DEVELOPMENT, ANALYSIS AND NUMERICAL TESTS OF A COMPOSITIONAL RESERVOIR SIMULATOR

ZHANGXIN CHEN AND YOUQIAN ZHANG

Abstract. The governing equations of a compositional model for three-phase multicomponent fluid flow in multi-dimensional petroleum reservoirs are cast in terms of a pressure equation and a set of component mass balance equations in this paper. The procedure is based on a pore volume constraint for component partial molar volumes, which is different from earlier techniques utilizing an equation of state for phase fluid volumes or saturations. The present technique simplifies the pressure equation, which is written in terms of various pressures such as phase, weighted fluid, global, and pseudo-global pressures. The different formulations resulting from these pressures are numerically solved; the numerical computations use a scheme based on the mixed finite element method for the pressure equation and the finite volume method for the component mass balance equations. A qualitative analysis of these formulations is also carried out. The analysis yields that the differential system of these formulations is of mixed parabolic-hyperbolic type, typical for fluid flow equations in petroleum reservoirs. Numerical experiments based on the benchmark problem of the third comparative solution project organized by the society of petroleum engineers are presented.

Key Words. compositional model, reservoir simulation, mixed finite elements, finite volume, thermodynamic equilibrium, numerical experiments.

1. Introduction

A compositional model for three-phase multicomponent fluid flow in petroleum reservoirs has been recently analyzed in [10]. This model incorporates compressibility, compositional effects, and mass interchange between phases. It consists of Darcy's law for volumetric flow velocities, mass balance for hydrocarbon components, thermodynamic equilibrium for mass interchange between phases, and an equation of state for phase 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 reservoirs, it has become increasingly important to study such a realistic model.

In this paper this compositional model is further studied. Instead of the equation of state for phase saturations, a pore volume constraint for component partial molar volumes is exploited for this model. Specifically, the governing equations of this model are cast in terms of a pressure equation and a set of component mass balance equations, and the procedure is based on this pore volume constraint. The advantages of using this constraint over the state equation for phase saturations

are that the saturations can be zero but the number of overall moles of each component appearing in this constraint is often positive, that the present development is practically well suited for multiphase flow since this constraint does not involve phases, and that the formulation of the pressure equation is simpler.

As in [10], the pressure equation is written in terms of various pressures such as phase, weighted fluid, global, and pseudo-global pressures. The emphasis here is to carry out numerical computations for the different formulations resulting from these pressures. The numerical computations use a scheme based on the mixed finite element method for the pressure equation and the finite volume method for the component mass balance equations. This scheme is suitable for numerical simulation of multiphase flow through geometrically complex geological petroleum reservoirs [11, 12]. Numerical experiments based on the benchmark problem of the third comparative solution project organized by the society of petroleum engineers [13] are presented.

A qualitative analysis of the differential system of these formulations is given. This system is of mixed parabolic-hyperbolic type, typical for fluid flow equations in petroleum reservoirs. We show that the pressure equation is a standard parabolic problem and the component mass balance 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. The mathematical structure of a one-dimensional two-phase multicomponent compositional model without capillary pressure effects was analyzed in [21] by a different approach.

The rest of the paper is organized as follows. In the next section, we review the governing equations for a compositional model. Then in the third section, we derive some lemmas from thermodynamic equilibrium conditions, which are used in the development of the pressure equation. In the fourth section, we derive the pressure and component mass balance equations. In the fifth section, we give a qualitative analysis of the derived differential system, and in the sixth section, we develop our numerical scheme. Finally, in the seventh section we report numerical experiments.

2. Governing Equations for Compositional Flow

There are books that develop the equations for compositional flow in petroleum reservoirs (e.g., [8, 15]). In this section, we briefly review these equations. The 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 reservoir fluids. These components associate as phases in the reservoirs. 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 is conserved:

$$(2.1) \quad \begin{aligned} &\partial_t(\phi n_w) + \nabla \cdot (\xi_w u_w) = q_w, \\ &\partial_t(\phi n_i) + \nabla \cdot (x_{ig}\xi_g u_g + x_{io}\xi_o u_o) = q_i, \qquad i = 2, \dots, N_c, \end{aligned}$$

where ∂_t denotes time differentiation, ϕ is the porosity of the reservoir, g, o, and w refer to gas, oil, and water phases, i is the component index, $N_c - 1$ is the number of hydrocarbon components, n_w and n_i denote the number of overall moles per

pore volume of the water and ith hydrocarbon component, x_{ig} and x_{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, $\alpha = g, o, w$. For notational convenience later, let water be the first component and $n_1 = n_w$. In (2.1), the volumetric velocity u_α in multiphase flow is given by Darcy's law:

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

where k is the effective permeability of the reservoir, $k_{r\alpha}$, 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), there are also algebraic constraints. Assume that the fluid volume completely fills the available pore volume as defined by

$$(2.3) \qquad \sum_{i=1}^{N_c} n_i v_i = 1,$$

where v_i represents the partial molar volume of component i. Equation (2.3) is referred to as the pore volume constraint and is used here. Previously, the equation of state for the phase saturations s_α has been used, as mentioned in the introduction:

$$s_g + s_o + s_w = 1.$$

The phase pressures are related by capillary pressures:

$$(2.4) \qquad p_{c\alpha o} = p_\alpha - p_o, \qquad \alpha = g, o, w,$$

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.

Other algebraic relations are stated as follows. The mass balance implies that

$$(2.5) \qquad n_i = n_{ig} + n_{io}, \qquad i = 2, \ldots, N_c,$$

where n_{ig} and n_{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 x_{ig} and x_{io} are defined by

$$(2.6) \qquad x_{i\alpha} = \frac{n_{i\alpha}}{\displaystyle\sum_{j=1}^{N_c} n_{j\alpha}}, \qquad i = 2, \ldots, N_c, \quad \alpha = g, o.$$

Finally, the saturations are expressed in terms of the phase compositions:

$$(2.7) \qquad s_w = \frac{n_w}{\xi_w}, \quad s_\alpha = \frac{\displaystyle\sum_{i=1}^{N_c} n_{i\alpha}}{\xi_\alpha}, \qquad \alpha = g, o.$$

It should be noted that there are more dependent variables than there are differential and algebraic relations; there are formally $5N_c + 5$ dependent variables: n_w, n_i, n_{ig}, n_{io}, x_{ig}, x_{io}, u_α, p_α, and s_α, $\alpha = g, o, i = 2, \ldots, N_c$. It is then necessary to have $5N_c + 5$ independent relations to determine a solution of the system. Equations (2.1)–(2.7) provide $4N_c + 6$ independent relations, differential or algebraic;

the additional $N_c - 1$ relations are provided by the equilibrium relations needed to relate the numbers of moles. However, as discussed in the fourth section later, the primary unknowns will be $(p, n_1, \ldots, n_{N_c})$, and other variables will be expressed in terms of them, where p is some as yet unspecified pressure.

3. Thermodynamic Equilibrium and Some Useful Lemmas

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 reservoir 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.

3.1. The Kuhn-Tucker condition. The total Gibbs free energy in the reservoir is defined by

$$\gamma = \gamma_g + \gamma_o,$$

where γ_α indicates the total Gibbs free energy of the α-phase. The constrained minimization problem for the Gibbs free energy of the compositional system under consideration is formulated as follows:

(3.1) Given $p, 0 \le n_i$, find (n_{ig}, n_{io}), $i = 2, \ldots, N_c$, such that
$$\gamma(n_{ig}, n_{io}) = \inf\{\gamma(v_{ig}, v_{io}) : 0 \le v_{ig}, v_{io} \text{ and } v_{ig} + v_{io} = n_i\}.$$

From this minimization problem, we can derive the Kuhn-Tucker condition [14] under the assumption that both the gas and oil phases are formed (see Lemma 3.2 in [10]):

$$f_{ig}(p, n_{2g}, \ldots, n_{N_c g}) = f_{io}(p, n_{2o}, \ldots, n_{N_c o}), \qquad i = 2, \ldots, N_c,$$

where $f_{i\alpha}$ is the chemical potential of the ith component in the α-phase, $i = 2, \ldots, N_c$, $\alpha = g, o$. This relation represents a set of necessary (but not sufficient) conditions at equilibrium. To guarantee that a minimum is achieved, the second order Kuhn-Tucker condition must be satisfied; i.e., the Hessian matrix $(\partial f_{ig}/\partial n_{jg} + \partial f_{io}/\partial n_{jo})_{(N_c-1)\times(N_c-1)}$ is symmetric and positive definite at (p, n_{ig}, n_{io}), where p is treated as a parameter.

3.2. Some useful relations. Let V be the volume of the overall fluid in the reservoir. Euler's Theorem implies that

$$(3.2) \qquad V = \sum_{i=1}^{N_c} n_i' v_i,$$

where n_i' is the number of overall moles of the ith hydrocarbon component and

$$(3.3) \qquad v_i = \frac{\partial V}{\partial n_i'}, \qquad i = 1, \ldots, N_c.$$

From (3.2) and (3.3), we can deduce the next lemma.

Lemma 3.1. *It holds that*

$$(3.4) \qquad \sum_{i=1}^{N_c} n_i \frac{\partial v_i}{\partial n_j} = 0, \qquad j = 1, \ldots, N_c.$$

PROOF. It follows from (3.2) that

$$\frac{\partial V}{\partial n'_j} = v_j + \sum_{i=1}^{N_c} n'_i \frac{\partial v_i}{\partial n'_j}, \qquad i = 1, \ldots, N_c.$$

Then (3.4) follows from (3.3) and the fact that $n_i = n'_i/V$.   []

The next lemma was proven in [10] (see Proposition 3.5 there).

Lemma 3.2. *For* α, $\beta = g$, o, *we have*

$$\sum_{j=2}^{N_c} n_{j\alpha} \frac{\partial s_\beta}{\partial n_j} = \begin{cases} s_\alpha & \text{if} \quad \alpha = \beta, \\ 0 & \text{if} \quad \alpha \neq \beta. \end{cases}$$

Let V_α represent the volume of the α-phase, $\alpha = g$, o, w. Note that

$$V = V_g + V_o + V_w.$$

We now show the following result.

Lemma 3.3. *It holds that*

$$\sum_{j=2}^{N_c} v_i x_{j\alpha} \xi_\alpha = 1, \qquad \alpha = g, \ o.$$

PROOF. Applying (3.3), we see that

$$v_j = \frac{\partial V}{\partial n'_j} = \frac{\partial}{\partial n'_j}(V_g + V_o + V_w), \qquad j = 2, \ldots, N_c.$$

From the definition of the saturations, this implies that

$$v_j = \frac{\partial}{\partial n_j}(s_g + s_o + s_w) = \frac{\partial}{\partial n_j}(s_g + s_o), \qquad j = 2, \ldots, N_c.$$

Thus by (2.6) and (2.7), we have

$$\sum_{j=2}^{N_c} v_i x_{j\alpha} \xi_\alpha = \frac{1}{s_\alpha} \sum_{j=2}^{N_c} n_{j\alpha} \frac{\partial}{\partial n_j}(s_g + s_o),$$

which, together with Lemma 3.2, yields the desired result.   []

4. The Pressure and Component Mass Balance Equations

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 choose our primary variables as $(p, n_1, \ldots, n_{N_c})$ and derive a compositional system for them. This system consists of the (various) pressure and component mass balance equations. We employ the usual total flow velocity

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

Several choices for p will be made later. For the time being, let us assume that p has been given. Also, for expositional convenience we assume that v_i depends on p instead of p_α, $\alpha = g, o, w$, $i = 1, \ldots, n_{N_c}$. This means that we neglect the errors (due to the capillary pressures) caused by calculating v_i at p instead of p_α. These small errors contribute to the lower order terms in the pressure equations, which does not affect the properties of these equations. The technique for handling these errors for a simpler problem in [5] applies here.

4.1. The pressure equation. The subsequent development is based on the constraint (2.3). Define

$$V_T = \sum_{i=1}^{N_c} n_i v_i.$$

Note that $V_T = V_T(p, n_1, \ldots, n_{N_c})$, as given, is a function of its arguments. Then it follows from the differentiation of (2.3) with respect to time that

$$\frac{\partial V_T}{\partial p} \partial_t p + \sum_{i=1}^{N_c} \frac{\partial V_T}{\partial n_i} \partial_t n_i = 0.$$

Apply (2.1) to see that

(4.2)
$$c_T \partial_t p + \frac{\partial V_T}{\partial n_w} \nabla \cdot (\xi_w u_w) + \sum_{i=2}^{N_c} \frac{\partial V_T}{\partial n_i} \nabla \cdot (x_{ig} \xi_g u_g + x_{io} \xi_o u_o)$$
$$= \frac{\partial V_T}{\partial n_w} q_w + \sum_{i=2}^{N_c} \frac{\partial V_T}{\partial n_i} q_i,$$

where c_T is the total fluid and rock compressibility given by

(4.3)
$$c_T = -\phi \frac{\partial V_T}{\partial p} + \left(n_w \frac{\partial V_T}{\partial n_w} + \sum_{i=2}^{N_c} n_i \frac{\partial V_T}{\partial n_i} \right) \frac{\mathrm{d}\phi}{\mathrm{d}p}.$$

By (3.4), we see that

(4.4)
$$\frac{\partial V_T}{\partial n_i} = v_i, \qquad i = 1, \ldots, N_c.$$

Now, apply (2.3), (4.1), (4.4), and Lemma 3.3 to (4.2) and (4.3) to obtain

$$c_T \partial_t p + \nabla \cdot u - \xi_w \nabla v_w \cdot u_w - \sum_{i=2}^{N_c} \nabla v_i \cdot (x_{ig} \xi_g u_g + x_{io} \xi_o u_o) = v_w q_w + \sum_{i=2}^{N_c} v_i q_i,$$

where

$$c_T = -\phi \frac{\partial V_T}{\partial p} + \frac{\mathrm{d}\phi}{\mathrm{d}p}.$$

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

(4.5)
$$c_T \partial_t p + \nabla \cdot u - \sum_{i=2}^{N_c} \nabla v_i \cdot (x_{ig} \xi_g u_g + x_{io} \xi_o u_o) = v_w q_w + \sum_{i=2}^{N_c} v_i q_i.$$

We remark that the pressure equation (4.5) is simpler than that derived in [10], where the state equations for the saturations was exploited to derived the pressure equation. Also, we do not see the saturations explicitly in (4.5). It now remains to express u in terms of p.

4.1.1. Phase pressure. Several choices for p have been made in [3, 10]. For the numerical simulation given in the seventh section, we consider these choices in this and the next three subsections for the compositional model under consideration. We first review the phase pressure. The water phase pressure is often used in petroleum reservoir simulation; to be consistent with (2.4), let us use the oil phase pressure

(4.6)
$$p = p_o;$$

the formulation for the water phase pressure is similar. 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), (2.4), and (4.6) that

$$(4.7) \qquad u = -k\lambda \left(\nabla p - G_\lambda + \sum_\alpha \frac{\lambda_\alpha}{\lambda} \nabla p_{c\alpha o} \right),$$

where $G_\lambda = g_c \sum_\alpha \rho_\alpha \lambda_\alpha / \lambda$. Substitution of (4.7) into (4.5) yields the equation for the phase pressure p. The analysis of the resulting equation will be described in subsection 5.1 later. The pressure equation as split in (4.5) and (4.7) into a first-order differential system is suitable to the application of the mixed finite element method considered in the sixth section.

From (2.2) and (2.4), we see that the phase velocity is related to the total velocity by

$$(4.8) \quad u_\alpha = \frac{\lambda_\alpha}{\lambda} \left(u + k \sum_\beta \lambda_\beta \left\{ \nabla(p_{c\beta o} - p_{c\alpha o}) - (\rho_\beta - \rho_\alpha)g_c \right\} \right), \quad \alpha = g,\, o,\, w.$$

4.1.2. Weighted fluid pressure. We now define a smoother pressure than the phase pressure given in (4.6). Namely, we define the weighted fluid pressure

$$(4.9) \qquad p = \sum_\alpha s_\alpha p_\alpha.$$

Note that even if some saturation is zero (i.e., some phase disappears), we still have a non-zero smooth variable p. By (2.4), 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

$$(4.10) \qquad u = -k\lambda \left(\nabla p - G_\lambda + \sum_\alpha \frac{\lambda_\alpha}{\lambda} \nabla p_{c\alpha o} - \sum_\alpha \nabla(s_\alpha p_{c\alpha o}) \right).$$

Finally, the relationships between the phase velocities and the total velocity are the same as in (4.8).

Observe that the pressure is strongly coupled to the saturations or to the compositions through the last term on the right-hand side of (4.7) (respectively, the last two terms of (4.10)). 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
(4.11)
$$\frac{\partial}{\partial s_g}\left(\frac{\lambda_w}{\lambda}\right)\frac{\partial p_{cwo}}{\partial s_w} + \frac{\partial}{\partial s_g}\left(\frac{\lambda_g}{\lambda}\right)\frac{\partial p_{cgo}}{\partial s_w} = \frac{\partial}{\partial s_w}\left(\frac{\lambda_w}{\lambda}\right)\frac{\partial p_{cwo}}{\partial s_g} + \frac{\partial}{\partial s_w}\left(\frac{\lambda_g}{\lambda}\right)\frac{\partial p_{cgo}}{\partial s_g}.$$

This condition is referred to as the total differential condition [2, 3], and it is a necessary and sufficient mathematical condition to write (2.2) and (2.4) in terms of (4.13) below (see the derivation of (4.13) and the reason that (4.11) is needed in [3] for a simpler problem). 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

(4.12)
$$p = p_o + p_c.$$

Apply (2.2), (2.4), (4.1), (4.11), and (4.12) to see that

(4.13)
$$u = -k\lambda(\nabla p - G_\lambda).$$

The phase velocity is determined by

(4.14)
$$u_\alpha = \frac{\lambda_\alpha}{\lambda}u + k\lambda_\alpha\big(\nabla(p_c - p_{c\alpha o}) - \delta_\alpha\big), \qquad \alpha = g,\, o,\, w,$$

where

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

While condition (4.11) is not always true, it has been shown [3] that it is satisfied for some simple three-phase relative permeability and capillary pressure functions. Also, a simple numerical procedure for constructing three-phase relative permeability and capillary pressure curves satisfying this condition has been given in [2], some of the numerical examples have been compared with the classical Stone's model [20], 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 (4.11) on the shape of three-phase relative permeability and capillary pressure functions. In this subsection, as introduced in [3], 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

(4.15)
$$p_{cwo} = p_{cwo}(s_w), \quad p_{cgo} = p_{cgo}(s_g).$$

We then introduce the mean values

(4.16)
$$\widehat{\left(\frac{\lambda_w}{\lambda}\right)}(s_w) = \frac{1}{1-s_w}\int_0^{1-s_w}\left(\frac{\lambda_w}{\lambda}\right)(s_w,\zeta)\mathrm{d}\zeta,$$
$$\widehat{\left(\frac{\lambda_g}{\lambda}\right)}(s_g) = \frac{1}{1-s_g}\int_0^{1-s_g}\left(\frac{\lambda_g}{\lambda}\right)(\zeta,s_g)\mathrm{d}\zeta,$$

and the pseudo-global pressure

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

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 (4.7) to find that

$$(4.17) \qquad u = -k\lambda \left\{ \nabla p - G_\lambda + \sum_\alpha \left(\frac{\lambda_\alpha}{\lambda} - \widehat{\left(\frac{\lambda_\alpha}{\lambda}\right)} \right) \frac{dp_{c\alpha o}}{ds_\alpha} \nabla s_\alpha \right\}.$$

The phase velocities in terms of the total velocity are expressed as in (4.8).

The global formulation seems 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 equations in this formulation is much less. The weakness of the global formulation is the need of the satisfaction of the total differential condition (4.11) by the three-phase relative permeability and capillary pressure curves. In general, the phase and weighted fluid formulations 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 (4.16), the pseudo-global formulation is more useful. In the (probably unphysical) case where the capillary pressures $p_{c\alpha}$ are zero, all the formulations are the same.

4.2. The component mass balance equations. The component mass balance equations are given as in (2.1); i.e.,

$$(4.18) \qquad \begin{aligned} &\partial_t(\phi n_w) + \nabla \cdot (\xi_w u_w) = q_w, \\ &\partial_t(\phi n_i) + \nabla \cdot (x_{ig}\xi_g u_g + x_{io}\xi_o u_o) = q_i, \qquad i = 2, \ldots, N_c. \end{aligned}$$

The phase velocities u_α are related to the total velocity u as in (4.8) or (4.14). Apply (4.11) and the definition of p_c, it can be checked that (4.8) and (4.14) have the same form

$$(4.19) \quad u_\alpha = \frac{\lambda_\alpha}{\lambda} u + \lambda_\alpha k \left(\frac{\lambda_w}{\lambda} \nabla p_{cwo} + \frac{\lambda_g}{\lambda} \nabla p_{cgo} - \nabla p_{c\alpha o} - \delta_\alpha \right), \quad \alpha = g, o, w.$$

In terms of ∇p_{cwo} and ∇p_{cgo}, the component mass balance equations are thus the same for all pressure formulations. Therefore, it suffices to analyze one of them, which is illustrated in the next section.

5. A Qualitative Analysis

In this section we carry out a qualitative analysis for the pressure and component mass balance equations.

5.1. Analysis of the pressure equation. The pressure equation is given by (4.5) and (4.7) (respectively, (4.10), (4.13), or (4.17), depending upon the formulation used). We analyze the global formulation in detail. Substitution of (4.13) into (4.5) yields

$$(5.1) \qquad \begin{aligned} &c_T \partial_t p - \nabla \cdot \left\{ k\lambda(\nabla p - G_\lambda) \right\} \\ &= \sum_{i=2}^{N_c} \nabla v_i \cdot (x_{ig}\xi_g u_g + x_{io}\xi_o u_o) + v_w q_w + \sum_{i=2}^{N_c} v_i q_i. \end{aligned}$$

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

$$c_T = -\phi \frac{\partial V_T}{\partial p} + \frac{d\phi}{dp} > 0.$$

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 reservoir is positive-definite, so is $k\lambda$. Consequently, it follows from (5.1) that the pressure equation is parabolic. Typically, the rock and fluid compressibility is quite small, and the pressure reaches a steady state very rapidly. The analysis for other formulations is exactly the same.

5.2. Analysis of the component mass balance equations. We first analyze the equation for the water phase, i.e., the first equation in (4.18). For notational simplicity, let p_{cwo} and p_{cgo} satisfy the usual assumption (4.15). Then it is obvious that

$$\nabla p_{cwo} = \frac{1}{\xi_w} \frac{\mathrm{d}p_{cwo}}{\mathrm{d}s_w} \nabla n_w,$$

(5.2)

$$\nabla p_{cgo} = \frac{\mathrm{d}p_{cgo}}{\mathrm{d}s_g} \left(\frac{\partial s_g}{\partial p} \nabla p + \sum_{j=2}^{N_c} \sum_{i=2}^{N_c} \frac{\partial s_g}{\partial n_{ig}} \frac{\partial n_{ig}}{\partial n_j} \nabla n_j \right).$$

Substitute (4.19) with $\alpha = w$ and the first equation in (5.2) into the water phase equation to see that

(5.3)
$$\partial_t(\phi n_w) + \nabla \cdot \left(\frac{\xi_w \lambda_w}{\lambda} u \right) - \nabla \cdot \left(\frac{\lambda_w(\lambda_o + \lambda_g)}{\lambda} \frac{\mathrm{d}p_{cwo}}{\mathrm{d}s_w} k \nabla n_w \right)$$
$$= q_w - \nabla \cdot \left(\xi_w \lambda_w k \left\{ \frac{\lambda_g}{\lambda} \nabla p_{cgo} - \delta_w \right\} \right).$$

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, we see that

$$\frac{\lambda_w(\lambda_o + \lambda_g)}{\lambda} \frac{\mathrm{d}p_{cwo}}{\mathrm{d}s_w} k$$

is positive semi-definite. Consequently, equation (5.3) is a degenerate parabolic problem. The degeneracy is caused by the fact that λ_w can be zero. Also, from the properties of the capillary pressure p_{cwo} and the phase mobility λ_w, the diffusion coefficient in (5.3) is small compared to the advection term in this equation. Thus (5.3) is advection-dominated.

We now consider the equation for the hydrocarbon components, i.e., the second equation in (4.18). Substitute (4.19) with $\alpha = g$ and o into this equation to see that

(5.4)
$$\partial_t(\phi n_i) + \nabla \cdot \left(\frac{1}{\lambda} \{ x_{ig} \xi_g \lambda_g + x_{io} \xi_o \lambda_o \} u \right)$$
$$+ \nabla \cdot \left(\frac{\lambda_g}{\lambda} \{ -x_{ig} \xi_g (\lambda_w + \lambda_o) + x_{io} \xi_o \lambda_o \} k \nabla p_{cgo} \right)$$
$$+ \nabla \cdot \left(\frac{\lambda_w}{\lambda} \{ x_{ig} \xi_g \lambda_g + x_{io} \xi_o \lambda_o \} k \nabla p_{cwo} \right)$$
$$- \nabla \cdot (x_{ig} \xi_g \lambda_g k \delta_g + x_{io} \xi_o \lambda_o k \delta_o) = q_i, \qquad i = 2, \ldots, N_c.$$

Introduce the column vectors

$$N = (n_i)_{i=\overline{2,N_c}}, \quad Q = (q_i)_{i=\overline{2,N_c}}, \quad H = \left(\frac{1}{\lambda} \{ x_{ig} \xi_g \lambda_g + x_{io} \xi_o \lambda_o \} u \right)_{i=\overline{2,N_c}},$$

and the matrix

$$D = - \left(\frac{\lambda_g}{\lambda} \frac{\mathrm{d}p_{cgo}}{\mathrm{d}s_g} \{ -x_{ig} \xi_g (\lambda_w + \lambda_o) + x_{io} \xi_o \lambda_o \} \sum_{l=2}^{N_c} \frac{\partial s_g}{\partial n_{lg}} \frac{\partial n_{lg}}{\partial n_j} \right)_{i,j=\overline{2,N_c}}.$$

Also, set

$$
\begin{aligned}
b_i = & \frac{\lambda_g}{\lambda} \frac{\mathrm{d}p_{cgo}}{\mathrm{d}s_g} \frac{\partial s_g}{\partial p} \left\{ -x_{ig}\xi_g(\lambda_w + \lambda_o) + x_{io}\xi_o\lambda_o \right\} k\nabla p \\
& + \frac{\lambda_w}{\lambda} \left\{ x_{ig}\xi_g\lambda_g + x_{io}\xi_o\lambda_o \right\} k\nabla p_{cwo} \\
& - (x_{ig}\xi_g\lambda_g k\delta_g + x_{io}\xi_o\lambda_o k\delta_o), \qquad i = 2, \ldots, N_c,
\end{aligned}
$$

and the column vector B to be

$$
B = (b_i)_{i=\overline{2,N_c}}.
$$

With these notation and substitution of the second equation in (5.2) into (5.4), we have the system

(5.5) $$\partial_t(\phi N) + \nabla \cdot H - \nabla \cdot (Dk\nabla N) = Q - \nabla \cdot B.$$

As in [21], it can be shown that $\frac{\partial H}{\partial N}$ has all real eigenvalues. Also, we want D to be positive semi-definite. This condition guarantees that (5.5) is a parabolic system and should be a consequence of thermodynamic analysis of real fluids. We do not, however, know how to prove the positive semi-definiteness of D for the time being. In the case where we move the off-diagonal terms in D to the right-hand side of (5.5), it can be proven that D is indeed positive semi-definite (see [10]). This is practically reasonable since the capillary pressures are quite small compared to the advection term in (5.5).

6. Numerical Scheme

In this section we briefly review a sequential procedure for numerically solving the differential system developed in the earlier sections. This sequential procedure was analyzed in detail in [10].

It is known that accurate numerical reservoir 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 finite element method [1] has a very satisfactory property in both this aspect and the treatment of the geometrically complex geological structure of reservoirs (see the references in [4]). Also, due to their advection-dominated features, more suitable methods than the standard finite difference and finite element methods need be exploited for the component mass balance equations. Here we use a finite volume method for these equations. This method is applicable to the solution of hyperbolic conservation laws [12]. Finally, as mentioned before, the phase compositions of the reservoir 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 Gibbs minimization problem (3.1).

We now state our sequential solution procedure as follows [10]:

(1) At time $t = 0$, the primary variables $(p, n_1, \ldots, n_{N_c})$ are computed from the initial data.

(2) Use the flash calculation to determine the phase compositions $n_{i\alpha}$, $i = 2, \ldots, N_c$, $\alpha = g, o$.

(3) Evaluate the phase viscosities μ_α by empirical correlations [16] and molar and mass densities $(\xi_\alpha, \rho_\alpha)$ by the equation of state [17], and then the mole fractions $x_{i\alpha}$ and saturations s_α by (2.6) and (2.7).

(4) Calculate the coefficients of the pressure equation and some of the coefficients of the mass balance equations and then proceed to the next time level.
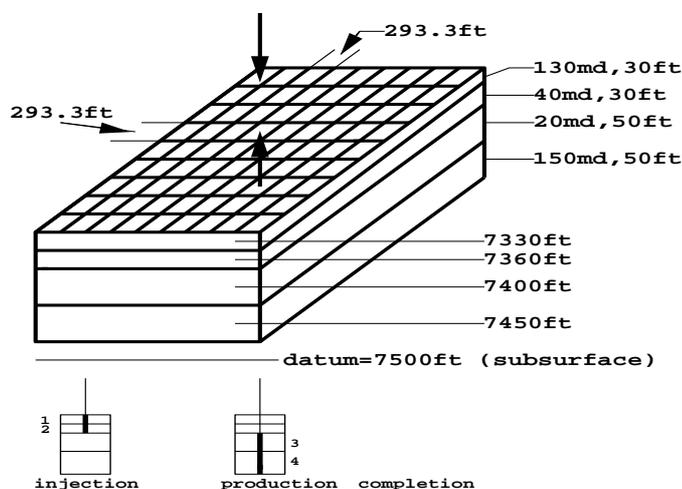
Fig. 1. A reservoir domain.

(5) Apply the mixed finite element method 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 mass balance system.

(7) Utilize the finite volume method to solve this system for $(n_1, \ldots, n_{N_c})$.

(8) Perform a few iterations between the pressure equation, the mass balance 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.

7. Numerical Experiments

The simulation problem considered is chosen from the benchmark problem of the third comparative solution project [13]. Nine companies participated in that comparison project. It is a study of gas cycling in a rich retrograde condensate reservoir. Two prediction cases are considered. The first case is gas cycling with constant sales gas removal, and the second case is cycling with some gas sales deferral to enhance pressure maintenance in the early life of the reservoir. The data are taken from [6, 7, 13]. The specification of the reservoir model can be found in [8, 13]. A reservoir grid with $9 \times 9 \times 4$ is shown in Fig. 1, and it is diagonally symmetrical, indicating that it would be possible to simulate half of this reservoir. We chose to model the full reservoir. Also, the reservoir layers are homogeneous and have a constant porosity, but there are permeability and thickness variations between layers, a factor leading to unequal sweepout. The two-well pattern is arbitrary and is employed to allow for some retrograde condensation without significant revaporization by recycling gas to simulate what occurs in sweep-inaccessible parts of a real reservoir.

The initial conditions, the location of the gas-water contact, and the capillary pressure data produce a water-gas transition zone extending to the pay zones [8]. However, the very small compressibility and water volume make water quite insignificant for the present problem. Relative permeability data are used under the assumption that the phase relative permeability function depends only on its own
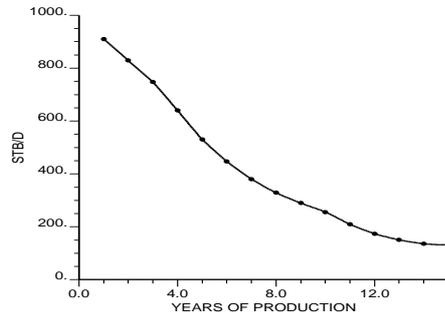
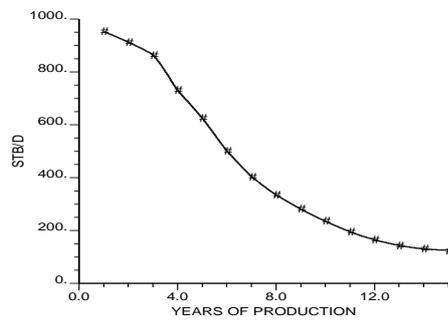Fig. 2. Stock-tank oil production rate in case 1.

Fig. 3. Stock-tank oil production rate in case 2.

phase saturation. Oil is immobile to 24% saturation, and k_{rg} is reduced from 0.74 to 0.4 as condensate builds to this saturation with irreducible water present.

Production is separator gas rate controlled. Liquid production through multistage separation is to be predicted. The separator train is given, and the primary separator pressure depends on reservoir pressure [9]. Sales gas is removed from the bulked separator gas, and the remaining gas is recycled. Volumetrically, the two cases under consideration provide for exactly the same amount of recycling gas to be reinjected over the cycling period (10 years), but more gas is recycled in the critical early years in the second case. Blowdown (all gas to sales) starts at the end of the tenth year of cycling, and simulations are run up to 15 years or 1,000 psi average reservoir pressure, whichever occurs first. The simulations are initialized at pressure about 100 psi above the dew point pressure 3,443 psia.

Simulation results for the compositional model considered are given in Figs. 2–6. The time step size used in the sequential solution procedure is about 30 days (in the first few time steps, it is smaller). Our compositional simulator can use either the ORTHOMIN (orthogonal minimum residual) [22] or GMRES (generalized minimum residual) [18] Krylov subspace methods, with incomplete LU factorization preconditioners, as the linear solver. The phase-pressure formulation given in Section 4.1.1 is used in the simulation, since this formulation applies to more general relative permeabilities and capillary curves.

Stock-tank oil rates for the first and second cases and the corresponding cumulative liquid production for these cases at the final simulation time of 15 years are shown in Figs. 2–5. Incremental stock-tank oil produced by gas-sales deferral (the second case minus the first) is given in Fig. 6. Primary separator switchout
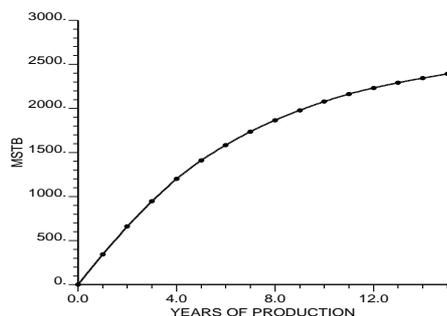
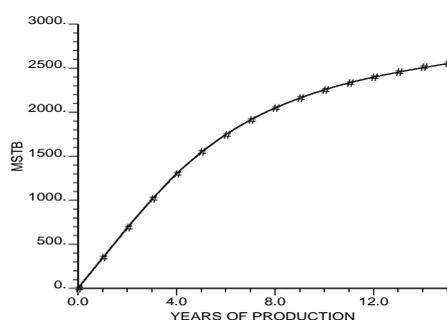Fig. 4. Cumulative stock-tank oil production in case 1.

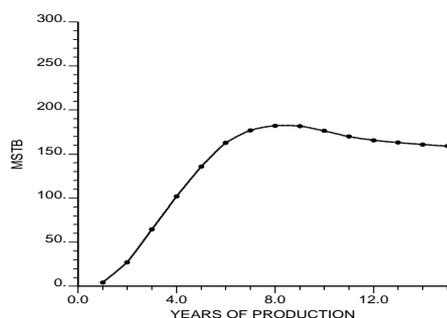Fig. 5. Cumulative stock-tank oil production in case 2.

Fig. 6. Incremental stock-tank oil produced by gas-sales deferral (case 2 minus case 1).

occurs late in the cycling phase (10 years). The predicted surface oil rate is closely correlated with the liquid yield predictions.

As noted earlier, the first case is gas cycling with constant sales gas removal, while the second case is cycling with some gas sales deferral to enhance pressure maintenance in the early life of the reservoir. The total sales gas removal is the same for the two cases; the difference lies in the way sales gas is removed in the first ten years. For a gas condensate reservoir, decreasing the occurring of retrograde condensate phenomena leads to less loss of heavy hydrocarbon components and more production of oil.

Fig. 6 gives incremental stock-tank oil produced by gas-sales deferral. In the peak of this curve (at the eighth year), the cumulative stock-tank oil produced by the second case is 182 Mstb more than that by the first case (i.e, 9.76% increase). At the final production time (the 15th year), the increase is down to 159 Mstb

(6.65%). This phenomenon can be seen from the observation that after injection of recycle gas stops, liquid production is due to depletion and the heavy end fractions vaporize into the vapor phase and are produced.

References

[1] F. Brezzi and M. Fortin, Mixed and Hybrid Finite Element Methods, Springer-Verlag, New York, 1991.

[2] G. Chavent and J. Jaffré, Mathematical Models and Finite Elements for Reservoir Simulation, North-Holland, Amsterdam, 1978.

[3] Z. Chen and R. E. Ewing, Comparison of various formulations of three-phase flow in porous media, *J. Comp. Phys.* **132** (1997), 362–373.

[4] Z. Chen and R. E. Ewing, From single-phase to compositional flow: applicability of mixed finite elements, *Transport in Porous Media* **27** (1997), 225-242.

[5] Z. Chen and R. E. Ewing, Fully-discrete finite element analysis of multiphase flow in groundwater hydrology, *SIAM J. Numer. Anal.* **34** (1997), 2228–2253.

[6] Z. Chen, G. Huan, and B. Li, A benchmark calculation of 3D horizontal well simulations, *International Journal of Numerical Analysis and Modeling*, **1** (2004), 189–202.

[7] Z. Chen, G. Huan, and B. Li, A pseudo function approach in reservoir simulation, *International Journal of Numerical Analysis and Modeling*, **2** (2005), 58–67.

[8] Z. Chen, G. Huan, and Y. Ma, Computational Methods for Multiphase Flows in Porous Media, Computational Science and Engineering Series, Vol. 2, SIAM, Philadephia, PA, 2006.

[9] Z. Chen, G. Huan, and H. Wang, Computer simulation of gas cycling of retrograde condensate reservoirs using an unstructured CVFE compositional model, *Computing* **78** (2006), 31–53.

[10] Z. Chen, G. Qin, and R. E. Ewing, Analysis of a compositional model for fluid flow in porous media, *SIAM J. Appl. Math.* **60** (2000), 747–777.

[11] J. Douglas, Jr., R. E. Ewing, and M. Wheeler, The approximation of the pressure by a mixed method in the simulation of miscible displacement, *RAIRO Anal. Numér.* **17** (1983), 17–33.

[12] L. J. Durlofsky and M. C. Chien, Development of a mixed finite element based compositional reservoir simulator, SPE 25253 in 12th SPE Symposium on Reservoir simulation, New Orleans, Louisiana, 1993, pp. 221–231.

[13] D. E. Kenyon and A. Behie, Third SPE comparative solution project: Gas cycling of retrograde condensate reservoirs, *J. Pet. Tech.* **39** (1987), 981–998.

[14] H. W. Kuhn and A. W. Tucker, Nonlinear programming, in Proc. 2nd Berkeley Symposium on Mathematical Statistics and Probability, University of California Press, Berkeley and Los Angeles, California, 1961, pp. 481–492.

[15] L. W. Lake, Enhanced Oil Recovery, Prentice-Hall, Englewood Cliffs, NJ, 1989.

[16] J. Lohrenz, B. G. Bray, and C. R. Clark, Calculating viscosities of reservoir fluids from their compositions, *J. Petroleum Tech.* **16** (1964), 1171–1176.

[17] D. Y. Peng and D. B. Robinson, A new two-constant equation of state, *Ind. Eng. Chem. Fundam.* **15** (1976), 59–64.

[18] Y. Saad and M. H. Schultz, GMRES: a generalized minimal residual algorithm for solving nonsymmetric linear systems, *SIAM J. Sci. Statist. Comput.* **7** (1986), 856–869.

[19] W. E. Smith and H. C. Van Ness, Introduction to Chemical Engineering Thermodynamics, McGraw Hill, New York, 1975.

[20] H. L. Stone, Estimation of three-phase relative permeability and residual oil data, *J. Can. Pet. Tech.* **12** (1973), 53–67.

[21] J. A. Trangenstein and J. B. Bell, Mathematical structure of compositional reservoir simulation, *SIAM J. Sci. Stat. Comput.* **10** (1989), 817–845.

[22] P. W. Vinsome, ORTHOMIN, An iterative method for solving sparse sets of simultaneous linear equations, Paper SPE 5729, presented at the SPE Symposium on Reservoir Simulation held in Los angles, California, February 19-20, 1976.

Department of Mathematics, Box 750156, Southern Methodist University, Dallas, TX 75275-0156, U.S.A.

E-mail: zchen@mail.smu.edu,yzhang@mail.smu.com

URL: faculty.smu.edu/zchen