

A Compositional Formulation of the Pressure and Saturation Equations

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Summary. This paper describes a sequential implicit formulation of the compositional reservoir flow equations. This procedure offers improved stability over implicit pressure, explicit saturation (IMPES) methods but, in general, is not as expensive computationally as fully implicit methods. It also possesses several other attractive features. It permits an efficient combination of compositional and black-oil capabilities in a single program. Important to this is the fact that it lends itself to a modular program design. Finally, it has a natural physical interpretation that can be very helpful in the understanding of model behavior.

Introduction

In black-oil reservoir simulation, there are currently three common approaches. The simplest is the IMPES procedure, in which an implicit pressure calculation is made at each timestep, followed by an explicit saturation calculation. The IMPES procedure is the fastest approach on a per-timestep basis, but it can have stability problems that restrict timestep size. The most stable procedure is the coupled implicit method, in which the nonlinear functions in the interblock flow terms are evaluated at the end of each timestep. This method is the slowest approach on a per-timestep basis, particularly on large models. The sequential implicit procedure combines the attractive features of the other two. It uses the same pressure calculation as IMPES but follows it with an implicit saturation calculation. It seems to be the best method for large models in which stability is a consideration. Coats¹ discusses these methods in more detail.

Young and Stephenson² proposed two categories of methods for compositional simulation—Newton-Raphson and non-Newton-Raphson. The difference in the methods lies in the way the pressure equations are formed. In Newton-Raphson methods, the pressure equation is an outgrowth of the iterative technique. In non-Newton-Raphson methods, the pressure equation is based on certain physical principles. In general, Newton-Raphson methods include compositional effects that are neglected in non-Newton-Raphson methods, and, as a result, require fewer iterations per timestep.² The method of Acs *et al.*³ is an exception to this statement, however. It is a non-Newton-Raphson, IMPES-type procedure in which the pressure equation includes the compositional effects mentioned above.

Young and Stephenson's categorization does not address the question of implicitness of interblock flow calculations. Most of the methods published (for example, those of Young and Stephenson,² Acs *et al.*,³ and Kazemi *et al.*⁴) use explicit relative permeabilities in these calculations. An exception is the Newton-Raphson-type model described by Coats.⁵

This paper describes a sequential implicit compositional formulation. Basically, it combines and extends the ideas of Acs *et al.*³ and Spillette *et al.*⁶ The procedure is as follows.

1. Construct a set of pressure equations and solve them for pressures at the new time level.
2. Compute interblock total fluid velocities with these pressures.
3. Use interblock total velocities and the Buckley-Leverett phase velocity relationship to construct a set of saturation equations having, in general, implicit treatment of relative permeabilities and capillary pressures. Solve these for saturations at the new time level.
4. Use the saturations to compute interblock phase velocities.
5. Use the phase velocities to compute interblock component transport and the amount of each component in each block at the end of the timestep.
6. Make the required fluid property and function evaluation calculations, and proceed to the next timestep.

A general-purpose simulator based on this procedure is described elsewhere.⁷ This paper presents the formulation in some detail. Particular attention is paid to demonstrating that the compositional formulation reduces to the common black-oil formulation when it is used with black-oil fluid properties. This is a very significant advantage, because it makes solving both types of problems in a single program practical.

The Pressure Equation

First, the compositional pressure equation is derived. Then it is shown to have a useful physical interpretation, which, in turn, can be used to write the equation directly.

The derivation seems overly long given the simplicity of the result. Unfortunately, no way to shorten it significantly has been found.

Derivation. The starting point for the compositional formulation is the molar continuity equation for Component m .

$$\frac{\partial}{\partial t}(\phi \rho_{MT} z_m) = \Theta_m \quad \dots \dots \dots (1)$$

The variable ρ_{MT} is the molar density and z_m is the mole fraction of Component m in the three phases combined. This is the fundamental equation that Kazemi *et al.*⁴ used, with the exception that here the water phase is treated in the same way as the two hydrocarbon phases; Kazemi *et al.* combined only the two hydrocarbon phases. The total molar density is given by

$$\rho_{MT} = \rho_{Mo} S_o + \rho_{Mg} S_g + \rho_{Mw} S_w \quad (2)$$

Θ_m is the rate of accumulation of Component m . This is equal to the negative of the divergence of the flux of Component m plus its rate of injection.

$$\begin{aligned} \Theta_m = & \nabla \cdot \left[x_m \rho_{Mo} \frac{k k_{ro}}{\mu_o} (\nabla p_o - g \rho_o \nabla D) \right] \\ & + \nabla \cdot \left[y_m \rho_{Mg} \frac{k k_{rg}}{\mu_g} (\nabla p_g - g \rho_g \nabla D) \right] \\ & + \nabla \cdot \left[w_m \rho_{Mw} \frac{k k_{rw}}{\mu_w} (\nabla p_w - g \rho_w \nabla D) \right] + q_m \quad (3) \end{aligned}$$

To work in terms of specific molar volumes, v_T , rather than molar densities is more convenient. The specific volume is defined by

$$\rho_{MT} = \frac{1}{v_T} \quad (4)$$

Substituting Eq. 4 into Eq. 1 yields

$$\frac{\partial}{\partial t} \left(\frac{\phi z_m}{v_T} \right) = \Theta_m \quad (5)$$

Breaking the time derivative into two parts yields

$$\frac{\phi}{v_T} \frac{\partial z_m}{\partial t} + z_m \frac{\partial}{\partial t} \left(\frac{\phi}{v_T} \right) = \Theta_m \quad (6)$$

Summing Eq. 6 over all components yields

$$\frac{\partial}{\partial t} \left(\frac{\phi}{v_T} \right) = \Theta_T \quad (7)$$

where Θ_T is Θ_m totalled over all components. This equation is equivalent to the pressure equation used by Kazemi *et al.*⁴

If Eq. 7 is multiplied by z_m and subtracted from Eq. 6, the following result is obtained:

$$\frac{\phi}{v_T} \frac{\partial z_m}{\partial t} = \Theta_m - z_m \Theta_T \quad (8)$$

Breaking the derivative term in Eq. 7 into its separate parts and multiplying the result by v_T yields

$$\frac{\partial \phi}{\partial t} - \frac{\phi}{v_T} \frac{\partial v_T}{\partial t} = v_T \Theta_T \quad (9)$$

At this point, it is necessary to introduce the concept of intensive and extensive variables. An extensive variable is one that depends on the amount of material present; an intensive variable does not. The specific volume v_T is an intensive variable. If it is multiplied by the total number of moles present, N_T , the extensive variable, V_T , is obtained:

$$V_T = N_T v_T \quad (10)$$

If the pressure dependency is ignored, V_T is a function only of the number of moles of each component present. Its differential can be written as

$$dV_T = \sum_m \frac{\partial V_T}{\partial N_m} dN_m \quad (11)$$

The partial derivative term is called the partial molal volume. It will be written as V_{Tm} . As a result,

$$dV_T = \sum_m V_{Tm} dN_m \quad (12)$$

This partial molal volume is not the same as that commonly seen in the thermodynamics literature. This one is defined for the multiple-phase case, whereas, in general, partial molal volumes apply only to a single phase. However, the principles involved are the same.

As Dodge⁸ has shown, the differential of the specific volume can be expressed in terms of the partial volumes as follows:

$$dv_T = \sum_m V_{Tm} dz_m \quad (13)$$

Dodge also shows that

$$v_T = \sum_m V_{Tm} z_m \quad (14)$$

Because the specific volume is a function of pressure and composition, its time derivative can be expressed as

$$\frac{\partial v_T}{\partial t} = \left(\frac{\partial v_T}{\partial p} \right)_z \frac{\partial p}{\partial t} + \sum_m V_{Tm} \frac{\partial z_m}{\partial t} \quad (15)$$

Substituting Eq. 8 into this equation yields

$$\begin{aligned} \frac{\partial v_T}{\partial t} = & \left(\frac{\partial v_T}{\partial p} \right)_z \frac{\partial p}{\partial t} + \frac{v_T}{\phi} \sum_m V_{Tm} (\Theta_m - z_m \Theta_T) \\ & \dots \dots \dots (16) \end{aligned}$$

Use of Eq. 14 yields

$$\begin{aligned} \frac{\partial v_T}{\partial t} = & \left(\frac{\partial v_T}{\partial p} \right)_z \frac{\partial p}{\partial t} \\ & + \frac{v_T}{\phi} \left[\left(\sum_m V_{Tm} \Theta_m \right) - v_T \Theta_T \right] \quad (17) \end{aligned}$$

Substituting Eq. 17 into Eq. 9 yields

$$\frac{\partial \phi}{\partial t} - \frac{\phi}{v_T} \left(\frac{\partial v_T}{\partial p} \right)_z \frac{\partial p}{\partial t} = \sum_m V_{Tm} \Theta_m. \quad (18)$$

Treating porosity as a function of pressure only permits

$$\phi \left[\frac{1}{\phi} \frac{\partial \phi}{\partial p} - \frac{1}{v_T} \left(\frac{\partial v_T}{\partial p} \right)_z \right] \frac{\partial p}{\partial t} = \sum_m V_{Tm} \Theta_m. \quad (19)$$

Eq. 19 is the compositional pressure equation. It is instructive to consider the differences between it and Eq. 7, the pressure equation used by Kazemi *et al.* The comparison is made most easily with modifications of Eqs. 9 and 19.

Eq. 20 shows Kazemi *et al.*'s form:

$$\frac{\partial \phi}{\partial p} \frac{\partial p}{\partial t} - \frac{\phi}{v_T} \frac{\partial v_T}{\partial t} = v_T \Theta_T. \quad (20)$$

Eq. 21 shows the new form:

$$\frac{\partial \phi}{\partial p} \frac{\partial p}{\partial t} - \frac{\phi}{v_T} \left(\frac{\partial v_T}{\partial t} \right)_z \frac{\partial p}{\partial t} = \sum_m V_{Tm} \Theta_m. \quad (21)$$

The right side of Eq. 20 treats all moles the same. It makes no distinction between a mole of methane and a mole of hexadecane, despite the fact that the two would occupy greatly different volumes in the reservoir. Eq. 21, on the other hand, specifically acknowledges this fact by the multiplication of each component by the corresponding partial molal volume.

Eq. 20 has the term $\partial v_T / \partial t$ on the left side. Because v_T is a function of composition as well as of pressure, $\partial v_T / \partial t$ depends on both composition and pressure changes with time. Eq. 20 should be viewed as a pressure/composition equation rather than as a pressure equation. Kazemi *et al.* are able to use it (or an equivalent) because they iterate on v_T . However, they implicitly assume that the dependence of v_T on composition is small compared with its dependence on pressure.

Physical Interpretation. The simplicity of the compositional pressure equation (Eq. 19) reveals that the pressure equation has a simple, natural physical interpretation. As noted by Acs *et al.*,³ the pressure equation is basically a volume balance. In the discretized case, it represents an attempt to find the pressure that causes the fluid volume in a block to fill the PV of that block exactly. If too much fluid is in the block, for instance, the equation should force the pressure to increase, thereby compressing the fluid as well as forcing some of it to leave the block. If the right pressure is found, the fluid remaining in the block at the end of the timestep should fill the PV of the block precisely. Eq. 22 expresses this for the *i*th block as follows:

$$V_{pi}^{n+1} = V_{Ti}^{n+1}. \quad (22)$$

Using the customary relationship for PV permits writing the left side of this equation as

$$\begin{aligned} V_{pi}^{n+1} &= V_{pi}^o [1 + c_f (p_i^{n+1} - p_i^o)] \\ &= V_{pi}^n + V_{pi}^o c_f (p_i^{n+1} - p_i^n). \quad (23) \end{aligned}$$

The volume of fluid in the block at the end of the timestep, V_{Ti}^{n+1} , is, to a first-order approximation, the (volume of fluid in the block at the beginning of the timestep) plus (volume change in that fluid caused by the pressure change that occurred during the timestep) plus (effective volume of the net fluid entering the block during the timestep). In equation form, this is written as

$$\begin{aligned} V_{Ti}^{n+1} &= V_{Ti}^n + \left[\frac{\partial}{\partial p} (V_{Ti}^n) \right]_N (p_i^{n+1} - p_i^n) \\ &\quad + \sum_m \left[\frac{\partial}{\partial N_m} (V_{Ti}^n) \right]_p (-N_{mi}^{n+1} - N_{mi}^n) \\ &= V_{Ti}^n + \left[\frac{\partial}{\partial p} (V_{Ti}^n) \right]_N (p_i^{n+1} - p_i^n) \\ &\quad + \sum_m V_{Tmi}^n (N_{mi}^{n+1} - N_{mi}^n). \quad (24) \end{aligned}$$

The term multiplying the pressure change in Eq. 24 corresponds to a compressibility. The equivalence can be seen by noting that the total fluid volume in the block is given by

$$V_{Ti}^n = N_{Ti}^n v_{Ti}^n. \quad (25)$$

Taking the partial derivative with respect to pressure and holding the number of moles of each component present constant yields

$$\left[\frac{\partial}{\partial p} (V_{Ti}^n) \right]_N = N_{Ti}^n \left(\frac{\partial v_{Ti}^n}{\partial p} \right)_z. \quad (26)$$

A simple substitution yields

$$\left[\frac{\partial}{\partial p} (V_{Ti}^n) \right]_N = V_{Ti}^n \left[\frac{1}{v_{Ti}^n} \left(\frac{\partial v_{Ti}^n}{\partial p} \right)_z \right]. \quad (27)$$

The term in brackets on the right side is the negative of the total compressibility.

A simple mole balance on Component m yields the following equation:

$$\begin{aligned}
 N_{mi}^{n+1} - N_{mi}^n = & \Delta t \left\{ \left(\frac{x_m T_x k_{ro}}{v_o \mu_o} \right)_{i-1/2}^n [p_{oi-1}^{n+1} - p_{oi}^{n+1}] \right. \\
 & - g_{p_{oi-1/2}} (D_{i-1} - D_i) \\
 & + \left(\frac{y_m T_x k_{rg}}{v_g \mu_g} \right)_{i-1/2}^n [p_{gi-1}^{n+1} - p_{gi}^{n+1}] \\
 & - g_{p_{gi-1/2}} (D_{i-1} - D_i) \\
 & + \left(\frac{w_m T_x k_{rw}}{v_w \mu_w} \right)_{i-1/2}^n [p_{wi-1}^{n+1} - p_{wi}^{n+1}] \\
 & - g_{p_{wi-1/2}} (D_{i-1} - D_i) \\
 & - \left(\frac{x_m T_x k_{ro}}{v_o \mu_o} \right)_{i+1/2}^n [p_{oi}^{n+1} - p_{oi+1}^{n+1}] \\
 & - g_{p_{oi+1/2}} (D_i - D_{i+1}) \\
 & - \left(\frac{y_m T_x k_{rg}}{v_g \mu_g} \right)_{i+1/2}^n [p_{gi}^{n+1} - p_{gi+1}^{n+1}] \\
 & - g_{p_{gi+1/2}} (D_i - D_{i+1}) \\
 & - \left(\frac{w_m T_x k_{rw}}{v_w \mu_w} \right)_{i+1/2}^n [p_{wi}^{n+1} - p_{wi+1}^{n+1}] \\
 & - g_{p_{wi+1/2}} (D_i - D_{i+1}) \\
 & \left. + q_m \right\}, \dots \dots \dots (28)
 \end{aligned}$$

or

$$N_{mi}^{n+1} - N_{mi}^n = \Delta t \Theta_{mi}^{n+1} \dots \dots \dots (29)$$

Here, $v_r = 1/\rho_{Mr}$. Also, Θ_{mi}^{n+1} corresponds to the divergence of the flux integrated over the PV of Block i , rather than the divergence of the flux at a point. In other words, it is the net flow of Component m into Block i .

Substituting Eq. 27 and 29 into Eq. 24 and combining it with Eq. 22 and 23 yields

$$\begin{aligned}
 V_{pi}^n + V_{pi}^o c_f (p_i^{n+1} - p_i^n) = & V_{Ti}^n \left[1 + \frac{1}{v_{Ti}^n} \left(\frac{\partial v_{Ti}^n}{\partial p} \right)_z (p_i^{n+1} - p_i^n) \right] \\
 & + \Delta t \sum_m V_{Tmi}^n \Theta_{mi}^{n+1} \dots \dots \dots (30)
 \end{aligned}$$

Eq. 30 can be rearranged in the following form:

$$\begin{aligned}
 & \left[V_{pi}^o c_f - \frac{V_{Ti}^n}{v_{Ti}^n} \left(\frac{\partial v_{Ti}^n}{\partial p} \right)_z \right] (p_i^{n+1} - p_i^n) \\
 & = (V_{Ti}^n - V_{pi}^n) + \Delta t \sum_m V_{Tmi}^n \Theta_{mi}^{n+1} \dots \dots \dots (31)
 \end{aligned}$$

Except for the term in parentheses on the right side, this equation is analogous to Eq. 19. Acs *et al.*³ call this term the volumetric error. It is a discrepancy at the beginning of the timestep. It reflects the fact that the pressures obtained at the previous time level may not have been exactly correct. To the extent to which they were incorrect, the fluid in the block will not have precisely filled it. This volume discrepancy provides a driving force to rectify the error on the next timestep. It appears in the equation in the same way a source would, but its contribution is not multiplied by the timestep size. It is analogous to the material-balance error term mentioned by Spillette *et al.*⁶

A similar physical interpretation can be used with the differential balance, which can be expressed as the (rate of change in PV)=(rate of change in fluid volume), which is defined as (rate of change in volume of fluid present caused by pressure changes)+(volumetric rate of fluid influx). This can be expressed in equation form as

$$\frac{\partial \phi}{\partial t} = \frac{\phi}{v_T} \left(\frac{\partial v_T}{\partial p} \right)_z \frac{\partial p}{\partial t} + \sum_m V_{Tm} \Theta_m \dots \dots \dots (32)$$

This equation is a slightly rearranged form of Eq. 18.

The Saturation Equation

The saturation equation is derived in much the same way as the pressure equation. The difference is that the calculations are based on the volume of a single phase rather than on the volume of the total mixture.

Previously, v_T , the total specific molar volume, was defined as the reservoir volume occupied by 1 mole of the mixture present. An analogous phase specific volume is needed. Let r be a subscript denoting a particular phase. Then v_r , the phase specific volume, is defined as the volume of that phase per mole of mixture present.

It must follow that

$$\sum_r v_r = v_T \dots \dots \dots (33)$$

In other words, the volumes of the phases must sum to the total volume. The saturation of phase r is

$$s_r = \frac{v_r}{v_T} \quad \dots\dots\dots (34)$$

Using Eqs. 33 and 34, it can be shown that the saturations sum to unity.

Like v_T , v_r is an intensive quantity. As a result,

$$v_r = \sum_m V_{rm} z_m \quad \dots\dots\dots (35)$$

Here, V_{rm} is the partial molar volume of Phase r with respect to Component m ; in other words, it is the increase in the volume of Phase r that results from the addition of a unit amount of Component m to the mixture.

The compositional saturation equation is written in terms of the time derivative of ϕS_r . With the use of Eq. 34, it can be expressed as follows:

$$\begin{aligned} \frac{\partial}{\partial t}(\phi S_r) &= \frac{\partial}{\partial t} \left(\frac{\phi v_r}{v_T} \right) \\ &= \frac{\phi}{v_T} \frac{\partial v_r}{\partial t} + v_r \frac{\partial}{\partial t} \left(\frac{\phi}{v_T} \right) \quad \dots\dots\dots (36) \end{aligned}$$

The quantity v_r is a function of pressure and composition. Using the chain rule makes it possible to write

$$\frac{\partial v_r}{\partial t} = \left(\frac{\partial v_r}{\partial p} \right)_z \frac{\partial p}{\partial t} + \sum_m V_{rm} \frac{\partial z_m}{\partial t} \quad \dots\dots\dots (37)$$

Substituting Eq. 8 into Eq. 37 yields

$$\begin{aligned} \frac{\partial v_r}{\partial t} &= \left(\frac{\partial v_r}{\partial p} \right)_z \frac{\partial p}{\partial t} \\ &+ \frac{v_T}{\phi} \sum_m V_{rm} (\Theta_m - z_m \Theta_T) \quad \dots\dots\dots (38) \end{aligned}$$

Substituting Eq. 35 into Eq. 38 yields

$$\begin{aligned} \frac{\partial v_r}{\partial t} &= \left(\frac{\partial v_r}{\partial p} \right)_z \frac{\partial p}{\partial t} \\ &+ \frac{v_T}{\phi} \left[\left(\sum_m V_{rm} \Theta_m \right) - v_r \Theta_T \right] \quad \dots\dots\dots (39) \end{aligned}$$

Substituting Eqs. 7 and 39 into Eq. 36 yields

$$\begin{aligned} \frac{\partial}{\partial t}(\phi S_r) &= \frac{\phi}{v_T} \left\{ \left(\frac{\partial v_r}{\partial p} \right)_z \frac{\partial p}{\partial t} \right. \\ &+ \frac{v_T}{\phi} \left[\left(\sum_m V_{rm} \Theta_m \right) - v_r \Theta_T \right] \} \\ &+ v_r \Theta_T \quad \dots\dots\dots (40) \end{aligned}$$

Rearranging yields

$$\frac{\partial}{\partial t}(\phi S_r) = \frac{\phi}{v_T} \left(\frac{\partial v_r}{\partial p} \right)_z \frac{\partial p}{\partial t} + \sum_m V_{rm} \Theta_m \quad \dots\dots\dots (41)$$

Eq. 41 is the compositional saturation equation. Summing it over all phases yields the pressure equation, Eq. 18.

Substituting Eq. 34 into Eq. 41 yields

$$\frac{\partial}{\partial t}(\phi S_r) = -\phi S_r c_r \frac{\partial p}{\partial t} + \sum_m V_{rm} \Theta_m \quad \dots\dots\dots (42)$$

where

$$c_r = \frac{-1}{v_r} \left(\frac{\partial v_r}{\partial p} \right)_z \quad \dots\dots\dots (43)$$

The phase compressibility, c_r , includes the effects of interphase mass transfer.

Eq. 42 has a convenient physical interpretation. The left side is the local rate of change of the volume of Phase r . This is a result of two effects: pressure change and change in what is present. These two effects are clearly represented by the two terms on the right side of the equation.

The Black Oil Equations

It is shown in this section that the conventional black-oil equations are obtained when the compositional formulation described above is used with black-oil fluid properties. First, the conventional equations are written and then equivalent equations are obtained with the compositional approach.

For the sake of simplicity, a relatively uncomplicated fluid model is used. Gas is permitted to go into solution in the oil, and a varying bubblepoint pressure is permitted. Solution of gas in water and volatilization of oil are not included. It can be shown that if these additional complications are included the same result is obtained—i.e., the conventional and compositional approaches yield the same set of equations.

Conventional Approach. The fundamental black-oil equations are component balances. The components are oil, gas, and water, all defined at surface conditions. Unfortunately, the phases in the reservoir go by the same names, which causes confusion. To avoid this confusion, these phases are called liquid, vapor, and aqueous, respectively.

The three continuity equations, one for each component, are

$$\frac{\partial}{\partial t} \left(\frac{\phi S_L}{B_L} \right) = \Theta_o \quad \dots\dots\dots (44)$$

$$\frac{\partial}{\partial t} \left(\frac{\phi S_v}{B_v} \right) + \frac{\partial}{\partial t} \left(\frac{\phi S_L R_{sL}}{B_L} \right) = \Theta_g \quad \dots\dots\dots (45)$$

and

$$\frac{\partial}{\partial t} \left(\frac{\phi S_a}{B_a} \right) = \Theta_w \quad \dots\dots\dots (46)$$

These can be rearranged into the following forms:

$$\frac{\partial}{\partial t}(\phi S_L) = -\phi S_L \left(-\frac{1}{B_L} \frac{\partial B_L}{\partial t} \right) + B_L \Theta_o, \dots (47)$$

$$\begin{aligned} \frac{\partial}{\partial t}(\phi S_v) = & -\phi S_v \left(-\frac{1}{B_v} \frac{\partial B_v}{\partial t} + \frac{S_L B_v}{S_v B_L} \frac{\partial R_{sL}}{\partial t} \right) \\ & + B_v \Theta_g - B_v R_{sL} \Theta_o, \dots (48) \end{aligned}$$

and

$$\frac{\partial}{\partial t}(\phi S_a) = -\phi S_a \left(-\frac{1}{B_a} \frac{\partial B_a}{\partial t} \right) + B_a \Theta_w, \dots (49)$$

If the system is saturated, the FVF's and gas/liquid ratio are functions of pressure only. Eqs. 47 through 49 can be written in a form analogous to that of Eq. 42 as follows:

$$\frac{\partial}{\partial t}(\phi S_L) = -\phi S_L c_L \frac{\partial p}{\partial t} + B_L \Theta_o, \dots (50)$$

$$\frac{\partial}{\partial t}(\phi S_v) = -\phi S_v c_v \frac{\partial p}{\partial t} + B_v \Theta_g - B_v R_{sL} \Theta_o, \dots (51)$$

and

$$\frac{\partial}{\partial t}(\phi S_a) = -\phi S_a c_a \frac{\partial p}{\partial t} + B_a \Theta_w, \dots (52)$$

Here

$$c_L = -\frac{1}{B_L} \frac{dB_L}{dp}, \dots (53)$$

$$c_v = -\frac{1}{B_v} \frac{dB_v}{dp} + \frac{S_L B_v}{S_v B_L} \frac{dR_{sL}}{dp}, \dots (54)$$

and

$$c_a = -\frac{1}{B_a} \frac{dB_a}{dp}, \dots (55)$$

If the system is not saturated, $S_v \neq 0$ and Eq. 48 becomes

$$\frac{\phi S_L}{B_L} \frac{\partial R_{sL}}{\partial t} = \Theta_g - R_{sL} \Theta_o, \dots (56)$$

In addition, B_L becomes a function of R_{sL} as well as of pressure, and

$$\frac{\partial B_L}{\partial t} = \frac{\partial B_L}{\partial p} \frac{\partial p}{\partial t} + \frac{\partial B_L}{\partial R_{sL}} \frac{\partial R_{sL}}{\partial t}, \dots (57)$$

Substituting from Eq. 56 yields

$$\frac{\partial B_L}{\partial t} = \frac{\partial B_L}{\partial p} \frac{\partial p}{\partial t} + \frac{\partial B_L}{\partial R_{sL}} \left(\frac{B_L}{\phi S_L} \right) (\Theta_g - R_{sL} \Theta_o), \dots (58)$$

Substituting Eq. 58 into Eq. 47 yields

$$\begin{aligned} \frac{\partial}{\partial t}(\phi S_L) = & -\phi S_L c_L \frac{\partial p}{\partial t} \\ & + \left(B_L - R_{sL} \frac{\partial B_L}{\partial R_{sL}} \right) \Theta_o + \frac{\partial B_L}{\partial R_{sL}} \Theta_g, \dots (59) \end{aligned}$$

with

$$c_L = -\frac{1}{B_L} \frac{\partial B_L}{\partial p}, \dots (60)$$

Compositional Approach. The compositional equations presented are derived and written in terms of molar quantities. This is a natural way to write them, but it is not necessary. The terms z , ρ_M , and v_s must be defined in some consistent way and must be based on some standard amount of each component, but this amount does not have to be a mole. It can be a pound or kilogram, as well as a pound-mole or kilogram-mole. In fact, the amount can even be a volume at standard conditions. In black-oil modeling, the standard amounts used are volumes at surface conditions. This makes it possible to use the compositional formulation in connection with standard black-oil fluid property treatment.

Consider a reservoir volume V_T made up of liquid, vapor, and aqueous volumes V_L , V_v , and V_a , respectively. Then the amount of each component present is given by the following set of equations:

$$N_o = \frac{V_L}{B_L}, \dots (61)$$

$$N_g = \frac{V_v}{B_v} + \frac{V_L R_{sL}}{B_L}, \dots (62)$$

and

$$N_w = \frac{V_a}{B_a}, \dots (63)$$

TABLE 1—PARTIAL VOLUMES AND COMPRESSIBILITIES—SATURATED BLACK OIL

r	V_{ro}	V_{rg}	V_{rw}	c_r
L	B_L	0	0	$-\frac{1}{B_L} \frac{dB_L}{dp}$
v	$-B_v R_{sL}$	B_v	0	$-\frac{1}{B_v} \frac{dB_v}{dp} + \frac{S_L B_v}{S_v B_L} \frac{dR_{sL}}{dp}$
a	0	0	B_a	$-\frac{1}{B_a} \frac{dB_a}{dp}$

Solving these equations for the phase volumes yields

$$V_L = B_L N_o, \quad (64)$$

$$V_v = B_v N_g - B_v R_{sL} N_o, \quad (65)$$

and

$$V_a = B_a N_w. \quad (66)$$

Noting that

$$V_T = V_L + V_v + V_a, \quad (67)$$

it follows that

$$S_r = \frac{V_r}{V_T}. \quad (68)$$

For saturated conditions, the FVF's and gas/liquid ratio are functions of pressure only. As a result, it is quite straightforward to evaluate the phase partial volumes by using the definition

$$V_{rm} = \frac{\partial V_r}{\partial N_m}. \quad (69)$$

The liquid- and aqueous-phase compressibilities are also easy to obtain. The vapor-phase compressibility is a little more complicated. First, Eq. 65 is differentiated with respect to pressure, yielding

$$\frac{\partial V_v}{\partial p} = N_g \frac{dB_v}{dp} - N_o \left(B_v \frac{dR_{sL}}{dp} + R_{sL} \frac{dB_v}{dp} \right). \quad (70)$$

Then Eqs. 61 and 62 are used to eliminate N_o and N_g :

$$\frac{\partial V_v}{\partial p} = \frac{V_v}{B_v} \frac{dB_v}{dp} - \frac{V_L B_v}{B_L} \frac{dR_{sL}}{dp}. \quad (71)$$

Rearranging and noting that saturation is proportional to phase volume yields

$$c_v = -\frac{1}{V_v} \frac{\partial V_v}{\partial p} = -\frac{1}{B_v} \frac{dB_v}{dp} + \frac{S_L B_v}{S_v B_L} \frac{dR_{sL}}{dp}. \quad (72)$$

TABLE 2—PARTIAL VOLUMES AND COMPRESSIBILITIES—UNDERSATURATED BLACK OIL

r	V_{ro}	V_{rg}	V_{rw}	c_r
L	$B_L R_{sL} \frac{\partial B_L}{\partial R_{sL}}$	$\frac{\partial B_L}{\partial R_{sL}}$	0	$-\frac{1}{B_L} \frac{\partial B_L}{\partial p}$
v	0	0	0	0
a	0	0	B_a	$-\frac{1}{B_a} \frac{\partial B_a}{\partial p}$

The saturated black-oil phase partial volumes and compressibilities are given in Table 1. Inserting these into Eq. 42 yields the black-oil saturation equations as shown in Eqs. 50 through 52.

If undersaturated conditions exist, $V_v = 0$ and Eq. 65 reduces to

$$R_{sL} = \frac{N_g}{N_o}. \quad (73)$$

B_L is a function of R_{sL} as well as of p . As a result,

$$\begin{aligned} V_{Lo} &= B_L + N_o \frac{\partial B_L}{\partial R_{sL}} \frac{\partial R_{sL}}{\partial N_o} \\ &= B_L + N_o \frac{\partial B_L}{\partial R_{sL}} \left(-\frac{N_g}{N_o^2} \right) \\ &= B_L - R_{sL} \frac{\partial B_L}{\partial R_{sL}}. \end{aligned} \quad (74)$$

Similarly,

$$V_{Lg} = N_o \frac{\partial B_L}{\partial R_{sL}} \frac{\partial R_{sL}}{\partial N_g} = \frac{\partial B_L}{\partial R_{sL}}. \quad (75)$$

The phase compressibilities are easily determined. The undersaturated black-oil phase partial volumes and compressibilities are given in Table 2. Substituting these into Eq. 42 yields the black-oil saturation equations (Eqs. 59 and 52).

Implicit Saturation Treatment

As shown above, the reservoir flow equations can be written as follows:

Pressure equation:

$$\frac{d\phi}{dp} \frac{\partial p}{\partial t} - \frac{\phi}{v_T} \left(\frac{\partial v_T}{\partial p} \right)_z \frac{\partial p}{\partial t} = \sum_m V_{Tm} \Theta_m.$$

Saturation equation:

$$\frac{\partial}{\partial t} (\phi S_r) = \frac{\phi}{v_T} \left(\frac{\partial v_r}{\partial p} \right)_z \frac{\partial p}{\partial t} + \sum_m V_{rm} \Theta_m.$$

Here, spatial pressure differences are contained within the Θ_m terms.

It is also shown that these equations apply equally to black-oil and compositional systems, and that in the black-oil case they are merely rearrangements of the conventional equations. In fact, experience has shown that the nature of these equations is essentially the same, regardless of whether the underlying problem is black-oil or compositional.

As a result, it appears that any of the commonly applied methods for solving black-oil problems can be used with these equations. These include IMPES, the coupled semi-implicit method, and the sequential semi-implicit procedure of Spillette *et al.*⁶ A fully implicit method can be obtained by performing an outer iteration with the coupled semi-implicit approach.

The only methods used to date are the IMPES and sequential approaches. Both start by solving for pressures. The IMPES approach can then be used to compute saturations or can go directly to the molar solution described below.

If the sequential approach is used, the pressure solution is followed by the computation of a set of interblock total velocities. The individual phase velocities are then written in terms of these with the Buckley-Leverett expression. In differential form, this is

$$u_r = f_r \left[u_T + kg \nabla D \sum_j \lambda_j (\rho_r - \rho_j) - k \sum_j \lambda_j \nabla (P_{cr} - P_{cj}) \right] \dots \dots \dots (76)$$

Here, u is phase flux. The j subscript is used in summing over the phases. The value $j=r$ can be included or not; it does not contribute to the expression. The mobility, λ , is given by

$$\lambda_r = \frac{k_{rr}}{\mu_r} \dots \dots \dots (77)$$

and

$$f_r = \frac{\lambda_r}{\lambda_T} = \frac{\lambda_r}{\lambda_L + \lambda_v + \lambda_a} \dots \dots \dots (78)$$

For the purposes of Eq. 76, capillary pressure is defined as

$$P_{cr} = p_r - p_L \dots \dots \dots (79)$$

As a result, the sign of the oil/water capillary pressure must be reversed for use in this equation.

The expression for phase flux given in Eq. 76 is substituted into Θ_m in the saturation equation. The resulting set of equations is discretized in the customary manner and solved for saturations at the new time level. In doing so, three of the saturation-dependent terms in Eq. 76 can be treated implicitly. These are the capillary pressures, f_r , and the λ_j 's in the gravitational terms. Any combination of these can be treated implicitly.

Once the new saturations have been obtained, they are used to compute semi-implicit fluid velocities at the new time level with the discretized form of Eq. 76. Obtaining these new-time-level fluid velocities is actually a major purpose of the saturation solution.

Once the final phase velocities have been obtained, the molar transport can be computed. The amount of each component in each gridblock at the end of the timestep can be computed with the following expression, given in discretized form:

$$N_{mi}^{n+1} = N_{mi}^n + \Delta t \left[\left(\frac{x_m^n u_L}{v_L^n} \right)_{i-1/2} - \left(\frac{x_m^n u_L}{v_L^n} \right)_{i+1/2} + \left(\frac{y_m^n u_v}{v_v^n} \right)_{i-1/2} - \left(\frac{y_m^n u_v}{v_v^n} \right)_{i+1/2} + \left(\frac{w_m^n u_a}{v_a^n} \right)_{i-1/2} - \left(\frac{w_m^n u_a}{v_a^n} \right)_{i+1/2} + q_m \right] \dots \dots \dots (80)$$

The velocities used in this expression can be at either time level. In other words, the same expression is used with both the IMPES and sequential procedures. It could also be used with the coupled semi-implicit method.

Also, note that the mole fractions used here are explicit in time. This is satisfactory in most cases, including those where implicit saturation treatment is needed to control potential instabilities related to capillary pressure or gas percolation. It is not adequate in cases with very high gridblock volume throughput rates. In such cases, an implicit molar equation is needed. So far, no equations that have been developed have been completely satisfactory. The one that is currently in use contains an inherent inconsistency that can lead to inaccuracies. This has not been a significant problem in applications to date, but it is a nagging concern. Work is continuing in this area.

At the end of the timestep, the pressure and amount of each component present are known for each gridblock. This is all the information required to compute the phase volumes. Given the phase-volumes and gridblock volumes, saturations can be computed. These will differ somewhat from those computed in the semi-implicit saturation calculation. These differences are phase-volume discrepancies and are resolved in much the same way as the volume discrepancies discussed in connection with the pressure equation are resolved.

Discussion

One of the best features of the new formulation is its simplicity. The pressure equation, for example, can be written

$$\frac{\partial \phi}{\partial t} - \frac{\phi}{v_T} \left(\frac{\partial v_T}{\partial p} \right)_T \frac{\partial p}{\partial t} = \sum_m V_{Tm} \Theta_m \dots \dots \dots (81)$$

This, obviously, is a very simple equation. Certainly, buried in some of the terms is some complexity, but each term has a clear physical meaning. For instance, the term

$$-\frac{1}{v_T} \left(\frac{\partial v_T}{\partial p} \right)_z$$

is the total fluid compressibility. The partial volume, V_{Tm} , is merely the increase in fluid volume that occurs when a unit amount of Component m is added. Using such easily understood terms makes the behavior of the resulting simulator easier to interpret. This can be an advantage in debugging the program, debugging the data, and in history matching.

Another nice feature is the formulation's natural modularity. Phase behavior and fluid property calculations essentially can be completely decoupled from transport calculations. All the transport package needs to know about phase behavior is how many phases and components there are and which components can be in each phase. This adds to the practicality of the use of a single simulator to model different types of processes.

As mentioned above, the only implicit saturation approach that has been used to date is the sequential method. However, it appears that the coupled method could be used as well. Doing so might offer an advantage over Coats'⁵ fully implicit method in multicomponent problems because the number of equations that must be solved simultaneously would be reduced. The number of unknowns per gridblock would be equal to the number of phases rather than to the number of components plus one, as required by Coats' method. If the number of components were large, the resulting reduction in the cost of solving the matrix equations could be dramatic.

A natural concern about combining multiple capabilities into a single program is efficiency. This does not seem to be a problem with this formulation. In comparisons that were made, a compositional simulator that used this formulation was actually found to run black-oil problems slightly faster than a similar black-oil simulator. Young and Stephenson² reported similar results for their compositional simulator.

The formulation described here has been used in two programs: a compositional simulator developed in 1979 and a multiple-application simulator⁷ that became operational on black-oil problems in 1982 and on compositional problems in mid-1983. These two programs have received considerable use. Black-oil applications have ranged from single-well coning models to three-dimensional field-scale models having up to nearly 33,000 gridblocks. Compositional applications have included small single-well models used to study productivity impairment as a result of condensate dropout around producing wells, typical partial-field models with several thousand gridblocks and with 8 to 12 components, and partial-field models with up to 6,000 gridblocks that represent the hydrocarbons with three components. Most of the compositional applications have been related to miscible flooding.

Overall, the formulation has performed well in these applications. In the high-velocity single-well problems, it has been stable enough to run economically. Its real strength has been in the large field-scale models. Some

of these had locally high velocities, usually caused by rapid gas movement. These would presumably have had severe timestep size problems if the IMPES formulation had been used.

Conclusions

1. The pressure and saturation equations have essentially the same form as the commonly used black-oil equations. This makes it possible to apply the implicit methods used in black-oil simulation directly to compositional problems. Only the IMPES and the sequential semi-implicit approaches have been used to date, but there is no apparent reason why the coupled semi-implicit and fully implicit approaches could not be used as well.

2. A major advantage of this formulation in compositional applications is that it reduces the number of equations that must be solved simultaneously if saturations are to be computed semi-implicitly. This is true regardless of the implicit treatment used. If, for example, the coupled semi-implicit approach were to be used, the number of unknowns per gridblock would be equal to the number of phases rather than to the number of components plus 1. This would avoid one of the major concerns in implicit multicomponent simulation.

3. The equations, though written in compositional form, reduce to the black-oil equations when black-oil fluid properties are substituted into them. This greatly increases the practicality of writing a single simulator to solve both black-oil and compositional problems.

4. The equations are quite simple. Furthermore, they and the terms used in them possess natural physical interpretations that are very helpful in understanding simulator behavior.

5. A possible drawback in certain applications is the lack of a completely satisfactory implicit molar equation.

Nomenclature *

- B = FVF, volume/volume
- c = compressibility, pressure⁻¹
- D = depth, L
- f = phase fractional flow in the absence of gravity and capillary pressure, dimensionless
- g = gravitational constant, used to convert density to pressure gradient, pressure-L²/m
- k = permeability, L²
- k_r = relative permeability, dimensionless
- N = amount of a given component, amount
- p = pressure
- P_c = capillary pressure
- q = injection rate, amount/time
- R_{sL} = solution gas/liquid ratio, amount/amount
- S = saturation, dimensionless

*These equations can be written with any consistent set of units. There is no need to limit their applicability by specifying a set because no numerical results are presented in the paper.

However, there is one source of potential confusion. Several quantities are, in essence, defined in terms of a standard amount of a given component. In the compositional case, this standard amount is the pound-mass-mole (or kilogram-mole, depending on the units used). In the black-oil case, it is the standard-conditions volume (stock-tank barrel or stock-tank cubic meter, for example). In either case, it is referred to in the dimensions given above as an "amount."

t = time
 T = interblock transmissibility
 u = phase flux, volume/area-time
 v = specific volume, volume/amount
 V = volume
 V_m = partial volume with respect to Component m , volume/amount
 w = mole fraction in the aqueous phase, dimensionless
 x = mole fraction in the liquid hydrocarbon phase, dimensionless
 y = mole fraction in the vapor phase, dimensionless
 z = overall mole fraction, dimensionless
 Θ = divergence of the flux of a given component, amount/volume-time
 λ = mobility, viscosity⁻¹
 μ = viscosity
 ρ = density, mass/volume
 ρ_M = molar density, amount/volume
 ϕ = porosity, dimensionless

Superscripts

n = time level
 o = initial condition

Subscripts

a = aqueous phase
 f = formation
 g = gas component
 i = gridblock number
 j = dummy phase index
 L = liquid hydrocarbon phase
 m = component
 o = oil component
 p = pore
 r = phase

s = specific
 T = total
 v = vapor
 w = water component

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