretical results. The fractional flow formulation for the two-phase flow can be derived without any hypothesis. The weakness of the global formulation for the three-phase flow is the need of the satisfaction of the total differential condition by the three-phase relative permeability and capillary pressure curves. The global formulation offers the potential for significant improvements in the efficiency of numerical schemes.

Appendix

In this Appendix we provide the derivation of Equations (3.5), (4.6)–(4.8), and (5.9)–(5.11).

A.1. DERIVATION OF (3.5)

Carry out the differentiation indicated in (3.1) and divide the resulting equation by ρ_i to see that

$$\phi c_i \frac{1}{\rho_i}\frac{\partial \rho_i}{\partial t} + \phi \frac{\partial c_i}{\partial t} + c_i \nabla \cdot u + \frac{c_i}{\rho_i} u \cdot \nabla \rho_i$$
$$+ u \cdot \nabla c_i - \frac{1}{\rho_i}(D\nabla c_i) \cdot \nabla \rho_i - \nabla \cdot (D \nabla c_i) = \tilde{c}_i q.$$

Consequently, by (3.3), we have

$$\phi c_i z_i \frac{\partial p}{\partial t} + \phi \frac{\partial c_i}{\partial t} + c_i \nabla \cdot u + z_i c_i u \cdot \nabla p +$$
$$+ u \cdot \nabla c_i - z_i (D\nabla c_i) \cdot \nabla p - \nabla \cdot (D \nabla c_i) = \tilde{c}_i q.$$

Now, by (3.4), we obtain

$$\sum_{i=1}^{N} \phi z_i c_i \frac{\partial p}{\partial t} + \nabla \cdot u + \sum_{i=1}^{N} z_i (c_i u - D\nabla c_i) \cdot \nabla p = q,$$

since

$$\sum_{i=1}^{N} \frac{\partial c_i}{\partial t} = \sum_{i=1}^{N} \nabla c_i = \sum_{i=1}^{N} \nabla \cdot (D \nabla c_i) = 0.$$

This shows (3.5).

A.2. DERIVATION OF (4.6)–(4.8)

First, (4.6a) is obtained directly by adding (4.1a) over α. Next, it follows from (4.4) that

$$\nabla p = \nabla p_n - f_w(x,s)\nabla p_c - \int_0^{p_c(s)} \nabla_x f_w(x, p_c^{-1}(\xi))\,\mathrm{d}\xi,$$

so that,

$$\nabla p_n = \nabla p + f_w \nabla p_c + \int_0^{p_c(s)} \nabla_x f_w(x, p_c^{-1}(\xi))\,\mathrm{d}\xi.$$

This, together with (4.3), yields that

$$\nabla p_w = \nabla p - f_n \nabla p_c + \int_0^{p_c(s)} \nabla_x f_w(x, p_c^{-1}(\xi))\,\mathrm{d}\xi.$$

Thus, by (4.1b), we have

$$\rho_w u_w = -k\lambda_w \left(\nabla p - f_n \nabla p_c + \int_0^{p_c(s)} \nabla_x f_w(x, p_c^{-1}(\xi))\,\mathrm{d}\xi - \rho_w \tilde{g} \right), \tag{A.1}$$

and

$$\rho_n u_n = -k\lambda_n \left(\nabla p + f_w \nabla p_c + \int_0^{p_c(s)} \nabla_x f_w(x, p_c^{-1}(\xi))\,\mathrm{d}\xi - \rho_n \tilde{g} \right). \tag{A.2}$$

Now, apply (4.5) to have

$$u = -k\lambda \left(\nabla p + \int_0^{p_c(s)} \nabla_x f_w(x, p_c^{-1}(\xi))\,\mathrm{d}\xi - (f_w\rho_w + f_n\rho_n)\tilde{g} \right), \tag{A.3}$$

which implies (4.6b) by the definition of $\omega(p,s)$. Also, substitute the expression of u in (A.3) into (A.1) to find that

$$\rho_w u_w = f_w u + k\lambda f_w f_n (\nabla p_c + \tilde{g}(\rho_w - \rho_n)),$$

which implies (4.8a), and, together with (4.1a) with $\alpha = w$, (4.7). Finally, substitute u in (A.3) into (A.2) to obtain (4.8b).

A.3. DERIVATION OF (5.9)–(5.11)

Again, (5.9a) is obtained directly by adding (5.1a) over α. Also, by (5.7), we observe that

$$\nabla p_o = \nabla p - \nabla p_c,$$

so that, by (5.3)

$$\nabla p_\alpha = \nabla p - \nabla p_c + \nabla p_{c\alpha o}, \quad \alpha = w, o, g.$$

Hence, by (5.1b), we see that

$$\rho_\alpha u_\alpha = -k\lambda_\alpha(\nabla p - \nabla p_c + \nabla p_{c\alpha o} - \rho_\alpha \tilde{g}). \tag{A.4}$$

Now, applying (5.8) and (5.4), we get

$$\begin{aligned} u &= -k \sum_\alpha \lambda_\alpha(\nabla p - \nabla p_c + \nabla p_{c\alpha o} - \rho_\alpha \tilde{g}) \\ &= -k \sum_\alpha \lambda_\alpha \left(\left\{ 1 - \frac{\partial p_c}{\partial p} \right\} \nabla p - \rho_\alpha \tilde{g} \right), \end{aligned} \tag{A.5}$$

which yields (5.9b). Next, insert the expression of u into (A.4) to have (5.11). Finally, utilize (5.1b) with $\alpha = w$ and g, (A.4) and (A.5) to prove (5.10).

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