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UNIVERSITY OF CALGARY

Development of a Four-Phase Compositional Simulator Using Equations of State

by

Yizheng Wei

A THESIS

SUBMITTED TO THE FACULTY OF GRADUATE STUDIES IN PARTIAL FULFILMENT OF THE REQUIREMENTS FOR THE DEGREE OF DOCTOR OF PHILOSOPHY

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Abstract

Compositional models are widely used in the simulation of gas injection processes where phase mole fractions and compositions at equilibrium change with space and time. Typically, the models are capable of handling three-phase flow (oil, gas and water), where the mole fractions and compositions of the oil and gas phases are determined by performing two-phase flash calculation using an equation of state. No mass interchange between the water and hydrocarbon phases is assumed.

Laboratory experiments, however, have observed that a second hydrocarbon liquid phase can coexist with oil and gas at equilibrium when CO_2 or rich gas is injected into a low temperature reservoir. This second liquid phase makes most conventional compositional models no longer suitable for the simulation of these processes. Using the two-phase flash calculation in a three-phase region provides false phase equilibrium solutions that can result in either erroneous simulation results or discontinuity in the calculation of phase properties over a time step, leaving the simulation fail to converge.

In this work, a new three-dimensional isothermal compositional simulator has been developed. Governing equations that describe compositional flow in porous media are reformulated for four coexisting equilibrium phases (oil, gas, 2nd liquid and aqueous). Water is treated as a component rather than an independent phase in the formulation of component flow and phase equilibrium. A component can exist in any phases as long as the thermodynamic equilibrium condition is satisfied. A robust and efficient four-phase equilibrium calculation algorithm consisting of stability analysis and phase split calculation is incorporated in the simulator to determine the number of phases, phase amounts and phase compositions. An equation of state is employed to calculate the densities and model the phase behavior of both

aqueous and hydrocarbon phases. The component flow equations are discretized using a finite difference method on the basis of a block-centered grid system and solved by an implicit pressure and explicit saturation and composition (IMPES) solution scheme. The proposed model has been validated with commercial software in both stand-alone flash calculation and simulation problems with two hydrocarbon phases.

The new four-phase simulator has been used to investigate the effects of complex phase behavior on displacement mechanisms in CO₂ injection processes. Both the multiphase behavior phenomena of the CO₂/crude oil/water mixtures and the multiphase flow during the injection have been addressed. Simulation results are in agreement with experimental observations in demonstrating the existence of a CO₂-rich liquid phase above a certain pressure and high oil recovery as a result of the formation of the CO₂-rich liquid phase. Compared to a conventional compositional simulator, the four-phase simulator focuses on a more realistic physical model of multiphase multicomponent flow. The simulation results not only provide more accurate predictions of reservoir performance but also promote a better understanding of the dynamic interactions between complex flow and phase behaviors.

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To My Family

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Chapter One: Introduction

Advances in computer hardware, numerical methods and simulation techniques make simulation of complex reservoir characteristics and recovery mechanisms possible. In the first part of this chapter, a brief introduction of reservoir simulation and its application in gas injection processes is presented. Then the phase behavior problems existing in conventional compositional models are described. Finally, research objectives for the development of a new four-phase compositional simulator are given.

1.1 Reservoir Simulation

Reservoir simulation has become a major tool in the oil and gas industry for field development and management since the 1950s. With the aid of digital computers, simulation results help engineers to study and predict production performance under various operation conditions by solving a set of nonlinear partial differential equations with appropriate initial and boundary conditions that describe a physical system of a hydrocarbon reservoir.

Based on the types of reservoir fluids, isothermal reservoir simulators can be classified into two categories: black-oil and compositional. The black oil simulator is used for recovery processes that are not sensitive to compositional changes in the reservoir fluids. In the black oil model, the oil and gas phases are treated as fixed composition systems and mass transfer between hydrocarbon phases relies on a pressure-dependent gas solubility factor. In contrast, the compositional simulator addresses complex multiphase flow in a reservoir where oil has a high volatility and phase compositions at equilibrium change significantly with space and time. Each phase is considered as a multi-component system and phase properties vary during production. Phase behavior and phase densities are calculated using an equation of state (EOS) because of its simplicity and accuracy. Compared to the black oil model, the compositional model is more complicated in its formulation that solves a coupled system of flow and phase equilibrium equations. The system involves more unknowns and requires additional computation for a proper determination of the number of phases, phase mole fractions and phase compositions in each gridblock.

1.2 Problem Description

Miscible gas flooding has been recognized as one of the most effective methods of enhanced oil recovery. Solvents, such as CO₂, enriched gas and nitrogen, are injected into a reservoir to establish miscibility between reservoir oil and injected fluid so that high displacement efficiency is achieved. The miscibility depends on the reservoir temperature and pressure and on the compositions of the oil in place and injected fluid. The simulation of this process requires a compositional model to handle both phase equilibrium and fluid flow parts of the reservoir because phase compositions and phase properties can vary greatly as a result of mass transfer between phases. The mixtures of crude-oil and solvent exhibit complicated multiphase behaviors. When CO₂ or rich gas is injected into a low temperature reservoir, a solvent-rich hydrocarbon liquid phase, called the 2nd liquid phase, is experimentally observed at equilibrium with the oil, gas and water phases. (Huang and Tracht, 1974; Shelton and Yarborough, 1977; Metcalfe and Yarborough, 1979; Gardener et al., 1981; Henry and Metcalfe, 1983; Orr and Jensen, 1984; Turek et al., 1988; Khan et al., 1992; Creek and Sheffield, 1993). However, most compositional models developed since the late 1970s are only capable of handling up to two hydrocarbon phases, which results in an incorrect fluid description and phase behavior prediction from the simulation. The incorrect phase equilibrium solutions can cause discontinuity in phase property calculation over a time step and make the simulation fail to converge. Even though there are some published four phase compositional simulators, water-free flash calculation is performed

and the aqueous phase is treated as an independent phase while four phases coexist. Waterhydrocarbon mutual solubilities and the effect of the water component on phase behavior are neglected in these models.

1.3 Research Objectives

The main objective of this work is to develop a new three-dimensional equation-of-state compositional reservoir simulator with a robust and efficient multiphase equilibrium calculation routine incorporated. Since gas injection is an isothermal process, the effect of temperature variations is not considered. To accurately model the equilibrium phase behavior, the water is considered as a component rather than an independent phase and components are allowed to partition into all phases in the system if thermodynamic equilibrium conditions are satisfied. The phase equilibrium calculation routine is able to predict and solve for up to four phases at equilibrium, and the simulator is capable of handling four-phase (oil, gas, solvent-rich liquid and aqueous) multi-component flow and simulating complex phase behaviors and flow mechanisms in the gas injection processes. From the simulation results, we can obtain a more accurate prediction of multiphase flow in porous media and achieve a better understanding of the effects of the second liquid on displacement efficiency.

The development of a reservoir simulator involves four major interrelated stages that include physical model, mathematical formulation, numerical method and computer algorithm. (Chen, 2007) To achieve the objectives, the following steps are conducted:

- 1. Derive the governing equations for a four-phase compositional model.
- 2. Develop a robust and efficient multiphase equilibrium calculation algorithm.
- 3. Discretize material balance equations using a finite difference method.
- 4. Solve a system of flow and equilibrium equations.

3

- 5. Validate simulation results with commercial reservoir simulators.
- Perform simulation studies to investigate the effect of the 2nd liquid phase on displacement efficiency.

Chapter Two: Literature Review

In this chapter, a literature review of published research is presented. The review consists of three related areas: compositional models, phase equilibrium calculation using equations of state, and phase behavior during CO_2 or rich-gas flooding.

2.1 Compositional Models

Compositional models are used to simulate oil recovery processes when mass transfer between equilibrium phases causes significant variations in phase compositions and phase properties. Typically, two types of reservoir problems require compositional treatment (Coats, 1980):

- 1. depletion and/or cycling of volatile oil and gas condensate reservoirs and
- 2. miscible flooding with multi-contact miscibility generated in situ.

One distinction between these two types of problems is that the first type commonly involves phase compositions far away from a critical point while the second type normally requires calculation of phase compositions and properties near the critical point. During the early stage, it is difficult to model the second type of problems because most compositional simulators that use table lookup equilibrium ratios (*K*-values) for phase equilibrium calculation result in unstable convergence of phase compositions and inconsistent phase densities and viscosities in the near-critical region. This difficulty has been overcome by applying an EOS thermodynamic model which provides a continuous and smooth transition of calculated *K*-values and phase densities through the critical point.

Since the late 1970s, numerous equation-of-state compositional models have been developed. Fussell and Fussell (1979) published the first EOS based compositional model that used an implicit pressure and explicit saturation and composition (IMPES) approach to solve a coupled system of flow and equilibria equations. A minimum variable Newton-Raphson iteration method was applied to update iteration variables. Coats (1980) developed a fully implicit (FIM) compositional model that solved a full set of material balance equations of hydrocarbon components and water, simultaneously. Nghiem et al. (1981) developed an IMPES compositional simulator using the Peng-Robinson EOS (1976). It is a variation of the K-value based IMPES method of Kazemi et al. (1978). The equations were solved by an iterativesequential method which decouples the solution of flow equations and the solution of equilibrium equations. Young and Stephenson (1983) presented a more efficient Newton-Raphson method-based IMPES model which differed from Fussell and Fussell's model in the ordering of the equations and unknowns. Nghiem (1983) modified Nghiem et al.'s (1981) model by implementing three-phase oil-gas-water flash calculation which allowed mass transfer from the hydrocarbon phases to the aqueous phase. A Quasi-Newton method was proposed to improve the convergence of solving a pressure equation and Henry's law was used to model gas solubility in water. Acs et al. (1985) combined Nghiem et al.'s and Young and Stephenson's techniques and developed an IMPES simulator where the pressure equation was derived from a volume balance, rather than overall mole balance. The K-values and liquid densities are looked up from input tables of experimental data and the gas phase density was calculated from an EOS. This model included dispersion by using the convection-diffusion equation. Chien et al. (1985) developed another FIM model which used different primary unknowns (pressure, overall concentrations and K-values) than what Coats used (pressure, saturations and phase compositions). It improved numerical stability by yielding a more diagonally dominant Jacobian matrix. Watts (1986) extended the volume-balance approach of Acs et al. and combined it with the high-stable sequential solution approach of Spillette et al.'s (1973) to develop a sequential

implicit compositional simulator. Nghiem and Li (1986) extended Nghiem et al.'s (1981) formulation to model three hydrocarbon phase flow, but the aqueous phase was not included in the system. The number of phases and the phase compositions were determined by a sequential method combining Michelson's (1982) phase stability analysis and a flash calculation. Collins et al. (1986) published an adaptive-implicit approach which solved a small number of blocks implicitly and the remaining blocks explicitly. Their approach also separated the task of solving flow equations from that of solving the equilibrium equations and allowed the use of various flash calculation methods. Chang et al. (1990) developed a four-phase IMPES compositional simulator based on full convection-diffusion equations, with a three-hydrocarbon-phase flash calculation algorithm where the aqueous phase was treated separately. Rajeev et al. (1993) modelled gas solubility in the aqueous phase for compositional simulators using Henry's law. Buchwalter and Miller (1993) added a compositional injection flow equation into the black oil equations to develop a FIM simulator. Branco and Rodrigues (1996) introduced a semi-implicit approach for compositional simulation with a level of implicitness intermediate to IMPES and FIM. Wang et al. (1997) developed a fully implicit equation of state compositional simulator for large scale reservoir simulations. The simulator used a multi-block, domain decomposition approach in which a reservoir is divided into non-overlapping sub-domains that are solved locally in parallel. Young (2001) presented a continuous form of the equations in the volumebalance method for a compositional model. Cao (2002) developed an implicit pressure and saturations and explicit component mole fraction (IMPSAT) model which is a balance between the IMPES model and the FIM model, stable and computationally cheap. Bowen and Crumpton (2003) published a more efficient implicit formulation which treated a single-phase hydrocarbon as a separate distinct phase. Varavei (2009) developed a four-phase equation-of-state FIM

thermal flooding simulator with three-phase flash calculation where the three hydrocarbon phases are at equilibrium and water is a separate phase. Wei *et al.* (2011) modified Nghiem and Li's three phase IMPES model and developed a three-phase equation-of-state compositional simulator with oil-gas-water flash calculation implemented by using Virtual Material Group Inc.'s property package. An advanced Peng-Robinson EOS (VMG, 2008) was used to model phase behavior and calculate phase density for both the hydrocarbon and aqueous phases.

Since a compositional reservoir model involves a large system of nonlinear partial differential equations, it is desirable to develop a solution scheme which can solve the system accurately and efficiently. From a numerical analysis point of view, a numerical algorithm is stable if errors do not propagate and increase as the iterations are continued. Based on the von Neumann stability analysis, explicit methods are generally unstable and require a Courant–Friedrichs–Lewy (CFL) condition to be satisfied to obtain correct results, while implicit methods are reasonably stable. Therefore, in the compositional reservoir simulations, a fully implicit model provides better stability but requires higher computational costs, while for a partially implicit model, the implicitness varies with the selection of the primary unknowns to be solved for. The choice of reasonable time steps becomes the key point in controlling convergence of the Newton-Raphson iteration and accelerating the simulation process (Chen *et al.*, 2006).

2.2 Multiphase Equilibrium Calculation Using an Equation of State

A fast and robust phase equilibrium calculation algorithm employed in a compositional model helps to determine the number of phases, phase amounts, and phase compositions at a given temperature, pressure and overall composition. The solution of a phase equilibrium problem can be obtained from two conventional formulations: minimization of the Gibbs free energy and solution of fugacity equations (Okuno, 2009). Because the equality of component

fugacity is a first-order necessary condition for a minimum of the Gibbs free energy, the solution of fugacity equations only indicates a stationary point of the Gibbs free energy. While failing to minimize the global Gibbs free energy, the solution of fugacity equations may predict an incorrect number of phases and false phase amounts and compositions. However, global minimization algorithms are not practical for compositional simulation due to their expensive computational costs. In contrast, solving fugacity equations is more efficient and the robustness can be increased by applying a tangent plan criterion (Baker *et al.*, 1982) and its numerical implementation, stability analysis (Michelsen, 1982a). In this dissertation, the minimization algorithms of the Gibbs free energy are not considered.

To solve fugacity equations, a classical successive substitution (SS) method (Henley and Rosen, 1969; Prausnitz *et al.*, 1980) was used by most simulators in the early days due to its robustness and simplicity. A standard SS procedure contains an inner loop and an outer loop at each iteration. A constant *K*-value flash calculation (Rachford and Rice, 1952) is performed to determine the phase mole fractions and compositions for currently specified *K*-values in the inner loop, and then component fugacities are calculated using an EOS to update the *K*-values in the outer loop. This method is stable but its convergence is extremely slow when the given condition is near a critical point (Michelsen, 1982b). Mehra *et al.* (1983) published an accelerated successive substitution (ACSS) algorithm by choosing an optimal step length and their results showed a significant reduction in the number of iterations for convergence. A few high-order methods have been developed to improve the convergence behavior. Fussell and Yanosik (1978) proposed a minimum variable Newton-Rapson (MVNR) iterative method with quadratic convergence that used either liquid or gas phase mole fractions and compositions as independent iteration variables. Fussel (1979) further generalized this two-phase MVNR method

to three-phase flash calculation. Similar approaches can be found in Michelsen (1982b) and Abhvani and Beaumont (1987) but different independent variables (*K*-values or logarithm of *K*-values) were selected. The high-order method usually requires an initial estimate in the vicinity of the solution to converge. To achieve both stability and efficiency, Nghiem *et al.* (1983) combined SS and Powell's hybrid methods and established a criterion for efficiently switching. Nghiem (1983) also developed an efficient quasi-Newton successive substitution method which does not require a good initial guess for convergence.

The equality of fugacity for each component in each phase is only a necessary but not sufficient condition for phase equilibrium. The system of predicted phases must also have the lowest Gibbs free energy at the system temperature and pressure, which is the statement of the second law of thermodynamics (Firoozabadi, 1999). Therefore, simply solving fugacity equations may provide an incorrect number of phases and/or wrong phase amounts and compositions. Baker *et al.* (1982) pointed out this deficiency and presented a tangent plane criterion to determine if predicted equilibrium has the global minimum Gibbs energy. Based on the tangent plane criterion of Gibbs energy, Michelsen (1982a) developed a stability test algorithm which not only checks if the phase splitting calculation results are thermodynamically stable but also provides a very good initial guess for incipient phase compositions for the next flash solution of the material balance equations if necessary. Since then, Nghiem and Li (1984) developed a general stage-wise three-phase equilibrium computation method which used rigorous stability tests to generate initial guesses and determined the number of phases. The quasi-Newton successive-substitution (Nghiem, 1983) is applied for solving flash calculation.

Effects of the water component on the phase behavior of hydrocarbon systems have been studied by Enick *et al.* (1986). They developed a technique for predicting one- to four-phase

equilibrium for multicomponent systems containing water and found significant changes in the phase distribution occurring by introducing water. The addition of water not only results in the formation of an aqueous phase, but also increases the width of the multiple-hydrocarbon-phase region and shifts it towards lower pressures.

For a compositional reservoir simulator, an EOS plays a critical role in the representation of volumetric, thermodynamic, and phase equilibrium properties. Since van der Waals (1873) first presented his EOS in 1873, many modifications have been presented in the literature. Among these equations, the Soave-Redlich-Kwong (Soave, 1972) and the Peng-Robinson (Peng and Robinson, 1976) equations of state are most commonly used in the petroleum industry due to their simplicity, solvability, accuracy and generalization. However, both of them have well known limitations in predicting liquid phase densities for polar compounds. A volume-shift technique was proposed by Peneloux *et al.* (1982) to improve density predictions. Translations were introduced along the volume axis without changing phase equilibrium results. Mathias *et al.* (1988) introduced an additional correction term necessary in the vicinity of the critical point for the Peng-Robinson EOS. A similar correction term can be applied to other equations of state as well.

2.3 Multiphase Behavior of Solvent/Crude Oil Mixtures

Various laboratory experiments have been conducted to study CO₂/crude-oil and richgas/crude-oil systems in the last four decades. Visual observations of the volumetric behavior of CO₂/crude-oil mixtures have shown multiple phases at equilibrium (Huang and Tracht, 1974; Shelton and Yarborough, 1977; Metcalfe and Yarborough, 1979; Gardener *et al.*, 1981; Henry and Metcalfe, 1983; Orr and Jensen, 1984; Turek *et al.*, 1988; Khan *et al.*, 1992; Creek and Sheffield, 1993). A maximum of four hydrocarbon phases together with the aqueous phase (w) have been observed. These hydrocarbon phases are oil (l_1) , gas (v), CO₂-rich liquid (l_2) and asphaltene (s). The l_2 phase, also known as 2nd liquid phase, is formed above a certain pressure at a high solvent composition and temperature not too far above the critical temperature of CO₂. Typically, mixtures of CO₂ and crude oil show liquid-liquid-vapor (l_1-l_2-v) and liquid-liquid (l_1-l_2) equilibria at temperatures below 120°F and exhibit only liquid-vapor (l_1-v) equilibria at higher temperatures (Orr *et al.*, 1981). The formation and deposition of solid-like asphaltene is an important problem in production because it can damage formation and plug wellbore and surface facilities (Nghiem, 1999). However, simulation of asphaltene precipitation that requires a different thermodynamic model for solid phase behavior is out of the scope of this research. In this dissertation, at most four non-solid phases are considered.

Several authors have measured oil displacement by CO₂ or rich-gas in a one-dimensional core and reported displacement efficiency of more than 90% (Yellig and Metcalfe, 1980; Shelton and Yarborough, 1977; Gardner *et al.*, 1981; Orr *et al.*, 1981; Henry and Metcalfe, 1983; Khan, 1992; Creek and Sheffield, 1993; DeRuiter *et al.*, 1994, Mohanty *et al.*, 1995). It is commonly believed that the multiphase behavior contributes to the high displacement efficiency in such a way that the CO₂-rich phase capably extracts a certain range of hydrocarbons from the oil phase (Huang and Tracht, 1974; Gardner *et al.*, 1981; Orr *et al.*, 1981; Turek *et al.*, 1988; Creek and Sheffield, 1993). Other proposed factors affecting the displacement efficiency include late breakthrough caused by a phase density, a volume charging effect, a sweep efficiency improvement and a viscosity reduction.

Chapter Three: Mathematical Formulation

This chapter describes a generalized mathematical formulation of multiphase, multicomponent compositional flow in porous media with appropriate initial and boundary conditions. The governing equations are derived from the physical relations:

- material balance
- volume consistency
- phase equilibrium conditions
- saturation and composition constraints

on the basis of the following assumptions:

- 1. isothermal reservoir
- 2. Darcy flow
- 3. non-flow boundary condition
- 4. no dispersion
- 5. no adsorption
- 6. no chemical reaction

In addition, water is treated as a component rather than an independent phase in our model. In both material balance and phase equilibrium relations, components are allowed to partition into any existing phase. The derived system of equations can be applied to describe compositional flow with any number of phases as long as they are thermodynamically at equilibrium. However, in this simulator, a maximum of four phases including oil, gas, the 2nd liquid and aqueous are considered.

3.1 Component Flow Equations

The governing partial differential equations describing multicomponent multiphase compositional flow in a porous medium are derived from the law of mass conservation for each component in the flow. In terms of moles, conservation of mass states that the accumulation rate of a component in a control volume *V* is equal to the total molar flux of that component across the boundary of *V* plus the moles of that component injected into or produced from *V* (sources or sinks). For component *m*, using ACC_m , $Flux_m$ and \bar{q}_m to represent the accumulation rate, flux and sink/source, respectively, the law of mass conservation can be described by the following equation:

Consider a fluid system that consists of n_c components and n_p equilibrium phases. Let $n_{m\alpha}$ be the moles of component m in phase α per unit bulk volume, n_{α} be the moles of phase α per unit bulk volume and n_m be the total moles of component m per unit bulk volume. According to material balance, n_{α} is the sum of $n_{m\alpha}$ over all components:

$$n_{\alpha} = \sum_{m=1}^{n_c} n_{m\alpha}$$
 3-2

and n_m is the sum of $n_{m\alpha}$ over all phases:

$$n_m = \sum_{\alpha=1}^{n_p} n_{m\alpha}$$
 3-3

The molar accumulation rate of component m can be expressed as

$$ACC_m = \frac{dn_m}{dt}$$
 3-4

The mole fraction of component m in phase α , called composition, is defined by

$$x_{m\alpha} = \frac{n_{m\alpha}}{n_{\alpha}}$$
 3-5

Let \vec{u}_{α} be the volumetric velocity of phase α with molar density ρ_{α} . The molar flux of component *m* carried by phase α is calculated using

$$Flux_{m\alpha} = -\nabla \cdot (x_{m\alpha} \rho_{\alpha} \vec{u}_{\alpha})$$
 3-6

where $\nabla \cdot$ denotes the divergence operator. In compositional flow, because components are transported in multiple fluid phases, the total molar flux of component *m* is the sum of $Flux_{m\alpha}$ over all phases:

$$Flux_{m} = \sum_{\alpha=1}^{n_{p}} Flux_{m\alpha} = -\nabla \cdot \left(\sum_{\alpha=1}^{n_{p}} x_{m\alpha} \rho_{\alpha} \vec{u}_{\alpha}\right)$$
3-7

Substituting Eqs. 3-4 and 3-7 into Eq. 3-1, we obtain the mass conservation equation for component m

$$\frac{dn_m}{dt} + \nabla \cdot \left(\sum_{\alpha=1}^{n_p} x_{m\alpha} \rho_\alpha \vec{u}_\alpha \right) - \bar{q}_m = 0$$
 3-8

Based on the assumption of Darcy flow, the volumetric velocity \vec{u}_{α} of phase α is evaluated using Darcy's law

$$\vec{u}_{\alpha} = -\frac{k_{r\alpha}}{\mu_{\alpha}} K \nabla (p_{\alpha} - \gamma_{\alpha} D)$$
3-9

where ∇ is the gradient operator, $k_{r\alpha}$ is the relative permeability of phase α , *K* is the absolute permeability tensor of the porous medium, μ_{α} is the viscosity of phase α , *D* is the depth, and $\gamma_{\alpha} = \tilde{\rho}_{\alpha}g$ is the specific weight of phase α . The phase pressures in Darcy's law are related by capillary pressures which determine the difference in pressure across the interface between two immiscible phases:

$$p_{c\alpha\beta} = p_{\alpha} - p_{\beta}, \qquad 3-10$$

Commonly, the oil phase pressure p_o is used as a reference pressure in the above equation. The capillary pressures and phase relative permeabilities are assumed to be known functions of phase saturations, which is the fraction of the void volume of a porous medium filled by the phase. Let ϕ , the porosity of the porous medium, denote the fraction of void volume available for the fluids. The porosity ϕ is a pressure dependent rock property that can be calculated as

$$\phi = \phi_0 \left(1 + C_R (p - p_{ref}) \right)$$
 3-11

where ϕ_0 is the porosity at the reference pressure p_{ref} . By definition, the saturation of phase α is evaluated using

$$s_{\alpha} = \frac{n_{\alpha}/\rho_{\alpha}}{\phi}$$
 3-12

Therefore, the total moles of component *m* per unit bulk volume, the composition of component *m* in phase α , the molar density and saturation of phase α , and the porosity of the porous medium are related by the following equation

$$n_m = \sum_{\alpha=1}^{n_p} \phi s_\alpha \rho_\alpha x_{m\alpha}$$
 3-13

For a four-phase system (oil, gas, 2^{nd} liquid and aqueous) that consists of n_c components including water, substituting Darcy's law Eq. 3-9 and capillary pressure relations Eq. 3-10 into Eq. 3-8 yields the component flow equations:

$$\frac{dn_m}{dt} - \nabla \cdot \left[\sum_{\alpha=o,g,l,w} \frac{Kk_{r\alpha}}{\mu_{\alpha}} \rho_{\alpha} x_{m\alpha} \nabla (p_o - p_{co\alpha} - \gamma_{\alpha} D) \right] - \bar{q}_m = 0$$
3-14

$$m = 1, \cdots n_c$$

where subscripts o, g, l and w are the phase indices which denote oil, gas, the 2nd liquid and aqueous, respectively. The oil phase pressure p_o is a primary variable in these equations and the pressure in the other phase is related by the capillary pressure. \bar{q}_m , the sink/source of component m, represents an injection/production well which can be either defined by a constant rate or a constant bottomhole pressure. \bar{q}_m is positive for injection, negative for production and set to zero for gridblocks which are not penetrated by wells.

To simplify the differential equations, define the transmissibility of component m in phase α as

$$T_{m\alpha} = \frac{Kk_{r\alpha}}{\mu_{\alpha}} \rho_{\alpha} x_{m\alpha},$$
 3-15

and the potential of phase α as

$$\Phi_{\alpha} = p_o - p_{co\alpha} - \gamma_{\alpha} D$$
 3-16

Substituting Eqs. 3-15 and 3-16 into Eq. 3-14 gives the final expressions for the component flow equations

$$\frac{dn_m}{dt} - \nabla \cdot \left(\sum_{\alpha=o,g,l,w} T_{m\alpha} \nabla \Phi_\alpha \right) - \bar{q}_m = 0 \qquad m = 1, \cdots n_c \qquad 3-17$$

Eqs. 3-17 compose a set of nonlinear partial differential equations describing flow and transport of multicomponents in multiple fluid phases. The formulation allows the use of overall properties $(n_1, ..., n_{n_c}, p_o)$ as primary variables for all gridblocks regardless of appearance and disappearance of phases and avoids additional work for tracking the phase existence and performing the switch of variables.
3.2 Volume Consistency Equation

A volume consistency equation is derived from the assumption that the pore volume of a porous medium is fully filled by reservoir fluids. In a unit bulk volume of the porous medium, the total volume of all the coexisting phases is equal to the porosity. This relationship can be formulated as

$$\sum_{\alpha=o,g,l,w} \frac{n_{\alpha}}{\rho_{\alpha}} - \phi = 0$$
 3-18

which is equivalent to the following saturation constraint equation:

$$\sum_{\alpha=o,g,l,w} s_{\alpha} = 1$$
 3-19

3.3 Phase Equilibrium Equations

Since mass interchange between phases happens much more rapidly than the fluid flow in porous media, it is physically reasonable to assume that all phases are at equilibrium. From the thermodynamic point of view, all equilibrium solution must satisfy three restrictions (Baker *et al.*, 1982):

- 1. Material balances hold for all components.
- 2. The chemical potentials for each component are the same in all phases.
- 3. The Gibbs free energy of the system is the minimum at given pressure and temperature.

For a n_p -phase system, the material balance means that the sum of the mole number of a component distributed in each phase is equal to the overall mole number of that component per unit bulk volume. Dividing both sides of Eq. 3-3 by the total mole number of the mixture per unit bulk volume $n_T = \sum_{m=1}^{n_c} n_m$ gives

$$\frac{n_m}{n_T} = \sum_{\alpha=1}^{n_p} \frac{n_\alpha}{n_T} \frac{n_{m\alpha}}{n_\alpha}$$
3-20

Here, we introduce the overall composition z_m of component m

$$z_m = \frac{n_m}{n_T}$$
 3-21

and the mole fraction of phase α

$$L_{\alpha} = \frac{n_{\alpha}}{n_T}$$
 3-22

Eq. 3-20 becomes

$$z_m = \sum_{\alpha=1}^{n_p} L_\alpha x_{m\alpha}$$
 3-23

which is the material balance equation frequently used in phase equilibrium calculation. From the definitions, the compositions and phase mole fractions satisfy the following constraint equations:

$$\sum_{m=1}^{n_c} z_m = 1$$
 3-24

$$\sum_{m=1}^{n_c} x_{m\alpha} = 1 \qquad \alpha = o, g, l, w \qquad 3-25$$

$$\sum_{\alpha=1}^{n_p} L_{\alpha} = 1$$
 3-26

The equality of chemical potentials indicates that there is no driving force to cause net movement of any component between phases at equilibrium. From fundamental thermodynamics equations, the chemical potential of a component is the partial derivative of the Gibbs free energy with respect to the component's mole number while holding temperature, pressure and the mole numbers of other components in the mixture constant. For an ideal gas mixture, it is determined by

$$\mu_m^{ig} = \tau_m(T) + RT \ln(x_m p)$$
 3-27

where *R* is the gas constant and $\tau_m(T)$ is an component-dependent integration constant at temperature *T*. To generalize it, a function f_m , called fugacity, was introduced by Lewis (1901) to allow the chemical potentials of components in a real fluid to have an analogous expression,

$$\mu_m = \tau_m(T) + RT \ln f_m \qquad 3-28$$

Therefore, the second equilibrium criterion, the equality of chemical potentials, is equivalent to the following fugacity equations:

$$f_{m1}(p_1, x_{11}, x_{21}, \dots, x_{n_c, 1}) = f_{m2}(p_2, x_{12}, x_{22}, \dots, x_{n_c, 2})$$

$$f_{m1}(p_1, x_{11}, x_{21}, \dots, x_{n_c, 1}) = f_{m3}(p_3, x_{13}, x_{23}, \dots, x_{n_c, 3})$$

$$\vdots$$

3-29

$$f_{m1}(p_1, x_{11}, x_{21}, \dots, x_{n_c, 1}) = f_{mn_p}(p_{n_p}, x_{1, n_p}, x_{2, n_p}, \dots, x_{n_c, n_p})$$

Since the effects of capillary pressures are ignored in the phase equilibrium calculation, p_{α} can be replaced by the system pressure in the evaluation of component fugacities in all phases. In the case of four-phase equilibrium, the system of fugacity equations for component *m* is reduced to:

$$f_{mo}(p_o, x_{1o}, x_{2o}, \dots, x_{n_c,o}) = f_{mg}(p_o, x_{1g}, x_{2g}, \dots, x_{n_c,g})$$

$$f_{mo}(p_o, x_{1o}, x_{2o}, \dots, x_{n_c,o}) = f_{ml}(p_o, x_{1l}, x_{2l}, \dots, x_{n_c,l})$$

$$f_{mo}(p_o, x_{1o}, x_{2o}, \dots, x_{n_c,o}) = f_{mw}(p_o, x_{1w}, x_{2w}, \dots, x_{n_c,w})$$
3-30

The fugacity of component *m* has the same unit as pressure and equals to the component's partial pressure $f_m^{ig} = x_m p$ in the ideal gas mixture. Define the fugacity coefficient φ_m as the dimensionless ratio of f_m to $x_m p$:

$$\varphi_m = \frac{f_m}{x_m p} \tag{3-31}$$

and combining Eqs. 3-27 and 3-28 gives

$$\mu_m = \mu_m^{ig} + RT \ln \varphi_m \qquad 3-32$$

which derives an equation to evaluate the fugacity and fugacity coefficient quantitatively (Prausnitz *et al.*, 1998)

$$RT\ln\varphi_m = RT\ln\frac{f_m}{x_m p} = \int_V^\infty \left[\left(\frac{\partial p}{\partial n_m}\right)_{T,V,\vec{n}_m} - \frac{RT}{V} \right] dV - RT\ln Z$$
 3-33

where Z = pv/RT is the compressibility factor of the mixture determined by an EOS.

As shown by Baker *et al.* (1982), an EOS can predict an incorrect number of phases or phase compositions even though the equilibrium solution satisfies the material balance and equality of chemical potentials while failing to minimize the Gibbs energy. They also presented a method, called a tangent plane distance (TPD) analysis, to determine when a phase equilibrium solution is incorrect. Based on the tangent plane criterion of the Gibbs free energy, Michelsen (1982a) developed a stability analysis algorithm which not only checks if the phase splitting calculation results are thermodynamically stable, but also provides an initial guess for incipient phase compositions for the next flash solution of the material balance equations if necessary. In the stability test, an equivalent stationarity criterion equation is solved to locate stationary points on the Gibbs free energy surface, and stability is verified by checking the vertical distance between the tangent hyperplane to the Gibbs energy surface for all stationary points. The detailed numerical implementations of the stability analysis and multiphase equilibrium calculation will be presented in Chapter Four.

3.4 Solution Method

The material balance equations (Eq. 3-23) and constraints on phase mole fractions and compositions (Eqs. 3-25 and 3-26) can be used to reduce the number of unknowns by eliminating

dependent variables x_{n_co} , x_{n_cg} , x_{n_cl} , x_{1w} , ..., x_{n_cw} , and L_w . As shown in Table 3-1, the coupled system of component flow and phase equilibrium for a four-phase compositional model includes $4n_c + 1$ independent equations and the same number of independent variables. Therefore, the system is complete and solvable. Out of $4n_c + 1$ equations, the component flow equations

$$F_m = \frac{dn_m}{dt} - \nabla \left[\sum_{\alpha = o, g, l, w} T_{m\alpha} \nabla \Phi_\alpha \right] - \bar{q}_m = 0$$
3-34

 $m = 1, \cdots n_c$

and the volume consistency equation

$$F_{n_c+1} = \sum_{\alpha=o,g,l,w} \frac{n_{\alpha}}{\rho_{\alpha}} - \phi = 0$$
3-35

are selected as the primary equation set:

$$\vec{F}_p = (F_1, F_2, \dots, F_{n_c}, F_{n_c+1})$$
 3-36

while the primary variables are all overall properties

$$\vec{x}_p = (n_1, \dots, n_{n_c}, p_o)$$
 3-37

The equilibrium equations

$$F_{n_c+1+m} = f_{mo} - f_{mg}$$

$$F_{2n_c+1+m} = f_{mo} - f_{ml}$$

$$F_{3n_c+1+m} = f_{mo} - f_{mw}$$
3-38

 $m = 1, ... n_c$

form the secondary equations

$$\vec{F}_{s} = (F_{n_{c}+2}, \dots, F_{2n_{c}+1}, F_{2n_{c}+2}, \dots, F_{3n_{c}+1}, F_{3n_{c}+2}, \dots, F_{4n_{c}+1})$$
3-39

and, consequently, the phase compositions and mole fractions compose the secondary variables

$$\vec{x}_{s} = (x_{1,0}, \dots, x_{n_{c}-1,0}, L_{0}, x_{1,g}, \dots, x_{n_{c}-1,g}, L_{g}, x_{1,l}, \dots, x_{n_{c}-1,l}, L_{l})$$
3-40

The remaining variables (porosity ϕ , overall composition z_m , phase molar density ρ_{α} , phase mass density $\tilde{\rho}_{\alpha}$, phase viscosity μ_{α} , phase saturation s_{α} , phase relative permeability $k_{r\alpha}$ and capillary pressure $p_{c\alpha o}$) are functions of the independent variables and can be evaluated after p, $\vec{n}, \vec{x}_{\alpha}$ and L_{α} are determined.

In a conventional compositional simulator, the component flow equations and phase equilibrium equations are solved simultaneously using the Newton-Raphson method for all variables and the phases are not at equilibrium until the convergence is achieved. For a multiphase model, this method sometimes fails to converge for the gridblocks where a phase change occurs during an iteration because the number of phases coexisting at the condition of converged pressure and overall composition are not known in advance. Also, solving $4n_c + 1$ equations together requires high computational costs during the iterations. To simplify the solution procedure and reduce the computational cost, it is desirable to decouple the phase equilibrium equations from the component flow equations and solve them separately. The solution method used in this model solves the primary equation set (Eqs. 3-34 and 3-35) for the primary variables $(n_1, ..., n_{n_c}, p_o)$ first in each Newton iteration. The Jacobian matrix of the system is evaluated using analytical derivatives and the chain rule. Once the primary variables are updated after each iteration, the overall component compositions $(z_1, ..., z_{n_c})$ are recalculated according to $(n_1, ..., n_{n_c})$ and the multiphase equilibrium calculation is then performed at the updated pressure and overall composition to determine the number of phases and the secondary variables $(x_{1\alpha},\ldots,x_{n_c-1\alpha},L_{\alpha}).$

This approach is advantageous to handle phase appearance and disappearance. If there exist fewer phases in the system, the primary equations and variables remain the same while the phase equilibrium equations and phase variables are reduced accordingly. For example, for an oil-gas- 2^{nd} liquid system, the equilibrium equations and variables of the non-existent aqueous phase are removed from the secondary set. In this case, the secondary equations are reduced to

$$f_{mo} = f_{mg}$$
$$f_{mo} = f_{ml}$$

and the secondary variables are

$$x_{1,o}, \dots, x_{n_c-1,o}, L_o, x_{1,g}, \dots, x_{n_c-1,g}, L_g$$

This method is similar to Collins *et al.*'s treatment for explicit blocks (1986) but differs in the maximum number of phases allowed in the system as well as the way for the Jacobian evaluation. It separates the solution of equilibrium equations from the solution of component flow equations so that we can implement a complex phase equilibrium calculation algorithm that sequentially applies a phase stability test and phase split calculation and overcome the difficulties of phase change during iteration.

3.5 Summary

A system of nonlinear equations that describe compositional flow in porous media has been derived from the law of mass conservation and the second law of thermodynamics. The full set of $4n_c + 1$ coupled component flow and phase equilibrium equations and variables is divided into the primary and secondary sets for a more efficient decoupled numerical approach. For a four-phase compositional model, this formulation using overall properties as the primary variables avoids phase tracking and variable switch during iteration. If fewer phases coexist in the system or phase disappearance happens during iteration, the primary set remains unchanged while the secondary set is reduced consequently. Details of numerical solutions are discussed in Chapter Five.

Equations	Number	Variables	Number
Component Flow (Eqs. 3-17)	n _c	p_o	1
Volume Consistency (Eq. 3-18)	1	n_1, n_2, \dots, n_{n_c}	n_c
Phase Equilibrium (Eqs. 3-30)	3n _c	$x_{1\alpha}, x_{2\alpha}, \dots, x_{n_c-1\alpha}$	$3n_{c} - 3$
		L_{lpha}	3
Total	$4n_{c} + 1$	Total	$4n_{c} + 1$

 $*\alpha = o, g, l$

Chapter Four: Phase Equilibrium and Property Calculation

In a compositional model, to solve the governing equations at each time step, the number of phases, phase amounts, phase compositions, and phase physical properties at a given temperature, pressure and overall composition are calculated. There are two thermodynamic models applied to phase equilibrium computations: an equilibrium ratio (*K*-values) model and an equation of state (EOS) model. The equilibrium ratio model, which can be easily tuned to fit experimental data, was widely used in compositional simulators at an early stage of compositional simulation due to its simplicity. However, this approach may be inconsistent in the near-critical region. On the other hand, the equation-of-state model offers a continuous and smooth transition of calculated *K*-values and densities through the critical point but it is not as easily fitted to data and additional computational efforts are required for root finding and property calculation. Recent developments of EOS methods have improved the accuracy of phase equilibrium and property calculation, and an explosion in computational power has overcome the high computational cost. Therefore, the interest in the application of the EOS for compositional simulations has significantly increased since the 1980s.

The solution of phase equilibrium has to satisfy three restrictions: material balance, equality of fugacity, and global minimum of the Gibbs energy. A stepwise method that sequentially applies a stability analysis and phase split calculation is used in this simulator. As shown in Fig. 4-1, a feed phase with overall composition is tested first for its stability. If the feed phase is unstable, another phase is introduced and a phase split calculation is performed to determine the mole fractions and compositions of each phase. When a multiphase system is obtained from the phase split calculation, it is necessary to select only one of the phases to perform the next stage stability test. The procedure repeats until the multiphase system obtained from the phase split

calculation is stable or the number of existing phases in the system reaches the maximum allowable number of phases.

4.1 Cubic Equations of State

An EOS is an algebraic expression that represents the PVT behavior of both liquid and vapor phases and satisfies the criterion of criticality. Since van der Waals introduced the first cubic EOS in 1873, numerous equations have been developed. Among these, the Soave-Redlich-Kwong (Soave, 1972) and the Peng-Robinson (Peng and Robinson, 1976) equations of state are most commonly used in the petroleum industry due to their simplicity, solvability, accuracy and generalization. Both of them are cubic equations and, in general, a cubic EOS can be written as:

$$p = \frac{RT}{\nu + \delta_1} - \frac{a(T)}{(\nu + \delta_2)(\nu + \delta_3)}$$
4-1

where *a*, an attraction parameter, represents the attractive force between molecules and δ_1 , δ_2 and δ_3 are volume correction parameters. In most cubic EOSs, δ_1 is related to a co-volume parameter *b*, which is the limiting volume of a fluid at infinite pressure and recognizes the role of repulsive force. These parameters are determined by matching available experimental PVT data.

4.1.1 Soave-Redlich-Kwong (SRK) Equation

The modified Redlich-Kwong EOS by Soave (1972) can be written explicitly in pressure as

$$p = \frac{RT}{v-b} - \frac{a(T)}{v(v+b)}$$
4-2

in which the attraction parameter a(T) and co-volume parameter b of the mixture are determined by linear mixing rules

$$a(T) = \sum_{m=1}^{n_c} \sum_{n=1}^{n_c} x_m x_n (1 - \kappa_{mn}) \sqrt{a_m a_n}$$
 4-3

and

$$b = \sum_{m=1}^{n_c} x_m b_m \tag{4-4}$$

where κ_{mn} is the binary interaction parameter between components *m* and component *n*, and a_m and b_m are, respectively, the attraction parameter and co-volume parameter for the pure component *m*. a_m and b_m are obtained from the criterion of criticality:

$$a_m = 0.42747 \alpha_m \frac{R^2 T_{cm}^2}{P_{cm}}$$
 4-5

$$b_m = 0.08664 \frac{RT_{cm}}{P_{cm}}$$
 4-6

where R is the universal gas constant and α_m is a temperature dependent parameter given by

$$\alpha_m = \left(1 + \lambda_m \left(1 - \sqrt{T/T_{cm}}\right)\right)^2$$
4-7

with

$$\lambda_m = 0.48 + 1.574\omega_m - 0.26992\omega_m^2$$
 4-8

The acentric factor ω_m of component *m* measures the deviation of the molecular shape from a spherically symmetric structure. Introducing

$$A = \frac{a \cdot p}{R^2 T^2}$$
 4-9

and

$$B = \frac{b \cdot p}{RT}$$
 4-10

Eq. 4-2 can be rewritten as a cubic equation in terms of the compressibility factor Z = pV/RT as follows

$$Z^{3} - Z^{2} + (A - B - B^{2})Z - AB = 0$$
4-11

which can be solved using the cubic formula (Chen, 2007). Once the compressibility factor of phase α is acquired, substituting Eq. 4-2 into Eq. 3-33 gives the fugacity coefficient of component *m* in the mixture:

$$\ln\frac{f_m}{x_m p} = \frac{b_m}{b}(Z-1) - \ln(Z-B) - \frac{A}{B}\left(\frac{1}{a}\frac{\partial a}{\partial x_m} - \frac{b_m}{b}\right)\ln\left(1 + \frac{B}{Z}\right)$$
4-12

4.1.2 Peng-Robinson (PR) Equation

The Peng-Robinson EOS is a two-constant pressure-explicit equation:

$$P = \frac{RT}{v-b} - \frac{a(T)}{v(v+b) + b(v-b)}$$
4-13

which can also be written in a cubic form in terms of the compressibility factor as

$$Z^{3} - (1 - B)Z^{2} + (A - 2B - 3B^{2})Z - (AB - B^{2} - B^{3}) = 0$$
4-14

When applied to a multi-component mixture, the same linear mixing rule as the SRK EOS is used to obtain the mixture's attraction parameter and co-volume parameter while the componentdependent parameters a_m , b_m and λ_m are calculated by

$$a_m = 0.44724 \alpha_m \frac{R^2 T_{cm}^2}{P_{cm}}$$
 4-15

$$b_m = 0.077796 \frac{RT_{cm}}{P_{cm}}$$
 4-16

and

$$\lambda_m = \begin{cases} 0.37464 + 1.5432\omega_m - 0.26992\omega_m^2 & \omega_m < 0.49\\ 0.3796 + 1.485\omega_m - 0.1644\omega_m^2 + 0.01666\omega_m^3 & \omega_m \ge 0.49 \end{cases}$$
4-17

respectively. The fugacity coefficient of component m in the mixture is given by

$$\ln\frac{f_m}{x_m p} = \frac{b_m}{b}(Z-1) - \ln(Z-B) - \frac{A}{2\sqrt{2}B} \left(\frac{1}{a}\frac{\partial a}{\partial x_m} - \frac{b_m}{b}\right) \ln\left(\frac{Z+(1+\sqrt{2})B}{Z+(1-\sqrt{2})B}\right)$$
 4-18

4.1.3 Solution and Root Selection

For a given pressure, a cubic equation has three real roots for the compressibility factor at a temperature below the pseudo critical temperature of a mixture while only one real root exists at a temperature above the pseudo critical temperature. No matter how many roots are obtained, the root corresponding to a molar volume less than the co-volume parameter b will be rejected since the co-volume parameter is defined as the molar volume when the pressure approaches infinity.

When an EOS has three real roots, the intermediate root is ignored and the one giving the lower Gibbs energy from the other two is selected. The phase type (liquid-like or vapor-like) of the selected root is determined based on its value compared to the other root. The larger root is assigned as a vapor-like phase whereas the smaller root implies a liquid-like phase. However, when the EOS only provides a single root for a given phase, Li's mixing rule (1971) is used to estimate the critical temperature of the phase

$$T_{c\alpha}^{L} = \frac{\sum_{m=1}^{n_{c}} x_{m\alpha} v_{cm} T_{cm}}{\sum_{m=1}^{n_{c}} x_{m\alpha} v_{cm}}$$
 4-19

Then, if the system temperature is less than $T_{c\alpha}^{L}$, the phase is considered liquid-like. Otherwise, the phase is vapor-like.

4.2 Phase Stability Analysis

To satisfy the minimum Gibbs free energy requirement in a multiphase equilibrium calculation, a stability analysis (Michelsen, 1982a) is carried out to decide whether a system is thermodynamically stable. The method is performed by adding a trial phase into the system and solving a phase splitting problem for the trial phase composition. If the total Gibbs free energy of the system is reduced by phase splitting, the original system is unstable and a phase is added into the phase split calculation.

Suppose that a system to be investigated has n_p phases with phase composition \vec{x}_{α} at equilibrium, and the overall molar Gibbs energy of the system is given by

$$G = RT \sum_{\alpha=1}^{n_p} \sum_{m=1}^{n_c} L_{\alpha} x_{m\alpha} \ln f_{m\alpha} + \sum_{m=1}^{n_c} z_m G_m^0$$
 4-20

where G_m^0 is the molar Gibbs energy of component *m* in the standard state. (Nghiem and Li, 1984) Since the n_p phases are at equilibrium, the surface *G* has the same tangent plane at each point of \vec{x}_{α} (Baker *et al.*, 1982) and the tangent plane criterion states that the Gibbs energy of a stable system lies entirely above its tangent plane. To implement this criterion numerically, define tangent plane distance as the vertical distance between the molar-Gibbs-energy surface and its tangent plane at composition $\vec{x}_t = (x_{1t}, x_{2t}, \dots, x_{n_ct})$ (Nghiem and Li, 1984)

$$TPD(\vec{x}_t) = RT \sum_{m=1}^{n_c} x_{mt} \ln \frac{f_m(\vec{x}_t)}{f_{m\beta}(\vec{x}_\beta)}$$

$$4-21$$

where β may represent any phase in the system due to the equality of fugacity at equilibrium. The tangent plane criterion implies that the system is stable if and only if the inequality

$$TPD(\vec{x}_t) \ge 0 \tag{4-22}$$

is valid for all \vec{x}_t . An exhaustive search in the composition space for values of \vec{x}_t which satisfy the above inequality is expensive and difficult to implement. Michelson (1982a) suggested locating stationary points of the tangent plane distance, and verifying the stability by checking whether Eq. 4-22 holds for all stationary points. The stationary points are obtained by solving the stationarity criterion equations:

$$\ln X_{mt} + \ln \varphi_m(\vec{x}_t) - \ln x_{m\beta} - \ln \varphi_{m\beta}(\vec{x}_\beta) = 0, \qquad m = 1, \cdots, n_c \qquad 4-23$$

where \vec{X}_t is interpreted as mole number,

$$x_{mt} = X_{mt} / \sum_{n=1}^{n_c} X_{nt}$$
 4-24

The stability of the investigated phase is determined by the sum of non-trivial solutions \vec{X}_t . Here, a trivial solution means $\vec{X}_t = \vec{x}_\beta$. If $\sum_{m=1}^{n_c} X_{mt}$ is greater than one, the phase is unstable. Otherwise, the phase is stable.

A combination of successive substitution (SS) and the Newton-Raphson (NR) method is used for solving Eq. 4-23. The SS is a linearly convergent stable method which converges slowly in a near-critical region, while the NR method is quadratically convergent only when an initial estimate close enough to the solution is provided. To take advantages of both methods, the combined iteration starts with the SS and switches to the Newton-Raphson method to accelerate convergence if the residual error is less than a certain tolerance.

For an application of the SS method, \vec{X}_t is updated by

$$X_{mt}^{(k+1)} = \exp\left(\ln x_{m\beta} + \ln \varphi_{m\beta}(\vec{x}_{\beta}) - \varphi_m(\vec{x}_t)\right), \qquad m = 1, \cdots, n_c$$
4-25

In the Newton-Raphson iteration, the residual of Eq 4-23 is given by

$$r_m = \ln X_{mt} + \ln \varphi_m(\vec{x}_t) - \ln x_{m\beta} - \ln \varphi_{m\beta}(\vec{x}_\beta), \qquad m = 1, \cdots, n_c \qquad 4-26$$

and the updated equation is

$$\vec{X}_t^{(k+1)} = \vec{X}_t^{(k)} - \left(J^{(k)}\right)^{-1} \vec{r}^{(k)}$$
4-27

where $J^{(k)}$ is the Jacobian matrix of the k-th iteration whose element is evaluated from

$$J_{ij}^{(k)} = \left(\frac{\partial r_i}{\partial X_j}\right)^{(k)} = \left(\frac{\partial \ln X_{it}\varphi_i(\vec{x}_t)}{\partial X_j}\right)^{(k)}$$
4-28

A number of initial estimates of \vec{X}_t are suggested for the stability analysis calculation to avoid trivial solutions for either phase (Michelsen, 1982a). They are applied in the following order:

1. The Wilson correlation:

$$X_{mt} = z_m K_m, \qquad m = 1, \cdots, n_c$$

where

$$K_m = \frac{p_{cm}}{p} \exp\left(5.37(1+\omega_m)\left(1-\frac{T_{cm}}{T}\right)\right)$$
4-30

2. The Inverse Wilson correlation:

$$X_{mt} = \frac{Z_m}{K_m}, \qquad m = 1, \cdots, n_c$$
4-31

3. Average compositions:

$$X_{mt} = \sum_{\alpha=1}^{n_p} \frac{x_{m\alpha}}{n_p}, \qquad m = 1, \cdots, n_c$$
4-32

4. A pure phase:

$$X_{mt} = 0.999$$
 and $X_{nt} = \frac{0.001}{n_c - 1}$, $n = 1, \dots, m - 1, m + 1, \dots, n_c$ **4-33**

5. A hypothetical ideal gas:

$$X_{mt} = \exp(\ln z_m + \ln \varphi_m(\vec{z})), \qquad m = 1, \cdots, n_c$$
4-34

- -

The calculation procedure of the stability analysis is as follows:

- 1. Calculate the compressibility factor and fugacity coefficient for the phase to be investigated with composition \vec{x}_{β} .
- 2. Obtain initial estimates for variable \vec{X}_t from Eqs. 4-29 through 4-34.
- 3. Calculate trial phase compositions \vec{x}_t using Eq. 4-24.
- 4. Calculate the compressibility factor and fugacity coefficient for the trial phase with compositions \vec{x}_t using Eq. 4-12 or Eq. 4-18 according to the selected EOS.
- 5. Calculate the residuals from Eq. 4-26 and check for the convergence:

$$\|\vec{r}\| \le \epsilon_{conv} \tag{4-35}$$

If the convergence criterion is satisfied, stop. Otherwise, continue to Step 6

6. Check the switching to NR iteration criterion

$$\|\vec{r}\| \le \epsilon_{switch}$$
 4-36

- 7. If the switching criterion is not satisfied, update \vec{X}_t using Eq. 4-25 and go to Step 3 to continue the SS iteration. Otherwise, go to Step 8 to start the NR iteration.
- 8. Evaluate the Jacobian matrix for the NR iteration from Eq. 4-28.
- 9. Update \vec{X}_t using Eq. 4-27.
- 10. Calculate the residuals from Eq. 4-26 and check for convergence by satisfying Eq. 4-35.If it converges, stop. Otherwise, go to Step 8.

4.3 Phase Split Calculation

A phase split calculation is performed based on stability test results to determine the mole fractions of each phase and phase compositions. Various methods have been developed during last a few decades but most of them are limited to a two-phase flash. In this section, first order and second order methods are presented and generalized for multiphase calculation.

4.3.1 Successive Substitution Method (SS)

In the early days, successive substitution (SS) was widely used in most compositional models to solve two-phase flash problems because of its robustness and simplicity. It is a first order method which converges linearly and the convergence becomes extremely slow in a near-critical region.

The independent variables used in the SS method are *K*-values, the ratios of the mole fractions of component *m* in phase α to those of the reference phase:

$$K_{m\alpha} = \frac{x_{m\alpha}}{x_{mr}}$$
, $m = 1, \dots, n_c$, $\alpha = 1, \dots, n_p$ and $\alpha \neq r$ 4-37

where subscript r indicates the reference phase and the K-value of the reference $K_{mr} = 1$. In each iteration, a constant K-value flash is performed to determine the phase mole fractions and compositions for the currently specified K-values in the inner loop. Component fugacities are calculated to update the K-values in the outer loop.

The equations for the constant *K*-value flash can be derived from material balance and mole fraction constraints. Substitution of Eq. 4-37 into Eq. 3-23 yields

$$x_{m\alpha} = \frac{K_{m\alpha} z_m}{\sum_{\beta=1}^{n_p} L_{\beta} K_{m\beta}}, \quad m = 1, \cdots, n_c$$
4-38

Using the phase mole fraction constraint to eliminate the dependent reference phase mole fraction and applying the constraint Eqs. 3-25 equations, we obtain a system of $n_p - 1$ nonlinear equations:

$$h_{\alpha} = \sum_{m=1}^{n_c} \frac{(K_{m\alpha} - 1)z_m}{1 + \sum_{\beta \neq r} L_{\beta} (K_{m\beta} - 1)}, \quad \alpha = 1, \cdots, n_p \text{ and } \alpha \neq r$$

$$4-39$$

which is also called the multiphase Rachford-Rice equations. The nonlinear system of Eq. 4-39 can be solved for unknowns L_{α} by the Newton-Raphson method

$$\vec{L}_{\alpha}^{(k+1)} = \vec{L}_{\alpha}^{(k)} - \left(\bar{\bar{J}}^{(k)}\right)^{-1} \vec{h}_{\alpha}^{(k)}$$
4-40

and the elements of the Jacobian matrix J are evaluated using

$$\bar{J}_{ij} = \sum_{m=1}^{n_c} \frac{(K_{mi} - 1)(K_{mj} - 1)z_m}{\left(1 + \sum_{\beta \neq r} L_\beta (K_{m\beta} - 1)\right)^2}$$
4-41

Once the L_{α} 's are solved for, the reference phase mole fraction phase L_r is computed from the constraint Eq. 3-26, the phase compositions are calculated using Eq. 4-38 and the component fugacities are obtained from Eq. 4-12 or Eq. 4-18 according to the selected EOS. Then the *K*-values are updated by

$$K_{m\alpha}^{(k+1)} = K_{m\alpha}^{(k)} \exp\left(-\frac{f_{mr}}{f_{ma}}\right), \quad m = 1, \cdots, n_c \text{ and } \alpha \neq r$$
4-42

where k is the iteration level in the SS.

The nature of the SS method is unclear until Mehra (1983) recognized that it is related to the steepest descent method which takes a unit step size for minimization of the Gibbs energy for the current system. The difference between them is that the SS method uses the descent direction which accounts only for the ideal mixing part of the Gibbs energy and does not consider the excess part of the Gibbs energy. This causes a slow convergence behavior when the given condition is near a critical region (Okuno, 2009).

4.3.2 Accelerated Successive Substitution Method (ACSS)

To improve the convergence behavior, Mehra *et al.* (1983) proposed an accelerated successive substitution (ACSS) method which modified the step size of the SS by introducing a non-negative acceleration parameter $\lambda^{(k+1)}$,

$$\lambda^{(k+1)} = \frac{\lambda^{(k)} \sum_{m=1}^{n_c} \sum_{\alpha \neq r}^{n_p} \left(g_{m\alpha}^{(k)} \right)^2}{\left| \sum_{m=1}^{n_c} \sum_{\alpha \neq r}^{n_p} \left(\left(g_{m\alpha}^{(k-1)} g_{m\alpha}^{(k)} \right) - \left(g_{m\alpha}^{(k)} \right)^2 \right)^2 \right|}, \quad m = 1, \cdots, n_c$$
4-43

where

$$g_{m\alpha} = \ln \frac{f_{mr}}{f_{m\alpha}}, \qquad m = 1, \cdots, n_c$$
 4-44

The acceleration parameter $\lambda^{(k+1)}$ is initialized with $\lambda^{(1)} = 1$ for the first iteration, and limited within the range $1 \le \lambda^{(k+1)} \le 3$. The *K*-values are updated using

$$K_{m\alpha}^{(k+1)} = K_{m\alpha}^{(k)} \exp\left(-\lambda^{(k+1)} \frac{f_{m\alpha}}{f_{mr}}\right) \qquad m = 1, \cdots, n_c \text{ and } \alpha \neq r$$
 4-45

It was reported that the ACSS algorithm gave a significant improvement in the convergence rate. The method may converge in a few iterations less than the second order method in certain cases but that is generally not to be expected.

4.3.3 Minimum Variable Newton-Raphson Method (MVNR)

The Minimum Variable Newton-Raphson method developed by Fussel and Yanosik (1978) solves the fugacity equations directly for independent unknowns L_{α} 's and $x_{m\alpha}$'s. The material balance equation and the constraints on phase mole fractions and compositions are used to eliminate dependent variables and reduce the number of unknowns. MVNR is a second order method which converges quadratically within the neighborhood of the solution. However, it may fail to converge when the initial estimate is not close enough to the solution of the system of the nonlinear equations.

For a n_p -phase flash problem, we have $n_c(n_p - 1)$ independent equations

$$f_{m1} = f_{m\alpha}, \qquad m = 1, \cdots, n_c, \alpha = 2, \cdots, n_p$$
 4-46

. . .

and $n_c(n_p - 1)$ independent unknowns after applying Eqs. 3-23, 3-25 and 3-26

$$\vec{X} = \left(x_{11}, \dots, x_{n_c-1,1}, L_1; \dots; x_{1\alpha}, \dots, x_{n_c-1,\alpha}, L_{\alpha}; \dots; x_{1,n_p-1}, \dots, x_{n_c-1,n_p-1}, L_{n_p-1}\right)^T.$$

Let the residual of Eq. 4-46 be

$$\vec{r} = \begin{pmatrix} f_{11} - f_{12} \\ \vdots \\ f_{n_c,1} - f_{n_c,2} \\ f_{11} - f_{13} \\ \vdots \\ f_{n_c,1} - f_{n_c,3} \\ \vdots \\ f_{11} - f_{1n_p} \\ \vdots \\ f_{n_c,1} - f_{n_c,n_p} \end{pmatrix}$$
4-47

The system $\vec{r}(\vec{X}) = 0$ can be solved by the Newton-Raphson (NR) method,

$$\vec{X}^{(k+1)} = \vec{X}^{(k)} - \left(\bar{J}^{(k)}\right)^{-1} \vec{r}^{(k)}$$
4-48

with the Jacobian matrix

$$\bar{J}^{(k)} = \begin{pmatrix} \frac{\partial r_1}{\partial x_{11}} & \cdots & \frac{\partial r_1}{\partial x_{n_c-1,1}} & \frac{\partial r_1}{\partial L_1} & \cdots & \frac{\partial r_1}{\partial x_{1,n_p-1}} & \cdots & \frac{\partial r_1}{\partial x_{n_c-1,n_p-1}} & \frac{\partial r_1}{\partial L_{n_p-1}} \\ \frac{\partial r_2}{\partial x_{11}} & \cdots & \frac{\partial r_2}{\partial x_{n_c-1,1}} & \frac{\partial r_2}{\partial L_1} & \cdots & \frac{\partial r_2}{\partial x_{1,n_p-1}} & \cdots & \frac{\partial r_2}{\partial x_{n_c-1,n_p-1}} & \frac{\partial r_2}{\partial L_{n_p-1}} \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots & \ddots & \vdots & \vdots \\ \frac{\partial r_{n_{cp}}}{\partial x_{11}} & \cdots & \frac{\partial r_{n_{cp}}}{\partial x_{n_c-1,1}} & \frac{\partial r_{n_{cp}}}{\partial L_1} & \cdots & \frac{\partial r_{n_{cp}}}{\partial x_{1,n_p-1}} & \cdots & \frac{\partial r_{n_{cp}}}{\partial x_{n_c-1,n_p-1}} & \frac{\partial r_{n_{cp}}}{\partial L_{n_p-1}} \end{pmatrix}^{(k)}$$

$$4-49$$

where $n_{cp} = n_c(n_p - 1)$ represents the dimension of residuals. The partial derivatives required to calculate the elements of the Jacobian matrix for the MVNR method are included in Appendix A.

4.3.4 Combined ACSS and MVNR Method

The MVNR method is very efficient for a two-phase flash even in the near-critical region. However, when there are more than two phases presenting in the system, the Newton-Raphson iteration is not reliable because it does not necessarily reduce the Gibbs free energy at each iteration (Michelsen, 1982b; Okuno, 2009). This problem is caused by the poor initial estimate which does not guarantee the positive definiteness of the matrix of second partial derivatives of the Gibbs energy. Therefore, the combination of ACSS and MVNR as in the stability analysis is used for the phase split calculation in the simulator. A tighter tolerance for switching is applied to ensure that MVNR converges to the exactly same solution which ACSS is solving for.

The calculation procedure of the combined ACSS-MNVR method is as follows:

1. Compute the *K*-values of the newly introduced phase from stability test results:

$$K_{mn_p} = \frac{x_{mn_p}}{x_{mr}}, \quad m = 1, \cdots, n_c$$
 4-50

2. Solve for the phase mole fraction L_{α} ($\alpha \neq r$) from Eq. 4-39 and calculate the reference phase mole fraction L_r from Eq. 3-26.

- 3. Calculate the phase compositions using Eq. 4-38.
- Calculate the component fugacities for each phase using Eq. 4-12 or Eq. 4-18 according to the EOS selected.
- 5. Calculate the acceleration parameter from Eq. 4-43.
- 6. Update the *K*-values using Eq. 4-45.
- Calculate the residuals from Eq. 4-47 and check whether the convergence criterion is satisfied

$$\|\vec{r}\| \le \epsilon_{conv} \tag{4-51}$$

If the convergence criterion is satisfied, stop. Otherwise, continue to Step 8.

8. Check the switching to the MVNR iteration criterion

$$\|\vec{r}\| \le \epsilon_{switch} \tag{4-52}$$

4 = 0

If the switching criterion is not satisfied, go to Step 2 to continue the ACSS iteration.

Otherwise, go to Step 9 to start the MVNR iteration.

- 9. Evaluate the Jacobian matrix for the MVNR iteration from Eq. 4-49.
- 10. Update \vec{X} using Eq. 4-48.
- 11. Calculate the residuals using Eq. 4-47 and check for convergence by satisfying Eq. 4-51.If it converges, stop. Otherwise, go to Step 9.

4.4 Phase Identification

The solution of the equilibrium equations provides the mole fractions and compositions of each phase and may also tell if a phase is vapor-like or liquid-like from the cubic equation root, but it does not label the phase as oil, gas, the second liquid or water. A consistent phase identification scheme is necessary therefore because the relative permeabilities and capillary pressures are modelled and assigned on the basis of the identity of the present phase and a phase swapping could cause divergence for the problem.

The phase identification for a traditional three-phase compositional simulator can be straightforward. Since the water phase is handled separately, it is only necessary to identify the two hydrocarbon phases according to the phase mass density. The oil phase is always assumed to be denser than the gas phase. In the single phase region, the phase is identified as the oil if the cubic equation root turns liquid-like, or as the gas otherwise. However, the method using the mass density alone is inappropriate for a four-phase model with multiple hydrocarbon liquid phases at equilibrium because an inversion of mass densities of the oil and second liquid phases can happen at higher pressure. Perschke et al. (1989) showed an example of mass density inversion using Maljamar separator oil (Orr et al., 1981) and found that the heavy hydrocarbon composition is always greatest in the oil phase. According to their result, the phase identification method implemented in the simulator is based on the following steps. Since the water phase mainly consists of the water component, a phase is labelled as water if the composition of the water component in the phase is greater than 85%. For mixtures that have three non-aqueous phases present, the phase with the highest composition of the heaviest hydrocarbon component is labelled as the oil phase. The mass densities help to differentiate the two remaining phases. The lighter phase is labelled as the gas phase and the denser phase is labelled as the second liquid. In the presence of two non-aqueous phases, the phase with a vapor-like cubic root is labelled as the gas phase and the liquid-like phase is labeled as either oil or the second liquid according to the composition of a key component. The key component is usually the major component which forms the second liquid phase and a threshold value of composition is required here. If the composition of the key component in the liquid-like phase is less than the threshold composition,

the phase is labelled as oil. Otherwise, it is labelled as the second liquid phase. In the case where both phases have a liquid-like cubic root, the phase with the higher composition of the heaviest hydrocarbon component is again labelled as oil and the remaining phase is labelled as the second liquid phase. The same logic applies to non-aqueous single-phase mixtures. The cubic root is used to distinguish between gas and liquid, and the key component composition helps identifying if the liquid-like phase is oil or the second-liquid.

4.5 Phase Properties Calculation

The physical properties of each phase in the governing equations (Eqs. 3-34 and 3-35) are evaluated based on the phase compressibility factors, phase mole fractions and compositions obtained from multiphase equilibrium calculation results.

4.5.1 Volume Shift

The volume shift method of Peneloux *et al.* (1982) is implemented to improve the density predictions. The calculated molar volume from the EOS is corrected by

$$v^{corr} = v - \sum_{m=1}^{n_c} x_m c_m$$

$$4-53$$

where c_m is the molar volume translation constant of component m. The translations along the volume axis do not change calculation results of phase equilibrium and the translation value for common hydrocarbons can be found in Peneloux *et al.* (1982) or obtained by fitting experimental density measurement through regressions.

4.5.2 Mass Density and Molar Density

The mass density $\tilde{\rho}_{\alpha}$ of phase α is related to its molar density ρ_{α} and average molecular weight mw_{α} by

$$\tilde{\rho}_{\alpha} = \rho_{\alpha} \cdot m w_{\alpha} \tag{4-54}$$

where mw_{α} is evaluated using the linear mixing rule

$$mw_{\alpha} = \sum_{m=1}^{n_c} x_{m\alpha} \cdot mw_m$$
 4-55

and ρ_{α} is the inverse of the molar volume v_{α} calculated from the EOS

$$\rho_{\alpha} = \frac{1}{v_{\alpha}} = \frac{p}{Z_{\alpha}RT}$$
 4-56

Note that if the volume shift method is applied, the corrected molar volume of phase α is used in Eq. 4-56.

4.5.3 Viscosity

The viscosity for a hydrocarbon phase is calculated from the Lohrenz-Bray-Clark (LBC) correlation (1964) which expresses the oil and gas viscosities as a fourth-degree polynomial in the reduced density $\rho_{r\alpha} = \rho_{\alpha} / p \rho_{c\alpha}$

$$[(\mu_{\alpha} - \mu_{\alpha}^{*})\xi_{\alpha} + 10^{-4}]^{1/4} = a_{1} + a_{2}\rho_{r\alpha} + a_{3}\rho_{r\alpha}^{2} + a_{4}\rho_{r\alpha}^{3} + a_{5}\rho_{r\alpha}^{4}$$
4-57

where the pseudo critical density $p \rho_{c\alpha}$ is calculated from the pseudo critical molar volume

$${}_{p}\rho_{c\alpha} = \frac{1}{{}_{p}v_{c\alpha}} = \frac{1}{\sum_{m=1}^{n_{c}} x_{m\alpha} \cdot v_{cm}}$$

$$4-58$$

 ξ_{α} is the phase viscosity-reducing parameter given by

$$\xi_{\alpha} = \frac{pT_{c\alpha}^{1/6}}{mw_{\alpha}^{1/2} \cdot pp_{c\alpha}^{2/3}}$$
 4-59

where $_{p}T_{c\alpha}$ is the pseudo critical temperature

$${}_{p}T_{c\alpha} = \sum_{m=1}^{n_{c}} x_{m\alpha} \cdot T_{cm}$$

$$4-60$$

and $_{p}P_{c\alpha}$ is the pseudo critical pressure

$${}_{p}p_{c\alpha} = \sum_{m=1}^{n_{c}} x_{m\alpha} \cdot p_{cm}.$$
4-61

 μ_{α}^{*} is the dilute gas viscosity of the phase at atmosphere pressure which can be determined from the equation developed by Herning and Zippener (1936)

$$\mu_{\alpha}^{*} = \frac{\sum_{m=1}^{n_{c}} x_{m\alpha} \mu_{m} m w_{i}^{1/2}}{\sum_{m=1}^{n_{c}} x_{m\alpha} m w_{i}^{1/2}}$$
4-62

in which the viscosity parameter of component m is calculated using the Stiel and Thodos correlation

$$\mu_m = 34 \times 10^{-5} \frac{T_{rm}^{0.94}}{\xi_m} \quad \text{for} \quad T_{rm} \le 1.5$$
 4-63

and

$$\mu_m = 17.78 \times 10^{-5} \frac{(4.58T_{rm} - 1.67)^{0.625}}{\xi_m} \quad \text{for} \quad T_{rm} > 1.5 \qquad 4-64$$

where ξ_m , the viscosity-reducing parameter of component *m*, is obtained by

$$\xi_m = \frac{T_{cm}^{1/6}}{m w_m^{1/2} \cdot P_{cm}^{2/3}}$$
 4-65

and $T_{rm} = T_m/T_{cm}$ is the reduced temperature of component *m*. The constants a_1 to a_5 in Eq. 4-57 are specified as follows:

$$a_1 = 0.1023, a_2 = 0.023364, a_3 = 0.058533, a_4 = -0.040758, a_5 = 0.0093324$$

For the aqueous phase, a modified Kestin-Khalifa-Correia correlation (1981) is applied for the viscosity calculation (Whitson and Brul é 2000):

$$\mu_{w} = (1 + A_{0}p)\mu_{w}^{*}$$

$$\log \frac{\mu_{w}^{*}}{\mu_{w}^{0}} = A_{1} + A_{2}\log \frac{\mu_{w}^{0}}{\mu_{w20}^{0}}$$

$$A_{0} = 10^{-3}[0.8 + 0.01(t - 90)\exp(-0.25c_{sw})]$$
4-66

$$A_{1} = \sum_{i=1}^{3} a_{1i} c_{sw}^{i}$$
$$A_{2} = \sum_{i=1}^{3} a_{2i} c_{sw}^{i}$$
$$\log \frac{\mu_{w}^{0}}{\mu_{w20}^{0}} = \sum_{i=1}^{3} a_{3i} \frac{(20-T)^{i}}{96+T}$$

where $\mu_{w20}^0 = 1.002$ cp is the aqueous phase viscosity at 20°C, c_{sw} is the salt concentration in the aqueous phase, and the empirical constants are

$$\begin{aligned} a_{11} &= 3.324 \times 10^{-2}, a_{12} = 3.624 \times 10^{-3}, a_{13} = -1.879 \times 10^{-4}, \\ a_{21} &= -3.96 \times 10^{-2}, a_{22} = 1.02 \times 10^{-2}, a_{23} = -7.02 \times 10^{-4}, \\ a_{31} &= 1.2378, a_{32} = -1.303 \times 10^{-3}, a_{33} = 3.06 \times 10^{-6}, a_{33} = 2.55 \times 10^{-8} \end{aligned}$$

with μ in cp, T in °C, and p in MPa.

4.5.4 Relative Permeability

Four relative permeability models: Stone's model II (1973), Baker's model (1988), Corey's model (1986) and modified Corey's model (Dria, 1989; Dria *et al.*, 1990) are implemented in the simulator. In all the models, the aqueous phase is always assumed to be the wetting phase. Alternatively, the relative permeability can also be defined by an analytical function of the phase saturation and interfacial tension.

For Stone's model II and Baker's model, two-phase relative permeability values k_{rw} and k_{row} are looked up as functions of s_w from a water-oil permeability table, and k_{rg} and k_{rog} are looked up as functions of s_g from a gas-liquid relative permeability table. In Stone's model II, the oil relative permeability is computed as

$$k_{ro} = k_{row}(s_{wc}) \left[\left(\frac{k_{row}}{k_{row}(s_{wc})} + k_{rw} \right) \left(\frac{k_{rog}}{k_{row}(s_{wc})} + k_{rg} \right) - k_{rw} - k_{rg} \right]$$
 4-67

where $k_{row}(s_{wc})$ is the oil relative permeability at the connate water saturation in the water-oil table. For Baker's model, the oil relative permeability is given by saturation-weighted interpolation between the two-phase relative permeabilities

$$k_{ro} = \frac{(s_w - s_{wr})k_{row} + (s_g - s_{gr})k_{rog}}{(s_w - s_{wr}) + (s_g - s_{gr})}$$
4-68

In our four-phase model, the second liquid phase can either share the oil phase relative permeability with the oil phase or share the gas phase relative permeability with the gas phase in proportion to their relative volumes:

$$k_{ro} = \frac{s_o}{s_o + s_l} k_{ro}$$
 and $k_{rl} = \frac{s_l}{s_o + s_l} k_{ro}$ 4-69

or

$$k_{rg} = \frac{s_g}{s_g + s_l} k_{rg}$$
 and $k_{rl} = \frac{s_l}{s_g + s_l} k_{rg}$ 4-70

A similar approach can be found in Gardner *et al.* (1981) and Nghiem and Li (1986) but only the gas relative permeability is shared by the gas and second liquid phases.

For Corey's model, the relative permeability of each phase depends only on the saturation of that phase. It can be calculated as follows:

$$k_{r\alpha} = k_{r\alpha}^{o} \left(\frac{s_{\alpha} - s_{\alpha r}}{1 - \sum_{\beta = o, g, l, w} s_{\beta r}} \right)^{e_{\alpha}}$$

$$4-71$$

$$\alpha = o, g, l, w$$

where $s_{\alpha r}$ is the residual saturation of phase α , $k_{r\alpha}^{o}$ is the endpoint relative permeability evaluated at $s_{\alpha} = 1 - \sum_{\beta \neq \alpha} s_{\beta}$ and e_{α} is the exponent of a relative permeability function.

For modified Corey's model, the phase relative permeabilities are calculated by

$$k_{rw} = k_{rw}^{o} (s_{we})^{e_w} 4-72$$

$$k_{ro} = k_{ro}^{o} (s_{oe})^{2} [1 - (1 - s_{oe})^{e_{o}}]$$
4-73

$$k_{rl} = k_{rl}^{o} (s_{le})^2 [1 - (1 - s_{le})^{e_l}]$$
4-74

$$k_{rg} = k_{rg}^{o} (s_{ge})^{2} [1 - (1 - s_{ge})^{e_{g}}]$$
4-75

where $s_{\alpha e}$, the effective saturations, are given by

$$s_{we} = \frac{s_w - s_{wr}}{1 - s_{wr} - s_{or}}$$
 4-76

$$s_{oe} = \frac{s_o - s_{or}}{1 - s_{wr} - s_{or}}$$
 4-77

$$s_{le} = \frac{s_l - s_{lr}}{1 - s_{wr} - s_{or} - s_{lr}}$$
 4-78

$$s_{ge} = \frac{s_g - s_{gr}}{1 - s_{wr} - s_{or} - s_{gr}}$$
 4-79

with the residual saturation $s_{\alpha r}$ of phase α .

4.5.5 Capillary Pressure

The oil-water and oil-gas capillary pressures can be looked up through input tables as a function of water saturation and gas saturation, respectively, and the capillary pressure between the oil and liquid phases is neglected. For water-second liquid-gas flow, the value of the oil-gas capillary pressure is assigned to the second liquid-gas pressure.

4.6 Treatment of Initial Water Saturation

Conventionally, the amount of water initially existing in a reservoir is often specified by the initial water saturation s_{wi} and the amounts of other components are specified by overall composition since the water is handled as a separate phase which is not involved in phase equilibrium calculation. The new four-phase model is fully component-based and uses the overall composition of all the components in both component flow and phase equilibrium

calculation. To make the conventional specification of the initial reservoir fluid properties compatible with our model, it is necessary to perform a conversion and normalize the overall composition.

Using the critical properties of the water component, the molar density of pure water at the reservoir condition can be obtained from an EOS and Eq. 4-56. The total moles of water per bulk volume are calculated as follows:

$$n_w = \phi s_{wi} \rho_w \tag{4-80}$$

Then a phase equilibrium calculation is performed at the initial reservoir conditions and the overall composition of non-water components to determine the number of phases as well as the mole fractions, compositions and physical properties of each non-aqueous phase. Since the pore volume is initially fully occupied by reservoir fluids, the saturation of non-aqueous phase can be found by applying Eqs. 3-12 and 3-18

$$s_{\alpha} = \frac{L_{\alpha}/\rho_{\alpha}}{\sum_{\beta=o,g,l} L_{\beta}/\rho_{\beta}} (1 - s_{wi}) \qquad \alpha = o, g, l \qquad 4-81$$

The total moles of each non-water component per unit bulk volume are found using Eq. 3-13. Last, water is added to the component list and its overall composition is given by

$$z_{n_{hc}+1} = \frac{n_{w}}{\sum_{m=1}^{n_{hc}} n_{m} + n_{w}}$$
 4-82

where n_{hc} is the total number of non-water components whose overall composition is normalized using

$$z_m = \frac{n_m}{\sum_{m=1}^{n_{hc}} n_m + n_w} \qquad m = 1, \dots n_{hc}$$
 4-83



Figure 4-1 Computational flowchart for the multiphase equilibrium calculation

Chapter Five: Numerical Solution of Compositional Flow Equations

The compositional flow in porous media is represented by a coupled nonlinear system of component flow, volume consistency and phase equilibrium equations. To solve the system numerically, a finite difference method is applied to divide the domain into a series of gridblocks and discretize the governing partial differential equations to an algebraic form. The Newton-Raphson method that linearly approximates the system by truncated Taylor series expansions is then used to obtain a numerical solution iteratively. In this chapter, detailed numerical approaches and solution schemes are presented.

5.1 Finite Difference Formulation

In general, a reservoir simulation problem involves a system of nonlinear partial differential equations that are not analytically solvable. Therefore, a numerical solution is to be sought instead. Often, the partial differential equations describing multiphase compositional flow in porous media can be solved numerically using a finite difference method.

5.1.1 Grid System

In order to apply the finite difference method to solve a reservoir simulation problem, it is necessary to divide the problem's domain into a finite set of gridblocks first. As illustrated in Fig. 5-1, a block-centered grid system (Chen, 2007) is selected as the base of the finite difference formulation and a seven-point stencil (Fig. 5-2) is used to represent a three-dimensional grid, where the integers *i*, *j*, and *k* denote the indices in the *x*-, *y*-, and *z*-directions in a Cartesian coordinate system, respectively, and operation $\pm \frac{1}{2}$ indicates a gridblock boundary in the corresponding direction.

The entire grid system is numbered in natural ordering, where i, j, and k increase in a nested manner: i is the innermost index, j is the intermediate index and k is the outermost index (Chen,

2007). Each gridblock is assigned a unique index number which determines the location of its equations and variables in the entire discretized nonlinear system. In general, for a $n_x \times n_y \times n_z$ grid where n_x , n_y and n_z are the numbers of gridblocks in the x-, y-, and z-directions, respectively, the index of a gridblock and its location (i, j, k) are related by a bijective function:

$$N = (kn_y + j)n_x + i 5-1$$

Fig. 5-3 shows the grid numbering for a $5 \times 4 \times 3$ grid as an example.

5.1.2 Finite Difference Equations

Based on the grid system introduced above, with temporal spacing Δt and mesh size Δx , Δy and Δz in the *x*-, *y*-, and *z*-directions respectively, an approximation of the derivative with respect to time is given by

$$\frac{dn_m}{dt} \cong \frac{(n_m)^{n+1} - (n_m)^n}{\Delta t}$$

where superscript n + 1 and n indicate the current and previous time levels, respectively, and the spatial derivatives can be approximated by

$$\nabla \left(T_{m\alpha} \nabla (\Phi_{\alpha}) \right) \cong \frac{1}{\Delta x^{2}} \left(T_{m\alpha,i,j,k}^{1} + \frac{1}{2},j,k} \left(\Phi_{\alpha,i,j,k} - \Phi_{\alpha,i,j,k} \right) - T_{m\alpha,i,j-\frac{1}{2},j,k}^{1} \left(\Phi_{\alpha,i,j,k} - \Phi_{\alpha,i,j,k} \right) \right) + \frac{1}{\Delta y^{2}} \left(T_{m\alpha,i,j+\frac{1}{2},k}^{1} \left(\Phi_{\alpha,i,j+1,k} - \Phi_{\alpha,i,j,k} \right) - T_{m\alpha,i,j-\frac{1}{2},k}^{1} \left(\Phi_{\alpha,i,j,k} - \Phi_{\alpha,i,j-1,k} \right) \right) + \frac{1}{\Delta z^{2}} \left(T_{m\alpha,i,j,k+\frac{1}{2}}^{1} \left(\Phi_{\alpha,i,j,k+1} - \Phi_{\alpha,i,j,k} \right) - T_{m\alpha,i,j,k-\frac{1}{2}}^{1} \left(\Phi_{\alpha,i,j,k} - \Phi_{\alpha,i,j,k-1} \right) \right)$$

Substituting the difference approximation into the component flow equations (Eq. 3-34) and multiplying the equations by the block volume $V_b = \Delta x \Delta y \Delta z$ converts the partial differential equations into finite difference equations at the n + 1 time level for each gridblock. In the IMPES solution scheme, the transmissibilities, sink/source terms, capillary pressures and gravity in the phase potentials are evaluated explicitly at the saturation and composition values of the previous timestep converged results. Therefore, superscript n that represents the previous time level is used for all explicit properties and the IMPES finite difference equations for the four-phase compositional model can be expressed as:

$$F_{m} = \frac{1}{\Delta t} (V_{b}[(n_{m})^{n+1} - (n_{m})^{n}])_{i,j,k} - \sum_{\alpha = o,g,l,w} T_{m\alpha, i+\frac{1}{2},j,k}^{n} \left(\Phi_{i+1,j,k}^{n+1} - \Phi_{i,j,k}^{n+1} \right) \\ + \sum_{\alpha = o,g,l,w} T_{m\alpha, i-\frac{1}{2},j,k}^{n} \left(\Phi_{i,j,k}^{n+1} - \Phi_{i-1,j,k}^{n+1} \right) - \sum_{\alpha = o,g,l,w} T_{m\alpha, i,j+\frac{1}{2},k}^{n} \left(\Phi_{i,j+1,k}^{n+1} - \Phi_{i,j,k}^{n+1} \right) \\ + \sum_{\alpha = o,g,l,w} T_{m\alpha, i,j-\frac{1}{2},k}^{n} \left(\Phi_{i,j,k}^{n+1} - \Phi_{i,j-1,k}^{n+1} \right) - \sum_{\alpha = o,g,l,w} T_{m\alpha, i,j,k+\frac{1}{2}}^{n} \left(\Phi_{i,j,k+1}^{n+1} - \Phi_{i,j,k}^{n+1} \right) \\ + \sum_{\alpha = o,g,l,w} T_{m\alpha, i,j,k-\frac{1}{2}}^{n} \left(\Phi_{i,j,k}^{n+1} - \Phi_{i,j,k-1}^{n+1} \right) - q_{m}^{n} = 0$$

 $m = 1 \dots n_c$ 5-2

$$F_{n_c+1} = \left(\sum_{\alpha=o,g,l,w} \frac{n_{\alpha}}{\rho_{\alpha}} - \phi\right)_{i,j,k}^{n+1} = 0$$
5-3

where

$$q_m = \bar{q}_m \Delta x \Delta y \Delta z \qquad 5-4$$

is the molar flow rate of component m injected or produced by wells. Also, the ratios of a perpendicular cross-sectional area A over the gridblock size are combined into the numerical transmissibility terms at the gridblock boundaries, namely,

$$T_{m\alpha, \ i\pm\frac{1}{2},j,k} = \left(\frac{\mathcal{A}_{x}}{\Delta x} \frac{K_{x}k_{r\alpha}}{\mu_{\alpha}} \rho_{\alpha} x_{m\alpha}\right)_{i\pm\frac{1}{2},j,k}$$

$$T_{m\alpha, \ i,j\pm\frac{1}{2},k} = \left(\frac{\mathcal{A}_{y}}{\Delta y} \frac{K_{y}k_{r\alpha}}{\mu_{\alpha}} \rho_{\alpha} x_{m\alpha}\right)_{i,j\pm\frac{1}{2},k}$$
5-5

$$T_{m\alpha, i, j, k \pm \frac{1}{2}} = \left(\frac{\mathcal{A}_z}{\Delta z} \frac{K_z k_{r\alpha}}{\mu_{\alpha}} \rho_{\alpha} x_{m\alpha}\right)_{i, j, k \pm \frac{1}{2}}$$

5.1.3 Treatment of Block Transmissibility

In Eqs. 5-2, the transmissibility terms at the interface between two adjacent gridblocks need to be carefully evaluated. According to Chen (2006), a harmonic average is used for the calculation of rock and grid properties in the transmissibilities,

$$\begin{pmatrix} \frac{\mathcal{A}_{x}}{\Delta x} K_{x} \end{pmatrix}_{i \pm \frac{1}{2} j, k} = \frac{2(A_{x}K_{x})_{i, j, k} (A_{x}K_{x})_{i \pm 1, j, k}}{(A_{x}K_{x})_{i, j, k} \Delta x_{i \pm 1, j, k} + (A_{x}K_{x})_{i \pm 1, j, k} \Delta x_{i, j, k}}$$

$$\begin{pmatrix} \frac{\mathcal{A}_{y}}{\Delta y} K_{y} \end{pmatrix}_{i, j \pm \frac{1}{2} k} = \frac{2(A_{y}K_{y})_{i, j, k} (A_{y}K_{y})_{i, j \pm 1, k}}{(A_{y}K_{y})_{i, j, k} \Delta y_{i, j \pm 1, k} + (A_{y}K_{y})_{i, j \pm 1, k} \Delta y_{i, j, k}}$$

$$\begin{pmatrix} \frac{\mathcal{A}_{z}}{\Delta z} K_{z} \end{pmatrix}_{i, j, k \pm \frac{1}{2}} = \frac{2(A_{z}K_{z})_{i, j, k} (A_{z}K_{z})_{i, j, k \pm 1}}{(A_{z}K_{z})_{i, j, k \pm 1} + (A_{z}K_{z})_{i, j, k \pm 1} \Delta z_{i, j, k}}$$
5.6

and fluid properties are obtained by one-point upstream weighting:

$$\left(\frac{k_{r\alpha}}{\mu_{\alpha}}\rho_{\alpha}x_{m\alpha}\right)_{i\pm\frac{1}{2},j,k} = \begin{cases} \left(\frac{k_{r\alpha}}{\mu_{\alpha}}\rho_{\alpha}x_{m\alpha}\right)_{i\pm1,j,k} & \text{if } \Phi_{\alpha,i+1,j,k} \ge \Phi_{\alpha,i,j,k} \\ \left(\frac{k_{r\alpha}}{\mu_{\alpha}}\rho_{\alpha}x_{m\alpha}\right)_{i,j,k} & \text{if } \Phi_{\alpha,i+1,j,k} < \Phi_{\alpha,i,j,k} \end{cases} \\ \left(\frac{k_{r\alpha}}{\mu_{\alpha}}\rho_{\alpha}x_{m\alpha}\right)_{i,j\pm1,k} & \text{if } \Phi_{\alpha,i,j+1,k} \ge \Phi_{\alpha,i,j,k} \\ \left(\frac{k_{r\alpha}}{\mu_{\alpha}}\rho_{\alpha}x_{m\alpha}\right)_{i,j,k} & \text{if } \Phi_{\alpha,i,j+1,k} < \Phi_{\alpha,i,j,k} \end{cases}$$
5-7

$$\left(\frac{k_{r\alpha}}{\mu_{\alpha}}\rho_{\alpha}x_{m\alpha}\right)_{i,j,k\pm\frac{1}{2}} = \begin{cases} \left(\frac{k_{r\alpha}}{\mu_{\alpha}}\rho_{\alpha}x_{m\alpha}\right)_{i,j,k\pm1} & \text{if } \Phi_{\alpha,i,j,k\pm1} \ge \Phi_{\alpha,i,j,k}\\ \left(\frac{k_{r\alpha}}{\mu_{\alpha}}\rho_{\alpha}x_{m\alpha}\right)_{i,j,k} & \text{if } \Phi_{\alpha,i,j,k\pm1} < \Phi_{\alpha,i,j,k} \end{cases}$$

5.2 Initial and Boundary Conditions

The initial conditions including pressure, temperature and overall composition are input data. Phase equilibrium calculation is performed for each gridblock during the initialization stage of a simulation to obtain fluid physical properties and determine the total moles per unit bulk volume for each component using Eq. 3-13. If vertical grid information has been input, the reservoir is assumed gravitationally stabilized. In this case, the fluid properties of the gridblocks at a reference depth are first calculated, and then other gridblocks are initialized inductively. For example, if the properties of the *k*-th gridblock in the *z*-direction is known, the pressure in the (k + 1)-th gridblock is approximated by

$$p_{i,j,k+1} = p_{i,j,k} - \gamma_{F,i,j,k} \Delta z_{i,j,k+\frac{1}{2}}$$

where γ_F is the total specific weight

$$\gamma_F = \sum_{\alpha = o, g, l, w} s_{\alpha} \gamma_{\alpha}$$

and $\Delta z_{i,j,k+\frac{1}{2}}$ is the average depth change given by

$$\Delta z_{i,j,k+\frac{1}{2}} = \frac{1}{2} \left(\Delta z_{i,j,k} + \Delta z_{i,j,k+1} \right)$$

The fluid physical properties of the (k + 1)-th gridblock are then determined from flash calculation (analogously for the (k - 1)-th gridblock).

The reservoir is assumed to be surrounded by impermeable rocks in the model and, therefore, non-flow boundary conditions are specified:

$$\nabla \cdot \vec{u} = 0$$

at the boundaries, numerically implemented by setting transmissibilities to zeroes for the boundary gridblocks:
$$T_{\alpha, i-\frac{1}{2},j,k} = 0 \quad \text{if } i = 1$$

$$T_{\alpha, i+\frac{1}{2},j,k} = 0 \quad \text{if } i = n_x$$

$$T_{\alpha, i,j-\frac{1}{2},k} = 0 \quad \text{if } j = 1$$

$$T_{\alpha, i,j+\frac{1}{2},k} = 0 \quad \text{if } j = n_y$$

$$T_{\alpha, i,j,k-\frac{1}{2}} = 0 \quad \text{if } k = 1$$

$$T_{\alpha, i,j,k+\frac{1}{2}} = 0 \quad \text{if } k = n_z$$

where n_x , n_y and n_z denote the numbers of gridblocks in the x-, y-, and z-directions, respectively (Chang, 1990).

5.3 Well Model

The molar flow rate of injection/production of component m, q_m , in the component flow equation is contributed by wells. In numerical reservoir simulations, a well flow equation which relates the reservoir volumetric flow rate Q_{α} of phase α , bottomhole pressure and gridblock pressure is derived by assuming a steady-state flow regime in a neighborhood of the well:

$$Q_{\alpha} = WI \frac{k_{r\alpha}}{\mu_{\alpha}} (p_{wf} - p_o)$$
 5-9

where WI is the well index and the sum of Eq. 5-9 over all phases results in the total volumetric rate

$$Q_t = \sum_{\alpha = o, g, l, w} WI \frac{k_{r\alpha}}{\mu_{\alpha}} (p_{wf} - p_o)$$
 5-10

The rates are positive for injection wells and negative for production wells.

The calculation of the well index depends on the grid properties, absolute permeabilities and well direction. For a one-dimensional slim tube (x-direction), applying Darcy's law for linear flow gives

$$WI = \frac{K_x \Delta y \Delta z}{\Delta x/2}$$
 5-11

In general, the well index of a well located in the center of a gridblock is obtained from the analytical solution of a steady-state radial flow and the direction it is parallel to

• *x*-direction

$$WI = \frac{2\pi\Delta x \sqrt{K_y K_z}}{\ln(r_e/r_w) + s}$$
5-12

• *y*-direction

$$WI = \frac{2\pi\Delta y \sqrt{K_x K_z}}{\ln(r_e/r_w) + s}$$
5-13

• *z*-direction

$$WI = \frac{2\pi\Delta z \sqrt{K_x K_y}}{\ln(r_e/r_w) + s}$$
5-14

where s is a skin factor, r_w is the wellbore radius and r_e is the equivalent radius given by Peaceman's equation (1983) for a non-square grid and an anisotropic porous medium:

• *x*-direction

$$r_{e} = \frac{0.14 \left(\left(K_{y} / K_{z} \right)^{\frac{1}{2}} (\Delta z)^{2} + \left(\left(K_{z} / K_{y} \right)^{\frac{1}{2}} (\Delta y)^{2} \right) \right)^{\frac{1}{2}}}{0.5 \left(\left(K_{y} / K_{z} \right)^{\frac{1}{4}} + \left(K_{z} / K_{y} \right)^{\frac{1}{4}} \right)}$$
5-15

• *y*-direction

$$r_{e} = \frac{0.14 \left(\left(K_{y} / K_{z} \right)^{\frac{1}{2}} (\Delta z)^{2} + \left((K_{z} / K_{x})^{\frac{1}{2}} (\Delta x)^{2} \right) \right)^{\frac{1}{2}}}{0.5 \left((K_{x} / K_{z})^{\frac{1}{4}} + (K_{z} / K_{x})^{\frac{1}{4}} \right)}$$
5-16

• *z*-direction

$$r_e = \frac{0.14 \left(\left(K_y / K_x \right)^{\frac{1}{2}} (\Delta x)^2 + \left(\left(K_x / K_y \right)^{\frac{1}{2}} (\Delta y)^2 \right) \right)^{\frac{1}{2}}}{0.5 \left(\left(K_y / K_x \right)^{\frac{1}{4}} + \left(K_x / K_y \right)^{\frac{1}{4}} \right)}$$
5-17

For a multilayer well which penetrates more than one gridblock, the total flow rate is distributed into each layer by using a mobility allocation method which assumes that the potential difference between the wellbore and a gridblock is the same for all blocks penetrated (Nolen and Berry, 1972; Chang, 1990).

5.3.1 Constant Molar Rate Wells

The total molar rate q_t and injection fluid composition \vec{z}_{inj} are specified for constant molar rate injection wells. According to the mobility allocation method, the injection rate of component m and the total injection rate for layer *iwl* are calculated using

$$q_{m,iwl} = \frac{\left(\sum_{\alpha=o,g,w,l} WI \frac{k_{r\alpha}}{\mu_{\alpha}}\right)_{iwl}}{\sum_{jwl=1}^{nwl} \left(\sum_{\alpha=o,g,w,l} WI \frac{k_{r\alpha}}{\mu_{\alpha}}\right)_{jwl}} q_t z_{m,inj}$$
5-18

and

$$q_{t,iwl} = \frac{\left(\sum_{\alpha=o,g,w,l} WI \frac{k_{r\alpha}}{\mu_{\alpha}}\right)_{iwl}}{\sum_{jwl=1}^{nwl} \left(\sum_{\alpha=o,g,w,l} WI \frac{k_{r\alpha}}{\mu_{\alpha}}\right)_{jwl}} q_t$$
5-19

where *nwl* is the total number of layers. To determine the bottomhole pressure, a flash calculation is performed at the reservoir conditions of layer *iwl* using \vec{z}_{inj} to determine the total molar density $(\rho_{F,inj})_{iwl} = \sum_{\alpha=o,g,w,l} s_{\alpha}\rho_{\alpha}$ of the injected fluid in the gridblock, and the bottomhole pressure of layer *iwl* is back computed from Eq. 5-10:

$$p_{wf,iwl} = p_{o,iwl} + \frac{q_{t,iwl} / (\rho_{F,inj})_{iwl}}{\left(\sum_{\alpha = o,g,w,l} WI \frac{k_{r\alpha}}{\mu_{\alpha}}\right)_{iwl}}$$
5-20

For constant molar rate production wells, only the total molar rate q_t needs to be specified, and the total production rate and component production rate for layer *iwl* are given by

$$q_{t,iwl} = \frac{\left(\sum_{\alpha=o,g,w,l} WI \frac{k_{r\alpha}}{\mu_{\alpha}} \rho_{\alpha}\right)_{iwl}}{\sum_{jwl=1}^{nwl} \left(\sum_{\alpha=o,g,w,l} WI \frac{k_{r\alpha}}{\mu_{\alpha}} \rho_{\alpha}\right)_{jwl}} q_t$$
5-21

and

$$q_{m,iwl} = \frac{\left(\sum_{\alpha=o,g,w,l} WI \frac{k_{r\alpha}}{\mu_{\alpha}} \rho_{\alpha} x_{m\alpha}\right)_{iwl}}{\left(\sum_{\alpha=o,g,w,l} WI \frac{k_{r\alpha}}{\mu_{\alpha}} \rho_{\alpha}\right)_{iwl}} q_t$$
5-22

The total volumetric flow rate and total production rate are related by

$$Q_{t,iwl} = \frac{\left(\sum_{\alpha=o,g,w,l} WI \frac{k_{r\alpha}}{\mu_{\alpha}}\right)_{iwl}}{\left(\sum_{\alpha=o,g,w,l} WI \frac{k_{r\alpha}}{\mu_{\alpha}}\rho_{\alpha}\right)_{iwl}} q_{t,iwl}$$
5-23

and the bottom hole pressure of layer *iwl* is found using

$$p_{wf,iwl} = p_{o,iwl} + \frac{Q_{t,iwl}}{\left(\sum_{\alpha=o,g,w,l} WI \frac{k_{r\alpha}}{\mu_{\alpha}}\right)_{iwl}}$$
5-24

5.3.2 Constant Surface Flow Rate Wells

The treatment of a constant surface flow rate well is similar to a constant molar rate well. For a constant surface flow rate injection well, the volumetric surface injection rate $q_{\beta,inj}$ is specified either for gas or water. A three-phase (oil-gas-water) flash calculation at surface conditions is performed for the injection stream \vec{z}_{inj} to obtain the mole fraction L_{β} and molar density ρ_{β} of the specified phase. Then the volumetric flow rate is converted to the total molar flow rate

$$q_t = \frac{q_\beta \rho_\beta}{L_\beta} \qquad \beta = g, w \qquad 5-25$$

and the molar injection rate and bottomhole pressure for each layer can be found using Eqs. 5-18 through 5-20.

The computation of a constant flow rate production well requires determining the production fluid composition first:

$$z_{m,prod} = \frac{\sum_{jwl=1}^{nwl} \left(\sum_{\alpha=o,g,w,l} WI \frac{k_{r\alpha}}{\mu_{\alpha}} \rho_{\alpha} x_{m\alpha} \right)_{jwl}}{\sum_{jwl=1}^{nwl} \left(\sum_{\alpha=o,g,w,l} WI \frac{k_{r\alpha}}{\mu_{\alpha}} \rho_{\alpha} \right)_{jwl}}$$
5-26

Similarly, the flash calculation is carried out at the specified separator conditions using \vec{z}_{prod} to get the mole fraction and molar density of the specified phase β (oil, gas or water). The total molar production rate is then calculated using Eq. 5-25 and the allocation of the molar production rate and bottomhole pressure for each layer are determined by applying Eqs. 5-22 through 5-24.

5.3.3 Constant Bottomhole Pressure Wells

For constant bottomhole pressure injection wells, the bottomhole pressure of a reference layer and the injection fluid composition \vec{z}_{inj} are specified. The bottomhole pressures for the layers below the reference layer are computed by

$$p_{wf,iwl} = p_{wf,iwl+1} + \gamma_{inj,iwl+\frac{1}{2}}(D_{iwl+1} - D_{iwl})$$
 5-27

and analogously for the layers above the reference layer

$$p_{wf,iwl} = p_{wf,iwl-1} - \gamma_{inj,iwl-\frac{1}{2}}(D_{iwl} - D_{iwl-1})$$
5-28

where *D* is the depth and $\gamma_{inj,iwl\pm\frac{1}{2}}$ is the volume-averaged specific weight of the injection fluid computed by

$$\gamma_{inj,iwl\pm\frac{1}{2}} = \frac{V_{b,l}\gamma_{inj,iwl} + V_{b,iwl\pm1}\gamma_{inj,iwl\pm1}}{V_{b,iwl} + V_{b,iwl\pm1}}$$
5-29

with $\gamma_{inj,iwl}$ and $\gamma_{inj,iwl\pm 1}$ determined by flash calculations at the layer block pressures. The total volumetric flow rate Q_t is determined from Eq. 5-10 and the molar injection rates are calculated using

$$q_{m,iwl} = \left[\sum_{\alpha=o,g,w,l} WI \frac{k_{r\alpha}}{\mu_{\alpha}} (p_{wf} - p_{o,iwl})\right]_{iwl} (\rho_{F,inj})_{iwl} Z_{m,inj}$$
5-30

for $p_{wf} > p_{o,iwl}$.

For the constant bottomhole pressure production wells, the bottomhole pressure of the reference layer is specified. The bottomhole pressures of other layers are computed in a similar way to the constant bottomhole pressure injection well:

$$p_{wf,iwl} = p_{wf,iwl+1} + \gamma_{prod,iwl+\frac{1}{2}}(D_{iwl+1} - D_{iwl})$$
 5-31

for the layers below the reference layer and

$$p_{wf,iwl} = p_{wf,iwl-1} - \gamma_{prod,iwl-\frac{1}{2}}(D_{iwl} - D_{iwl-1})$$
5-32

for the layers above the reference layer. The volume-averaged specific weight of the production fluid is calculated by

$$\gamma_{prod,iwl\pm\frac{1}{2}} = \frac{V_{b,l}\gamma_{prod,iwl} + V_{b,iwl\pm1}\gamma_{prod,iwl\pm1}}{V_{b,iwl} + V_{b,iwl\pm1}}$$
5-33

where $\gamma_{prod,iwl}$ is related to the well block fluid properties and evaluated using

$$\gamma_{prod,iwl} = \left(\frac{\sum_{\alpha=o,g,w,l} WI \frac{k_{r\alpha}}{\mu_{\alpha}} \gamma_{\alpha}}{\sum_{\alpha=o,g,w,l} WI \frac{k_{r\alpha}}{\mu_{\alpha}}}\right)_{iwl}$$
5-34

The molar production rate is found by

$$q_{m,iwl} = \left[\sum_{\alpha=o,g,w,l} WI \frac{k_{r\alpha}}{\mu_{\alpha}} \rho_{\alpha} x_{m\alpha} \left(p_{wf} - p_{o,iwl} \right) \right]_{iwl}$$
 5-35

for $p_{wf} < p_{o,iwl}$.

5.4 Numerical Solution

Eqs. 5-2 and 5-3 form a decoupled system of $n_b(n_c + 1)$ flow equations to be solved iteratively using the Newton-Raphson method for the primary variables $(n_1, ..., n_{n_c}, p_o)_N$ for $N = 1 ... n_b$. After each iteration of the primary variables, the overall component compositions $(z_1, ..., z_{n_c})$ are recalculated according to the updated values of $(n_1, ..., n_{n_c})$ and the phase equilibrium calculation described in Chapter Four are performed for all gridblocks at the updated pressure and overall composition to determine the number of phases, phase mole fractions, phase compositions and phase properties. For the IMPES method, since the volume consistency equation always holds, the variables involved in Eq. 5-3 need to be treated implicitly and updated thereafter. In contrast, the well and transmissibility terms are not recalculated until the current time step is converged

5.4.1 Jacobian Structure and Evaluation

To solve the system by the Newton-Raphson method, it is necessary to calculate the Jacobian of the system in each iteration. The Jacobian matrix J_F of the problem is generated by computing the partial derivatives of Eqs. 5-2 and 5-3 of all the gridblocks with respect to all the primary variables. For a simulation model with n_b gridblocks, J_F is a block matrix which consists of $n_b \times n_b$ submatrices:

$$\bar{J}_{F} = \begin{pmatrix} \bar{J}_{1,1} & \bar{J}_{1,2} & \cdots & \bar{J}_{1,n_{b}} \\ \bar{J}_{2,1} & \bar{J}_{2,2} & \cdots & \bar{J}_{2,n_{b}} \\ \vdots & \vdots & \ddots & \vdots \\ \bar{J}_{n_{b},1} & \bar{J}_{n_{b},2} & \cdots & \bar{J}_{n_{b},n_{b}} \end{pmatrix}$$
5-36

where the block Jacobian $J_{M,N}$ storing the partial derivatives of equations of the *M*-th gridblock with respect to the primary variables of the *N*-th gridblock can be expressed as

$$\bar{J}_{MN} = \begin{pmatrix} \frac{\partial F_1|_M}{\partial n_1|_N} & \frac{\partial F_1|_M}{\partial n_2|_N} & \cdots & \frac{\partial F_1|_M}{\partial n_{N_c}|_N} & \frac{\partial F_1|_M}{\partial p_0|_N} \\ \frac{\partial F_2|_M}{\partial n_1|_N} & \frac{\partial F_2|_M}{\partial n_2|_N} & \cdots & \frac{\partial F_2|_M}{\partial n_{N_c}|_N} & \frac{\partial F_2|_M}{\partial p_0|_N} \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ \frac{\partial F_{N_c}|_M}{\partial n_1|_N} & \frac{\partial F_{N_c}|_M}{\partial n_2|_N} & \cdots & \frac{\partial F_{N_c}|_M}{\partial n_{N_c}|_N} & \frac{\partial F_{N_c}|_M}{\partial p_0|_N} \\ \frac{\partial F_{N_c+1}|_M}{\partial n_1|_N} & \frac{\partial F_{N_c+1}|_M}{\partial n_2|_N} & \cdots & \frac{\partial F_{N_c+1}|_M}{\partial n_{N_c}|_N} & \frac{\partial F_{N_c+1}|_M}{\partial p_0|_N} \end{pmatrix}$$
5-37

Since the finite difference equations derived are written for each gridblock and the adjacent gridblocks are coupled through the flux terms, the off-diagonal blocks are zero matrices for the nonadjacent gridblocks. The Jacobian matrix has a block heptadiagonal sparse structure for three-dimensional flow based on the grid system selected. For one-dimensional and two-dimensional problems, the Jacobian matrices are block tridiagonal and block pentadiagonal, respectively. To obtain the Jacobian, both diagonal and off-diagonal blocks are evaluated using analytical differentiation and the chain rule.

5.4.1.1 Off-diagonal Block

For the off-diagonal block J_{MN} where $M \neq N$ and gridblock M and gridblock N are connected, it is necessary to compute derivatives of the component flow equations only while the derivatives of the volume consistency equation are all zero because the volume consistency holds at every gridblock. In IMPES where the transmissibilities are evaluated explicitly from conditions at the old time level, the only non-zero entries remaining in $J_{M,N}$ are the partial derivatives of the flux terms in the component flow equations with respect to the pressure

$$\bar{J}_{MN} = \begin{pmatrix} 0 & \dots & 0 & \frac{\partial F_1|_M}{\partial p_o|_N} \\ \vdots & \ddots & \vdots & \vdots \\ 0 & \dots & 0 & \frac{\partial F_N_c|_M}{\partial p_o|_N} \\ 0 & \dots & 0 & 0 \end{pmatrix}$$
 5-38

 $\partial F_m|_M / \partial p_o|_N$ can be obtained from

$$\frac{\partial F_m|_M}{\partial p_o|_N} = -\sum_{\alpha=o,g,l,w} (T^n_{m\alpha,MN})$$
 5-39

where $T_{m\alpha,MN}^n$ is the transmissibility of component *m* in phase α evaluated at the interface between gridblock *M* and gridblock *N* at the old time level.

5.4.1.2 Diagonal Block

The diagonal block J_{MM} has a sparse arrowhead-like structure which contains zeroes in all entries except for the diagonal, last row and last columns when the IMPES approach is used because the flow equation for component m only involves n_m and p_o in the gridblock. The structure and Jacobian elements can be illustrates as follows:

$$\bar{J}_{MM} = \begin{pmatrix} \frac{\partial F_1|_M}{\partial n_1|_M} & \cdots & 0 & \frac{\partial F_1|_M}{\partial p_o|_M} \\ \vdots & \ddots & \vdots & \vdots \\ 0 & \cdots & \frac{\partial F_{n_c}|_M}{\partial n_{n_c}|_M} & \frac{\partial F_{n_c}|_M}{\partial p_o|_M} \\ \frac{\partial F_{n_c+1}|_M}{\partial n_1|_M} & \cdots & \frac{\partial F_{n_c+1}|_M}{\partial n_{n_c}|_M} & \frac{\partial F_{n_c+1}|_M}{\partial p_o|_M} \end{pmatrix}$$
5-40

To evaluate the diagonal block Jacobian, the partial derivatives of the component equation of component m with respect to n_m and p_o are calculated using

$$\frac{\partial F_m|_M}{\partial n_m|_M} = \frac{V_b|_M}{\Delta t}, \qquad m = 1 \dots n_c$$
5-41

and

$$\frac{\partial F_m|_M}{\partial p_o|_M} = \sum_{N=1}^{cnt} \sum_{\alpha=o,g,l,w} (T^n_{m\alpha,MN}), \qquad m = 1 \dots n_c$$
 5-42

respectively. In Eq. 5-42, $\sum_{N=1}^{cnt} \sum_{\alpha=o,g,l,w} (T_{m\alpha,MN}^n)$ is the sum of component transmissibilities over all the connections and *cnt* is the number of gridblocks connected to gridblock *M*. For instance, if gridblock *M* is located at (i, j, k),

$$\sum_{N=1}^{n_{cnt}} \sum_{\alpha=o,g,l,w} (T_{m\alpha,MN}^{n}) = \sum_{\alpha=o,g,l,w} \left(T_{m\alpha,i-\frac{1}{2},j,k}^{n} + T_{m\alpha,i+\frac{1}{2},j,k}^{n} + T_{m\alpha,i,j+\frac{1}{2},k}^{n} + T_{m\alpha,i,j+\frac{1}{2},k}^{n} + T_{m\alpha,i,j,k+\frac{1}{2}}^{n} + T_{m\alpha,i,j,k-\frac{1}{2}}^{n} \right)$$
5-43

For the gridblock penetrated by a constant bottomhole pressure well, a term generated by the well needs to be added to $\partial F_m|_M/\partial p_o|_M$

$$\frac{\partial F_m|_M}{\partial p_o|_M} = \sum_{N=1}^{cnt} \sum_{\alpha=o,g,l,w} (T^n_{m\alpha,MN}) - \sum_{\alpha=o,g,w,l} \left(WI \frac{k_{r\alpha}}{\mu_{\alpha}} \rho_{\alpha} x_{m\alpha} \right)^n$$

$$m = 1 \dots n_c$$
5-44

Computation of the last row of the diagonal block Jacobian is the most complicated part. The partial derivative of the volume consistency equation with respect to n_m can be expressed as

$$\frac{\partial F_{n_c+1}\big|_M}{\partial n_m\big|_M} = \left(\sum_{\alpha=o,g,l,w} \left(\frac{1}{\rho_\alpha} \frac{\partial n_\alpha}{\partial n_m} - \frac{1}{\rho_\alpha^2} \frac{\partial \rho_\alpha}{\partial n_m}\right)\right)_M^{(l)}$$
 5-45

where

$$n_{\alpha} = \sum_{m=1}^{n_c} n_{m\alpha}$$
 3-2

l denotes the current iteration level and ρ_{α} is a function of the phase mole number and pressure

$$\rho_{\alpha} = \rho_{\alpha}(n_{1\alpha}, \dots, n_{n_{c}\alpha}, p_{o})$$

Therefore, applying the chain rule

$$\frac{\partial}{\partial n_m} = \sum_{n=1}^{n_c} \left(\frac{\partial}{\partial n_{n\alpha}}\right)_{p,\vec{n}_{n\alpha}} \left(\frac{\partial n_{n\alpha}}{\partial n_m}\right)_{p,\vec{n}_n}$$
 5-46

to Eq. 5-45 results in

$$\frac{\partial F_{n_c+1}}{\partial n_m}\Big|_M = \left(\sum_{\alpha=o,g,l,w} \sum_{n=1}^{n_c} \left(\frac{1}{\rho_\alpha} \left(\frac{\partial n_\alpha}{\partial n_{n\alpha}}\right)_{p,\vec{n}_{n\alpha}} - \frac{1}{\rho_\alpha^2} \left(\frac{\partial \rho_\alpha}{\partial n_{n\alpha}}\right)_{p,\vec{n}_{n\alpha}}\right) \left(\frac{\partial n_{n\alpha}}{\partial n_m}\right)_{p,\vec{n}_n}\right)_M^{(l)}$$
5-47

where $\vec{n}_{n\alpha} = (n_{1\alpha}, ..., n_{n-1,\alpha}, n_{n+1,\alpha}, ..., n_{n_c,\alpha})$, $\vec{n}_n = (n_1, ..., n_{n-1}, n_{n+1}, ..., n_{n_c})$ and all variables in the subscript are held constant when calculating the partial derivatives. Eq. 3-2 indicates that

$$\left(\frac{\partial n_{\alpha}}{\partial n_{n\alpha}}\right)_{p,\vec{n}_{n\alpha}} = 1$$
5-48

and the partial derivative of the phase molar density can be calculated from the EOS selected:

$$\left(\frac{\partial \rho_{\alpha}}{\partial n_{n\alpha}}\right)_{p,\vec{n}_{n\alpha}} = -\frac{\rho_{\alpha}}{Z_{\alpha}} \left(\frac{\partial Z_{\alpha}}{\partial n_{n\alpha}}\right)_{p,\vec{n}_{n\alpha}}$$
5-49

Substituting Eqs. 5-48 and 5-49 into Eq. 5-47 gives

$$\frac{\partial F_{n_c+1}\big|_M}{\partial n_m\big|_M} = \left(\sum_{\alpha=o,g,l,w} \sum_{n=1}^{n_c} \left(\frac{1}{\rho_\alpha} + \frac{1}{\rho_\alpha Z_\alpha} \left(\frac{\partial Z_\alpha}{\partial n_{n\alpha}}\right)_{p,\vec{n}_{n\alpha}}\right) \left(\frac{\partial n_{n\alpha}}{\partial n_m}\right)_{p,\vec{n}_n}\right)_M^{(l)}$$
5-50

The remaining task is to evaluate the partial derivatives of the phase mole number with respect to n_m holding the pressure and total mole number of other components constant. These can be obtained by solving a linear system derived from phase equilibrium conditions. In the case of four-phase equilibrium, using the chain rule to differentiate Eqs. 3-30 with respect to n_m yields

$$\frac{\partial f_{io}}{\partial n_m} - \frac{\partial f_{ig}}{\partial n_m} = \sum_{n=1}^{n_c} \frac{\partial f_{io}}{\partial n_{no}} \frac{\partial n_{no}}{\partial n_m} - \sum_{n=1}^{n_c} \frac{\partial f_{ig}}{\partial n_{ng}} \frac{\partial n_{ng}}{\partial n_m} = 0$$

$$\frac{\partial f_{io}}{\partial n_m} - \frac{\partial f_{il}}{\partial n_m} = \sum_{n=1}^{n_c} \frac{\partial f_{io}}{\partial n_{no}} \frac{\partial n_{no}}{\partial n_m} - \sum_{n=1}^{n_c} \frac{\partial f_{il}}{\partial n_{nl}} \frac{\partial n_{nl}}{\partial n_m} = 0$$

$$\frac{\partial f_{io}}{\partial n_m} - \frac{\partial f_{iw}}{\partial n_m} = \sum_{n=1}^{n_c} \frac{\partial f_{io}}{\partial n_{no}} \frac{\partial n_{no}}{\partial n_m} - \sum_{n=1}^{n_c} \frac{\partial f_{iw}}{\partial n_{nw}} \frac{\partial n_{nw}}{\partial n_m} = 0$$

$$5.51$$

for $i = 1, ..., n_c$ and $m = 1, ..., n_c$. From Eq. 3-3, we see that

$$n_n = n_{no} + n_{ng} + n_{nl} + n_{nw}$$
 5-52

for $n = 1, ..., n_c$ and $\partial n_{nw} / \partial n_m$ can be replaced by

$$\frac{\partial n_{nw}}{\partial n_m} = \delta_{mn} - \frac{\partial n_{no}}{\partial n_m} - \frac{\partial n_{ng}}{\partial n_m} - \frac{\partial n_{nl}}{\partial n_m}$$
5-53

where δ_{mn} is the Kronecker delta function. Substituting Eq. 5-53 into Eq. 5-51 gives a set of linear equations to be solved

$$\sum_{n=1}^{n_c} \frac{\partial f_{io}}{\partial n_{no}} \frac{\partial n_{no}}{\partial n_m} - \sum_{n=1}^{n_c} \frac{\partial f_{ig}}{\partial n_{ng}} \frac{\partial n_{ng}}{\partial n_m} = 0$$

$$\sum_{n=1}^{n_c} \frac{\partial f_{io}}{\partial n_{no}} \frac{\partial n_{no}}{\partial n_m} - \sum_{n=1}^{n_c} \frac{\partial f_{il}}{\partial n_{nl}} \frac{\partial n_{nl}}{\partial n_m} = 0$$
5.54
$$\sum_{n=1}^{n_c} \left(\frac{\partial f_{io}}{\partial n_{no}} + \frac{\partial f_{iw}}{\partial n_{nw}}\right) \frac{\partial n_{no}}{\partial n_m} + \sum_{n=1}^{n_c} \frac{\partial f_{iw}}{\partial n_{nw}} \frac{\partial n_{ng}}{\partial n_m} + \sum_{n=1}^{n_c} \frac{\partial f_{iw}}{\partial n_{nw}} \frac{\partial n_{ng}}{\partial n_m} + \sum_{n=1}^{n_c} \frac{\partial f_{iw}}{\partial n_{nw}} \frac{\partial n_{ng}}{\partial n_m} + \sum_{n=1}^{n_c} \frac{\partial f_{iw}}{\partial n_{nw}} \frac{\partial n_{nl}}{\partial n_m} = \frac{\partial f_{iw}}{\partial n_{mw}}$$

$$i = 1 \dots n_c \text{ and } m = 1 \dots n_c$$

In matrix form, Eqs. 5-54 can be expressed as

$$\begin{pmatrix} \frac{\partial \vec{f}_o}{\partial \vec{n}_o} & -\frac{\partial \vec{f}_g}{\partial \vec{n}_g} & \overline{0} \\ \frac{\partial \vec{f}_o}{\partial \vec{n}_o} & \overline{0} & -\frac{\partial \vec{f}_l}{\partial \vec{n}_l} \\ \frac{\partial \vec{f}_o}{\partial \vec{n}_o} & \frac{\partial \vec{f}_w}{\partial \vec{n}_w} & \frac{\partial \vec{f}_w}{\partial \vec{n}_w} \end{pmatrix} \begin{pmatrix} \frac{\partial \vec{n}_o}{\partial n_m} \\ \frac{\partial \vec{n}_g}{\partial n_m} \\ \frac{\partial \vec{n}_l}{\partial n_m} \end{pmatrix} = \begin{pmatrix} \vec{0} \\ \vec{0} \\ \frac{\partial \vec{f}_w}{\partial n_{mw}} \end{pmatrix}$$
5-55

where $\vec{f}_{\alpha} = (f_{1\alpha}, ..., f_{n_c\alpha})$ and $\vec{n}_{\alpha} = (n_{1\alpha}, ..., n_{n_c\alpha})$ for $\alpha = o, g, l, w$. This system of the linear equations needs to be solved n_c times for $\partial \vec{n}_{\alpha} / \partial n_m$ as m goes from 1 to n_c and a different right-hand side is applied when m changes. The solution of Eqs. 5-55 is used in Eq. 5-50 to evaluate the partial derivative of the volume consistency equation with respect to n_m .

Last, the partial derivative of the volume consistency equation with respect to p_o is calculated. Similar to Eq. 5-45, the partial derivative of the volume consistency equation with respect to p_o can be written as

$$\frac{\partial F_{n_c+1}}{\partial p_o|_M} = \left(\sum_{\alpha=w,o,g,l} \left(\frac{1}{\rho_\alpha} \frac{\partial n_\alpha}{\partial p_o} - \frac{1}{\rho_\alpha^2} \frac{\partial \rho_\alpha}{\partial p_o}\right)\right)_M^{(l)}$$
 5-56

Using the chain rule

$$\frac{\partial}{\partial p_o} = \left(\frac{\partial}{\partial p_o}\right)_{\vec{n}_{\alpha}} + \sum_{n=1}^{n_c} \left(\frac{\partial}{\partial n_{n\alpha}}\right)_{p,\vec{n}_{n\alpha}} \left(\frac{\partial n_{n\alpha}}{\partial p_o}\right)_{p,\vec{n}_n}$$
5-57

to express the derivatives in Eq. 5-56 gives

$$\frac{\partial F_{n_c+1}|_{M}}{\partial p_o|_{M}} = \left(\sum_{\alpha=o,g,l,w} \left(\sum_{n=1}^{n_c} \left(\frac{1}{\rho_{\alpha}} + \frac{1}{\rho_{\alpha} Z_{\alpha}} \left(\frac{\partial Z_{\alpha}}{\partial n_{n\alpha}}\right)_{p,\vec{n}_{n\alpha}}\right) \left(\frac{\partial n_{n\alpha}}{\partial p_o}\right)_{\vec{n}} - \frac{n_{\alpha}}{\rho_{\alpha}^{-2}} \left(\frac{\partial \rho_{\alpha}}{\partial p_o}\right)_{\vec{n}_{\alpha}}\right) - \phi_0 C_R\right)_{M}^{(l)}$$
5-58

where the partial derivatives of the phase molar density with respect to the pressure holding the phase mole number constant can be computed from the EOS:

$$\left(\frac{\partial \rho_{\alpha}}{\partial p_{\alpha}}\right)_{\vec{n}_{\alpha}} = \frac{\rho_{\alpha}}{Z_{\alpha}} \left(\frac{Z_{\alpha}}{p_{\alpha}} - \left(\frac{\partial Z_{\alpha}}{\partial p_{\alpha}}\right)_{\vec{n}_{\alpha}}\right)$$
 5-59

The partial derivatives of the phase mole number with respect to p_o holding the total component mole number constant are obtained from the fugacity equations in the same way as that of the molar partial derivatives. If there are four equilibrium phases in the gridblock, differentiating Eqs. 3-30 with respect to p_o and applying the chain rule yields

$$\sum_{n=1}^{n_c} \frac{\partial f_{io}}{\partial n_{no}} \left(\frac{\partial n_{no}}{\partial p_o}\right)_{\vec{n}} + \left(\frac{\partial f_{io}}{\partial p_o}\right)_{\vec{n}_o} - \sum_{n=1}^{n_c} \frac{\partial f_{ig}}{\partial n_{ng}} \left(\frac{\partial n_{ng}}{\partial p_o}\right)_{\vec{n}} - \left(\frac{\partial f_{ig}}{\partial p_o}\right)_{\vec{n}_g} = 0$$

$$\sum_{n=1}^{n_c} \frac{\partial f_{io}}{\partial n_{no}} \left(\frac{\partial n_{no}}{\partial p_o}\right)_{\vec{n}} + \left(\frac{\partial f_{io}}{\partial p_o}\right)_{\vec{n}_o} - \sum_{n=1}^{n_c} \frac{\partial f_{il}}{\partial n_{nl}} \left(\frac{\partial n_{nl}}{\partial p_o}\right)_{\vec{n}} - \left(\frac{\partial f_{il}}{\partial p_o}\right)_{\vec{n}_l} = 0$$

$$\sum_{n=1}^{n_c} \frac{\partial f_{io}}{\partial n_{no}} \left(\frac{\partial n_{no}}{\partial p_o}\right)_{\vec{n}} + \left(\frac{\partial f_{io}}{\partial p_o}\right)_{\vec{n}_o} - \sum_{n=1}^{n_c} \frac{\partial f_{iw}}{\partial n_{nw}} \left(\frac{\partial n_{nw}}{\partial p_o}\right)_{\vec{n}} - \left(\frac{\partial f_{iw}}{\partial p_o}\right)_{\vec{n}_w} = 0$$

$$\sum_{n=1}^{n_c} \frac{\partial f_{io}}{\partial n_{no}} \left(\frac{\partial n_{no}}{\partial p_o}\right)_{\vec{n}} + \left(\frac{\partial f_{io}}{\partial p_o}\right)_{\vec{n}_o} - \sum_{n=1}^{n_c} \frac{\partial f_{iw}}{\partial n_{nw}} \left(\frac{\partial n_{nw}}{\partial p_o}\right)_{\vec{n}} - \left(\frac{\partial f_{iw}}{\partial p_o}\right)_{\vec{n}_w} = 0$$

for $i = 1, ..., n_c$. According to Eq. 5-52, eliminating $\partial n_{nw} / \partial p_o$ in the system using

$$\frac{\partial n_{nw}}{\partial p_o} = -\frac{\partial n_{no}}{\partial p_o} - \frac{\partial n_{ng}}{\partial p_o} - \frac{\partial n_{nl}}{\partial p_o}$$
5-61

gives a linear system to be solved for $(\partial n_{n\alpha}/\partial p_o)_{\vec{n}_{\alpha}}$:

$$\sum_{n=1}^{n_c} \frac{\partial f_{io}}{\partial n_{no}} \left(\frac{\partial n_{no}}{\partial p_o} \right)_{\vec{n}} - \sum_{n=1}^{n_c} \frac{\partial f_{ig}}{\partial n_{ng}} \left(\frac{\partial n_{ng}}{\partial p_o} \right)_{\vec{n}} = - \left(\frac{\partial f_{io}}{\partial p_o} \right)_{\vec{n}_o} + \left(\frac{\partial f_{ig}}{\partial p_o} \right)_{\vec{n}_g}$$

$$\sum_{n=1}^{n_c} \frac{\partial f_{io}}{\partial n_{no}} \left(\frac{\partial n_{no}}{\partial p_o} \right)_{\vec{n}} - \sum_{n=1}^{n_c} \frac{\partial f_{il}}{\partial n_{nl}} \left(\frac{\partial n_{nl}}{\partial p_o} \right)_{\vec{n}} = - \left(\frac{\partial f_{io}}{\partial p_o} \right)_{\vec{n}_o} + \left(\frac{\partial f_{il}}{\partial p_o} \right)_{\vec{n}_l}$$
5-62
$$\sum_{n=1}^{n_c} \left(\frac{\partial f_{io}}{\partial n_{no}} + \frac{\partial f_{iw}}{\partial n_{nw}} \right) \left(\frac{\partial n_{no}}{\partial p_o} \right)_{\vec{n}} + \sum_{n=1}^{n_c} \frac{\partial f_{iw}}{\partial n_{nw}} \left(\frac{\partial n_{ng}}{\partial p_o} \right)_{\vec{n}} + \sum_{n=1}^{n_c} \frac{\partial f_{iw}}{\partial n_{nw}} \left(\frac{\partial n_{ng}}{\partial p_o} \right)_{\vec{n}} + \sum_{n=1}^{n_c} \frac{\partial f_{iw}}{\partial n_{nw}} \left(\frac{\partial n_{ng}}{\partial p_o} \right)_{\vec{n}} + \sum_{n=1}^{n_c} \frac{\partial f_{iw}}{\partial n_{nw}} \left(\frac{\partial n_{nl}}{\partial p_o} \right)_{\vec{n}}$$

$$= - \left(\frac{\partial f_{io}}{\partial p_o} \right)_{\vec{n}_o} + \left(\frac{\partial f_{iw}}{\partial p_o} \right)_{\vec{n}_w}$$

$$i = 1 \dots n_c$$

whose coefficients are the same as those of the system used to calculate molar derivatives. In matrix form, Eqs. 5-62 can be written as:

$$\begin{pmatrix} \frac{\partial \vec{f_o}}{\partial \vec{n_o}} & -\frac{\partial \vec{f_g}}{\partial \vec{n_g}} & \bar{0} \\ \frac{\partial \vec{f_o}}{\partial \vec{n_o}} & \bar{0} & -\frac{\partial \vec{f_l}}{\partial \vec{n_l}} \\ \frac{\partial \vec{f_o}}{\partial \vec{n_o}} & \bar{0} & -\frac{\partial \vec{f_l}}{\partial \vec{n_l}} \\ \frac{\partial \vec{f_o}}{\partial \vec{n_o}} + \frac{\partial \vec{f_w}}{\partial \vec{n_w}} & \frac{\partial \vec{f_w}}{\partial \vec{n_w}} & \frac{\partial \vec{f_w}}{\partial \vec{n_w}} \end{pmatrix} \begin{pmatrix} \frac{\partial \vec{n_o}}{\partial p_o} \\ \frac{\partial \vec{n_g}}{\partial p_o} \\ \frac{\partial \vec{n_l}}{\partial p_o} \end{pmatrix} = \begin{pmatrix} -\left(\frac{\partial \vec{f_o}}{\partial p_o}\right)_{\vec{n_o}} + \left(\frac{\partial \vec{f_l}}{\partial p_o}\right)_{\vec{n_l}} \\ -\left(\frac{\partial \vec{f_o}}{\partial p_o}\right)_{\vec{n_o}} + \left(\frac{\partial \vec{f_l}}{\partial p_o}\right)_{\vec{n_l}} \end{pmatrix}$$
5-63

Since the coefficient matrices of Eqs. 5-55 and 5-63 are the same, it is necessary to perform the LU decomposition once when solving both systems. The solution of Eqs. 5-63 is then substituted into Eq. 5-58 to calculate the partial derivative of the volume consistency equation with respect to p_o . The partial derivatives of the component fugacity and phase compressibility factor required in the above equations are computed analytically from the equations of state selected using formulas provided in Appendix A.

If there are fewer phases at equilibrium, the linear system to be solved for the partial derivatives of the phase mole number can be derived in a similar way; however, the dimension of the system is reduced accordingly. The calculation for two-phase and three-phase mixtures can be found in Subramanian *et al.* (1987) and Chang (1990), respectively. For single-phase mixtures, assuming phase α , there is no equilibrium relation and the phase mole number

$$n_{n\alpha} = n_n, \qquad n = 1, \dots, n_c \tag{5-64}$$

is independent of pressure. Therefore, the partial derivatives of the last row of the diagonal block Jacobian can be evaluated as follows:

$$\frac{\partial F_{n_c+1}}{\partial n_m|_M} = \left(\frac{1}{\rho_\alpha} + \frac{1}{\rho_\alpha Z_\alpha} \left(\frac{\partial Z_\alpha}{\partial n_{m\alpha}}\right)_{p,\vec{n}_{m\alpha}}\right)_M^{(l)}$$
5-65

and

$$\frac{\partial F_{n_c+1}}{\partial p_o|_M} = \left(-\frac{n_\alpha}{\rho_\alpha Z_\alpha} \left(\frac{Z_\alpha}{p_\alpha} - \left(\frac{\partial Z_\alpha}{\partial p_\alpha} \right)_{\vec{n}_\alpha} \right) - \phi_0 C_R \right)_M^{(l)}$$
5-66

5.4.2 Jacobian Reduction

The primary set can be reduced to an implicit set with the pressure as the only variable by carrying out a partial elimination process. As shown before, the Jacobian structure of two adjacent gridblocks can be illustrated by the following incidence matrix:

where asterisk denotes nonzero elements. For the diagonal blocks, eliminating the first n_c elements of the last row using the diagonal elements by row operations results in

/*				*						*\	$n_{1,M}$
1	·.			*						*	:
		*		*						*	$n_{n_c-1,M}$
			*	*	i					*	$n_{n_c,M}$
				~	i					~	$p_{o,M}$
-	_	_	_	_	+	_	_	_	_	_	
				*	İ	*				*	$n_{1.N}$
				*			•.			*	
				*				*		*	$n_{n_c-1,N}$
				*					*	*	$n_{n_c,N}$
\				¥	Ì					ĩ/	$p_{o,N}$

where the accent tilde indicates the elements that have been modified during the elimination. This structure allows extracting the implicit variable pressure p_o from the primary variables and the system is reduced to the implicit set which contains the pressures as the only unknowns to be solved for first by the Newton-Raphson iteration using either direct elimination or an iterative method (Saad, 2003). The rest primary variables $(\Delta n_1, ..., \Delta n_{n_c})$ are then calculated using back substitution based on the upper triangular diagonal block once Δp_o is acquired.

5.4.3 Computational Procedure

As shown in Fig. 5-4, the computational procedure of an IMPES four-phase compositional model can be summarized as follows:

- Input simulation data that includes grid information, dimensions, reservoir conditions, fluid components, rock-fluid properties and well specifications.
- 2. Initialize simulation, allocate storage, generate grids and calculate the pressure of each gridblock according to vertical grid information.
- 3. Initialize the Newton iteration
 - a) Perform multiphase equilibrium calculation to determine the number of phases, phase mole fractions L_{α} and phase compositions $x_{m\alpha}$;
 - b) Compute phase physical properties: ρ_{α} , γ_{α} , s_{α} , μ_{α} and ρ_{F} ;
 - c) Calculate ϕ , $k_{r\alpha}$, and $p_{c\alpha o}$.
- 4. Calculate well terms q_m according to the well specifications.
- 5. Calculate residuals $\vec{R} = (F_1, \dots F_{n_c}, F_{n_c+1})^T$.
- 6. Check for convergence

$$\|\vec{R}\| \le \epsilon_{conv} \tag{5-67}$$

If the convergence criterion is satisfied, go to Step 3 and proceed to next time step. Otherwise, continue to Step 7.

7. Evaluate the Jacobian J_F .

- 8. Reduce the Jacobian J_F using partial elimination.
- 9. Extract the implicit set which contains the pressures as the only unknowns and solve for Δp_o .
- 10. Calculate $(\Delta n_1, ..., \Delta n_{n_c})$ using back substitution based on the upper triangle diagonal block.
- 11. Update the primary variables

$$\vec{x}_p^{(l+1)} = \vec{x}_p^{(l)} - \Delta \vec{x}_p^{(l+1)}.$$
 5-68

- 12. Recalculate $(z_1, \dots, z_{n_c})^{(l+1)}$ according to $(n_1, \dots, n_{n_c})^{(l+1)}$.
- 13. Perform multiphase flash calculation at the updated pressure and overall composition to determine the number of phases and the secondary variables $(x_{1\alpha}, ..., x_{n_c-1\alpha}, L_{\alpha})^{(l+1)}$.
- 14. Go to Step 5 for the next Newton iteration.



Figure 5-1 A block centered grid



Figure 5-2 Seven-point stencil



Figure 5-3 Numbering of a 5×4×3 grid system



Figure 5-4 Computational flowchart for the four-phase compositional model

Chapter Six: Simulator Validation

This chapter presents validation examples with commercial software developed by Computer Modelling Groups Ltd. (CMG). Both stand-alone multiphase equilibrium calculation and compositional simulations involving two hydrocarbon phases are tested to verify different aspects of the simulator.

6.1 Comparison of Multiphase Equilibrium Calculation Results

Multiphase equilibria of two CO₂-hydrocarbon-water mixtures are calculated isothermally at various pressures to verify the robustness and accuracy of the routine developed in this work for different types of phase behaviors. Both cases involve three-phase oil-gas-aqueous equilibrium, oil-gas- 2^{nd} liquid-aqueous equilibrium, and oil- 2^{nd} liquid-aqueous equilibrium that are commonly observed in CO₂ injection processes. Calculation results from CMG-WinProp are considered as reference standards of numerical tests. The WinProp is CMG's equation of state multiphase equilibrium property package (WinProp, 2013). Comparisons of the calculated phase mole fractions for water-in and water-free systems are presented to demonstrate the effect of the water component on the phase distribution.

6.1.1 Five-Component CO₂-Hydrocarbon-Water Mixture

Multiphase equilibria of a five-component CO₂-hydrocarbon-H₂O system are calculated at temperature of 70°F and pressures between 835 to 925 psia using the Peng-Robinson EOS. This multicomponent system is similar to the four-component CO₂-C₁-nC₁₆-H₂O system which Enick *et al.* (1986) used to demonstrate the four-phase equilibrium calculation results. Component compositions and properties are listed in Table 6-1. Calculation results show that the system has three phases: oil, gas and aqueous phases at equilibrium initially. At 855 psia, a CO₂-rich 2nd liquid phase is formed and four-phase equilibrium is established. As pressure further increases, the 2nd liquid phase keeps growing while the amount of the gas phase gradually decreases. The

oil phase expands at first and then diminishes once the 2nd liquid phase appears. However, the changes in oil phase fraction are small. The aqueous phase remains almost the same. The gas phase disappears at 897.5 psia where the four-phase region ends and only oil, the 2nd liquid phase and aqueous phases remain at equilibrium. Calculation results of phase mole fractions and phase compositions at pressures of 850 psia, 875 psia and 900 psia are presented and compared quantitatively in Tables 6-2, 6-3 and 6-4, respectively. Figs. 6-1 and 6-2 compare the calculated phase mole fractions versus pressure with CMG-WinProp's results. Predictions of both three-phase and four-phase equilibria of this work are highly consistent with those of CMG-WinProp.

At all pressures, the predicted solubility of CO_2 in the aqueous phase and water content in hydrocarbon phases are very small, and hydrocarbon solubility in water is negligible. The effect of the water component on phase distribution is substantial. When water is removed from the system and water-free equilibrium calculation is carried out at normalized overall composition as shown in the last column in Table 6-1, the phase behavior exhibits significant changes. Fig. 6-3 shows the comparison of the phase mole fraction versus pressure from water-in and water-free equilibrium calculation. Both phase distributions present the same trend of transition from oilgas to oil-2nd liquid-gas to oil-2nd liquid equilibrium as the pressure increases; the water-free equilibrium calculation results, however, enter the oil-2nd liquid-gas and oil-2nd liquid region at higher pressures of 857.25 and 900 psia, respectively. Similar to Enick *et al.*'s observation (1986), the addition of water to the system in the multiphase equilibrium calculation not only forms the aqueous phase but also shifts the multiple hydrocarbon phase region to a lower pressure.

6.1.2 Sixteen-Component CO₂-Hydrocarbon-Water Mixture

A three-phase flash calculation case from CMG-WinProp templates is selected as the second validation case to test the multiphase equilibrium calculation routine developed in this work. The mixture is originally composed of 15 components including CO_2 and light, intermediate and heavy hydrocarbons. The water component (H₂O) with composition of 0.1 is added to the mixture to generate an aqueous phase, and compositions of other components are normalized accordingly. Multiphase behaviors of the sixteen-component mixture are calculated at a constant temperature of 94°F and pressures between 1,150 psia and 1,200 psia. Phase densities and component fugacities are computed using the Peng-Robinson EOS. Table 6-5 gives component overall composition and properties required. Typical multiphase behavior of the CO₂/crude-oil mixture is observed in calculation results. The mixture exhibits three-phase oil-gas-aqueous equilibrium at pressures below 1,157.5 psia. A 2nd liquid phase is formed at 1,157.5 psia and four-phase equilibrium is recognized. The 2nd liquid phase expands and the gas phase steadily diminishes as pressure increases. Meanwhile, the oil phase slightly increases at the beginning, and then starts slightly shrinking after the 2^{nd} liquid phase appears. The aqueous phase barely changes. The gas phase vanishes at 1,185 psia, resulting in three-phase oil-2nd liquid-aqueous equilibrium thereafter. Plots of calculated phase mole fractions versus pressure are compared with CMG-WinProp in Figs. 6-4 and 6-5. Tables 6-6, 6-7 and 6-8 present calculation results of phase mole fractions and compositions at pressures of 1,155 psia, 1,175 psia and 1,190 psia which cover both the three-phase and four-phase regions. An excellent agreement in multiphase equilibrium predictions with CMG-WinProp demonstrates the robustness and accuracy of the multiphase equilibrium calculation routine developed in this work.

Similar to the calculation results of the five-component mixture, the solubility of CO_2 in the aqueous phase is very small and hydrocarbon solubility in water is negligible at all pressures. Comparison of the phase distribution from water-in and water-free equilibrium calculation is presented in Fig. 6-6. In the water-free system, the formation of the 2nd liquid phase happens at a higher pressure of 1,116.25 psia and the three-phase oil-2nd liquid-gas equilibrium ends at the same pressure of 1,185 psia. For this mixture, the introduction of water lowers the boundary between the oil-gas and oil-2nd liquid-gas equilibria and expands the oil-2nd liquid-gas region to a wider pressure range.

6.2 Comparison of Reservoir Simulation Results

Simulations of slim tube methane injection and the SPE Third Comparative Solution Project (Kenyon and Behie, 1987) are carried out to validate the simulator for one-dimensional and three-dimensional problems with two hydrocarbon phases at equilibrium. Data sets for both cases can be found in CMG-GEM templates (gmspr001.dat and gmflu001.dat) (GEM, 2013).

6.2.1 One-dimensional Methane Injection

A one-dimensional slim tube with the size of $60 \times 0.025 \times 0.025$ ft³ is used to test the simulator for one-dimensional problems. Input data for reservoir properties are provided in Table 6-9. As depicted in Fig. 6-7, the slim tube is discretized into 20 equal gridblocks with a porosity of 0.3, permeability of 1,000 md. Rock compressibility is set to zero. The initial temperature and pressure of the slim tube are 160°F and 2,260 psia and the initial oil in place consists of three components C₁, nC₄ and nC₁₀ with critical properties given in Table 6-10 and the compositions of 0, 0.64 and 0.36, respectively. There is no water in the system. Pure C₁ is injected into one end of the slim tube at a constant injection rate of 0.001125 ft³ (0.1 pore volume) per day and the reservoir fluid is produced from the other end at a constant pressure of 2,260 psia. Two phase relative permeabilities are looked up through Table 6-11 and Stone's Model II is used to calculate the oil phase relative permeability. Capillary pressure between the oil phase and gas phase is ignored. The Peng-Robinson EOS is used to model oil/gas equilibrium and phase densities.

Saturation profiles in the slim tube at 0.6 and 1.2 pore volume injected (PVI) are compared in Figs. 6-8 and 6-9, respectively. The comparisons of gas production, oil production and the gas-oil ratio at standard conditions are shown in Figs. 6-10, 6-11 and 6-12, respectively. Results of both saturation profiles and production data obtained from this simulator are consistent with those of CMG-GEM. In this case, the mixture of oil in place and injected gas exhibits two-phase equilibrium during the injection and it is demonstrated that the four-phase model proposed can correctly simulate the compositional flow with fewer phases than assumed.

6.2.2 The Third SPE Comparative Project

The third SPE comparative project is an artificial modeling study of gas cycling in a rich retrograde-gas-condensate reservoir (Kenyon and Behie, 1987). The study presented and compared fluid characterization results as well as reservoir simulation results from nine companies. Case 1 of the project is used to test the three-dimensional capability of our simulator. According to the CMG-GEM template for this problem, a three-dimensional reservoir with the size of $2639.7 \times 2639.7 \times 160$ ft³ is discretized into $9 \times 9 \times 4$ gridblocks with homogeneous properties in each layer but permeability and thickness vary among layers. The initial reservoir temperature is 200 °F and the initial pressure at a datum of 7,500 ft is 2,550 psia. Porosity at the initial reservoir condition is 0.13 for all gridblocks and rock compressibility is 4×10^{-6} psi⁻¹. Fig. 6-13 depicts the discretized gridblocks, and locations and penetrations of injection and production wells. A three-stage separator is used to separate produced reservoir fluids into oil, gas and water

surface streams. Reservoir fluids are produced from two bottom layers at a surface gas rate of 6,200 MSCF/day for 15 years and the separator-gas is injected back to two top layers of the reservoir at 4,700 MSCF/day for 10 years. The original reservoir fluid presented consists of 16 components which were characterized into different groups to match PVT data by different companies. Since the purpose of this chapter is to validate the simulator, the fluid characterization is skipped and the properties and compositions of 10 characterized components from the CMG template are directly used. The input data for reservoir properties, component properties and separator conditions are given in Tables 6-12 through 6-14. Modified relative permeabilities by CMG are used for the simulation. Two phase relative permeabilities are looked up through Table 6-15 and Stone's Model II is used to calculate the oil phase relative permeability. Table 6-15 also provides the water-oil capillary pressure while the capillary pressure between the oil and gas phases is assumed to be zero. The oil/gas equilibrium and phase densities are modelled by the Peng-Robinson EOS.

Since the production well is controlled by the surface gas rate, only the oil production rate and cumulative oil production at surface conditions are compared. As shown in Fig. 6-14 for the comparison of the predicted oil production rate and cumulative oil production at standard conditions, there is a good match between our model and CMG-GEM. Fig. 6-15 shows the comparison of oil saturation in gridblock (7, 3, 1) which is the bottom gridblock of the production completion and corresponds to gridblock (7, 7, 4) in the paper of Kenyon and Behie (1987). The oil saturation predicted by our simulator exhibits the same trend as that of CMG-GEM but is slightly lower. This can be caused by the different formulations in the numerical solution. CMG-GEM uses an adaptive-implicit solution scheme which treats well blocks and their neighbors fully implicitly while our simulator uses IMPES for all blocks. Additionally, the effect of the water component on phase distribution should also be taken into account because in our simulator, water is considered as a component rather than an independent phase in the phase equilibrium calculation. To summarize, this simulator presents a satisfactory range of accuracy agreeable with CMG-GEM in the simulation results and the three-dimensional capability is validated.

	p_c (psia)	T_c (°F)	v_c (ft ³ /lbmol)	mw	ω	<i>z_m</i> Water-in	<i>z_m</i> Water-Free
CO_2	1069.87	87.89	1.5057	44.01	0.225	0.72	0.9
C_1	667.2	-116.59	1.5859	16.043	0.008	0.016	0.02
C ₃	615.76	205.97	3.2518	12.3757	0.152	0.024	0.03
nC_{16}	252.04	862.43	12.3757	222	0.6837	0.04	0.05
H ₂ O	3197.84	705.47	0.8971	18.015	0.344	0.2	0.0

 Table 6-1 Component properties and overall composition for the five-component CO2hydrocarbon-water mixture

Binary interaction parameters:

	CO ₂	C1	C ₃	nC_{16}	H ₂ O
CO ₂	0.0	0.105	0.125	0.115	0.2
C_1	0.105	0.0	0.00854	0.0715	0.4907
C ₃	0.125	0.00854	0.0	0.0325	0.5469
nC_{16}	0.115	0.0715	0.0325	0.0	0.48
H ₂ O	0.2	0.4907	0.5469	0.48	0.0

Table 6-2 Predicted phase mole fractions and compositions at 70 °F	and 850 psia f	or the
five-component CO ₂ -hydrocarbon-water mixture		

	Oil, Mole %		Gas, N	Iole %	2 nd Liquid	l, Mole %	Aqueous, Mole %	
	This Work	This WinProp Work		WinProp	This Work	WinProp	This Work	WinProp
Phase	12.4198	12.4199	67.6383	67.6383	0.00000	0.00000	19.9418	19.9418
CO ₂	61.56579	61.56595	95.14002	95.14002	0.00000	0.00000	0.01253	0.01253
C_1	0.64735	0.64735	2.24666	2.24666	0.00000	0.00000	0.00000	0.00000
C_3	5.53295	5.53293	2.53232	2.53232	0.00000	0.00000	0.00000	0.00000
nC_{16}	32.19897	32.19883	0.00139	0.00139	0.00000	0.00000	0.00000	0.00000
H ₂ O	0.05494	0.05494	0.07962	0.07962	0.00000	0.00000	99.98747	99.98747

Table 6-3 Predicted phase mole fractions and compositions at 70 °F and 875 psia for the five-component CO₂-hydrocarbon-water mixture

	Oil, Mole %		Gas, N	Iole %	2 nd Liquid	l, Mole %	Aqueous	Aqueous, Mole %		
	This Work	WinProp	Prop This Work W		This Work	WinProp	This Work	WinProp		
Phase	11.6105	11.6104	25.5090	25.5020	42.9795	42.9867	19.9010	19.9010		
CO ₂	61.70635	61.70622	94.32238	94.32214	94.86467	94.86461	0.01258	0.01258		
C_1	1.00651	1.00659	3.39062	3.39090	1.43842	1.43855	0.00000	0.00000		
C ₃	4.78382	4.78372	2.20544	2.20539	2.98279	2.98272	0.00000	0.00000		
nC_{16}	32.44839	32.44853	0.00171	0.00171	0.54011	0.54010	0.00000	0.00000		
H ₂ O	0.05494	0.05494	0.07985	0.07985	0.17401	0.17401	99.98742	99.98742		

	Oil		G	as	2 nd L	iquid	Aqu	Aqueous	
	This Work	WinProp	This Work	WinProp	This Work	WinProp	This Work	WinProp	
Phase	11.1543	11.1543	0.00000	0.00000	68.9678	68.9678	19.8779	19.8779	
CO_2	61.43061	61.43052	0.00000	0.00000	94.45762	94.45762	0.01256	0.01255	
C_1	1.44498	1.44498	0.00000	0.00000	2.08622	2.08622	0.00000	0.00000	
C ₃	4.43204	4.43205	0.00000	0.00000	2.76308	2.76308	0.00000	0.00000	
nC_{16}	32.63765	32.63774	0.00000	0.00000	0.52125	0.52125	0.00000	0.00000	
H ₂ O	0.05471	0.05471	0.00000	0.00000	0.17183	0.17183	99.98744	99.98744	

Table 6-4 Predicted phase mole fractions and compositions at 70 °F and 900 psia for the
five-component CO2-hydrocarbon-water mixture

	p _c (psia)	<i>T_c</i> (°F)	v_c (ft ³ /lbmol)	mw	ω	<i>z_m</i> Water-in	z _m Water-Free
CO_2	1069.87	87.89	1.5058	44.01	0.225	0.71055	0.7895
N_2	492.31	-232.51	1.4337	28.013	0.04	0.0009	0.001
C_1	667.2	-116.59	1.5859	16.043	0.008	0.030915	0.03435
C_2	708.35	-90.05	2.3708	30.07	0.098	0.007641	0.00849
C ₃	615.76	205.97	3.2518	44.097	0.152	0.005634	0.00626
iC ₄	529.05	274.91	4.2129	58.124	0.176	0.000684	0.00076
nC ₄	551.1	305.69	4.0848	58.124	0.193	0.006237	0.00693
iC5	490.85	369.05	4.9017	72.151	0.227	0.002997	0.00333
nC ₅	489.37	385.61	4.8697	72.151	0.251	0.004077	0.00453
nC_6	430.59	453.65	5.9269	86.178	0.296	0.0063	0.007
C ₇ -C ₁₁	393.85	598.73	6.1031	121.77	0.36958	0.049599	0.05511
C_{12} - C_{16}	289.31	798.584	10.0277	191.8	0.54918	0.029799	0.03311
C ₁₇ -C ₂₂	217.76	927.14	14.1606	267.75	0.6958	0.020448	0.02272
C ₂₃ -C ₂₉	168.77	1046.41	18.7419	357.38	0.95945	0.01233	0.0137
C ₃₀₊	111.94	1260.82	22.4839	549.6	1.2843	0.011889	0.01321
H ₂ O	3197.84	705.47	0.8971	18.015	0.344	0.1	0.0

Table 6-5 Component properties and overall composition for the sixteen-component CO2-hydrocarbon-water mixture

Binary interaction	parameters:

	CO ₂	N_2	C_1	C_2	C ₃	iC ₄	nC ₄	iC ₅	nC ₅	nC_6	C ₇ -C ₁₁	C ₁₂ -C ₁₆	C ₁₇ -C ₂₂	C ₂₃ -C ₂₉	C ₃₀₊	H ₂ O
CO ₂	0.0	-0.02	0.1	0.13	0.135	0.13	0.13	0.125	0.125	0.125	0.12	0.12	0.12	0.12	0.12	0.2
N_2	-0.02	0.0	0.1	0.042	0.091	0.095	0.095	0.095	0.095	0.1	0.1	0.1	0.1	0.1	0.1	0.275
C_1	0.1	0.1	0.0	0.002	0.007	0.013	0.012	0.017	0.017	0.024	0.025	0.045	0.063	0.079	0.09	0.491
C_2	0.13	0.042	0.002	0.0	0.001	0.005	0.004	0.007	0.007	0.012	0.012	0.028	0.043	0.057	0.066	0.491
C ₃	0.135	0.091	0.007	0.001	0.0	0.001	0.001	0.002	0.002	0.005	0.005	0.017	0.029	0.041	0.05	0.547
iC4	0.13	0.095	0.013	0.005	0.001	0.0	0.0	0.0	0.0	0.002	0.002	0.01	0.02	0.03	0.038	0.508
nC ₄	0.13	0.095	0.012	0.004	0.001	0.0	0.0	0.0	0.0	0.002	0.002	0.011	0.021	0.031	0.039	0.508
iC ₅	0.125	0.095	0.017	0.007	0.002	0.0	0.0	0.0	0.0	0.001	0.001	0.007	0.015	0.024	0.031	0.5
nC ₅	0.125	0.095	0.017	0.007	0.002	0.0	0.0	0.0	0.0	0.001	0.001	0.007	0.016	0.025	0.032	0.5
nC_6	0.125	0.1	0.024	0.012	0.005	0.002	0.002	0.001	0.001	0.0	0.0	0.004	0.01	0.018	0.024	0.45
C ₇ -C ₁₁	0.12	0.1	0.025	0.012	0.005	0.002	0.002	0.001	0.001	0.0	0.0	0.003	0.01	0.017	0.023	0.0
C_{12} - C_{16}	0.12	0.1	0.045	0.028	0.017	0.01	0.011	0.007	0.007	0.004	0.003	0.0	0.002	0.005	0.009	0.0
C ₁₇ -C ₂₂	0.12	0.1	0.063	0.043	0.029	0.02	0.021	0.015	0.016	0.01	0.01	0.002	0.0	0.001	0.003	0.0
C ₂₃ -C ₂₉	0.12	0.1	0.079	0.057	0.041	0.03	0.031	0.024	0.025	0.018	0.017	0.005	0.001	0.0	0.0	0.0
C ₃₀₊	0.12	0.1	0.09	0.066	0.05	0.038	0.039	0.031	0.032	0.024	0.023	0.009	0.003	0.0	0.0	0.0
H ₂ O	0.2	0.275	0.491	0.491	0.547	0.508	0.508	0.5	0.5	0.45	0.0	0.0	0.0	0.0	0.0	0.0

	Oil, M	Iole %	Gas, N	Iole %	2 nd Liquic	l, Mole %	Aqueous	, Mole %
	This Work	WinProp	This Work	WinProp	This Work	WinProp	This Work	WinProp
Phase	41.8997	41.8999	48.7260	48.7259	0.000000	0.000000	9.3743	9.3743
CO ₂	61.97053	61.9706	92.53301	92.53297	0.00000	0.00000	0.02011	0.02010
N_2	0.03819	0.03819	0.15187	0.15187	0.00000	0.00000	0.00000	0.00000
C_1	2.06629	2.06633	4.56785	4.56782	0.00000	0.00000	0.00000	0.00000
C_2	0.84996	0.84996	0.83727	0.83727	0.00000	0.00000	0.00000	0.00000
C ₃	0.81692	0.81692	0.45378	0.45379	0.00000	0.00000	0.00000	0.00000
iC ₄	0.11311	0.11311	0.04311	0.04311	0.00000	0.00000	0.00000	0.00000
nC ₄	1.08468	1.08467	0.34730	0.34730	0.00000	0.00000	0.00000	0.00000
iC5	0.57132	0.57131	0.12380	0.12380	0.00000	0.00000	0.00000	0.00000
nC ₅	0.79631	0.79630	0.15197	0.15197	0.00000	0.00000	0.00000	0.00000
nC_6	1.32477	1.32475	0.15377	0.15378	0.00000	0.00000	0.00000	0.00000
C7-C11	11.34809	11.34801	0.42089	0.42093	0.00000	0.00000	0.00000	0.00000
C_{12} - C_{16}	7.07915	7.07913	0.02823	0.02823	0.00000	0.00000	0.00000	0.00000
C ₁₇ -C ₂₂	4.87619	4.87617	0.00347	0.00347	0.00000	0.00000	0.00000	0.00000
C ₂₃ -C ₂₉	2.94258	2.94257	0.00014	0.00000	0.00000	0.00000	0.00000	0.00000
C ₃₀₊	2.83749	2.83748	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
H ₂ O	1.28443	1.28442	0.18354	0.18354	0.00000	0.00000	99.97989	99.97989

Table 6-6 Predicted phase mole fractions and compositions at 94 °F and 1,155 psia for the sixteen-component CO₂-hydrocarbon-water mixture

	Oil, M	Iole %	Gas, N	Iole %	2 nd Liquic	l, Mole %	Aqueous, Mole %		
	This Work	WinProp	This Work	WinProp	This Work	WinProp	This Work	WinProp	
Phase	40.2718	40.2715	18.9916	18.9810	31.3764	31.3872	9.3602	9.3602	
CO ₂	61.56869	61.56868	91.98986	91.98970	91.75042	91.75035	0.02008	0.02008	
N_2	0.04720	0.04720	0.17757	0.17758	0.11878	0.11879	0.00000	0.00000	
C_1	2.34763	2.34772	4.99906	4.99919	3.81391	3.81409	0.00000	0.00000	
C_2	0.86440	0.86440	0.84775	0.84775	0.81268	0.81269	0.00000	0.00000	
C ₃	0.79264	0.79263	0.44918	0.44918	0.50638	0.50637	0.00000	0.00000	
iC ₄	0.10770	0.10770	0.04265	0.04265	0.05395	0.05395	0.00000	0.00000	
nC ₄	1.02783	1.02781	0.34447	0.34446	0.46008	0.46007	0.00000	0.00000	
iC5	0.53863	0.53862	0.12458	0.12458	0.18844	0.18843	0.00000	0.00000	
nC ₅	0.75111	0.75110	0.15388	0.15388	0.24219	0.24218	0.00000	0.00000	
nC_6	1.26067	1.26065	0.16071	0.16071	0.29253	0.29252	0.00000	0.00000	
C7-C11	11.11236	11.11226	0.47831	0.47833	1.25545	1.25539	0.00000	0.00000	
C_{12} - C_{16}	7.23461	7.23463	0.03707	0.03708	0.18916	0.18915	0.00000	0.00000	
C ₁₇ -C ₂₂	5.04102	5.04104	0.00503	0.00503	0.04378	0.04378	0.00000	0.00000	
C ₂₃ -C ₂₉	3.05791	3.05793	0.00023	0.00023	0.00473	0.00472	0.00000	0.00000	
C ₃₀₊	2.95196	2.95198	0.00000	0.00000	0.00030	0.00030	0.00000	0.00000	
H ₂ O	1.29566	1.29565	0.18964	0.18964	0.26723	0.26722	99.97992	99.97992	

Table 6-7 Predicted phase mole fractions and compositions at 94 °F and 1,175 psia for the sixteen-component CO₂-hydrocarbon-water mixture

	Oil, Mole %		Gas, Mole %		2 nd Liquid, Mole %		Aqueous, Mole %	
	This Work	WinProp	This Work	WinProp	This Work	WinProp	This Work	WinProp
Phase	39.4327	39.4327	0.00000	0.00000	51.2146	51.2147	9.3526	9.3526
CO_2	61.35167	61.35173	0.00000	0.00000	91.49820	91.49812	0.02006	0.02006
N_2	0.05352	0.05352	0.00000	0.00000	0.13452	0.13452	0.00000	0.00000
C_1	2.52175	2.52178	0.00000	0.00000	4.09474	4.09471	0.00000	0.00000
C_2	0.87230	0.87231	0.00000	0.00000	0.82032	0.82032	0.00000	0.00000
C ₃	0.78067	0.78067	0.00000	0.00000	0.49900	0.49900	0.00000	0.00000
iC ₄	0.10506	0.10506	0.00000	0.00000	0.05266	0.05266	0.00000	0.00000
nC ₄	0.99988	0.99987	0.00000	0.00000	0.44796	0.44797	0.00000	0.00000
iC5	0.52242	0.52241	0.00000	0.00000	0.18295	0.18295	0.00000	0.00000
nC ₅	0.72849	0.72848	0.00000	0.00000	0.23516	0.23517	0.00000	0.00000
nC_6	1.22736	1.22735	0.00000	0.00000	0.28511	0.28512	0.00000	0.00000
C7-C11	10.96525	10.96519	0.00000	0.00000	1.24184	1.24190	0.00000	0.00000
C_{12} - C_{16}	7.3083	7.30830	0.00000	0.00000	0.19141	0.19143	0.00000	0.00000
C ₁₇ -C ₂₂	5.12770	5.12771	0.00000	0.00000	0.04453	0.04453	0.00000	0.00000
C ₂₃ -C ₂₉	3.12059	3.12060	0.00000	0.00000	0.00481	0.00481	0.00000	0.00000
C ₃₀₊	3.01461	3.01462	0.00000	0.00000	0.00030	0.00030	0.00000	0.00000
H ₂ O	1.30042	1.30040	0.00000	0.00000	0.26648	0.26648	99.97993	99.97993

Table 6-8 Predicted phase mole fractions and compositions at 94 °F and 1,190 psia for the sixteen-component CO₂-hydrocarbon-water mixture
Dimensions (ft)	
Length×Width×Thickness	60×0.025×0.025
Grid Number	
$n_x \times n_y \times n_z$	20×1×1
Grid Size (ft)	
dx dy dz	3 0.025 0.025
Permeability (md)	1000
Relative Permeability Model	Stone II
Porosity	0.3
Rock Compressibility (psi ⁻¹)	0.0
Initial Temperature (°F)	160
Initial Pressure (psia)	2260
Initial Oil Composition	
$C_1 nC_4 nC_{10}$	0.0 0.64 0.36
Injected Composition	
$C_1 nC_4 nC_{10}$	1.0 0.0 0.0
Injection Rate (ft ³ /day)	0.001125
Production Pressure (psia)	2260
Final Time (day)	12

Table 6-9 Summary of reservoir properties for the one-dimensional methane injection process

 v_c (ft³/lbmol) T_c (°F) p_c (psia) mwω C_1 1.5859 667.2 -116.59 16.043 0.008 nC_4 551.1 305.69 4.0848 58.124 0.193 nC_{10} 367.55 660.11 8.3458 134 0.443774

Table 6-10 Component properties for the one-dimensional methane injection process

	C_1	nC ₄	nC_{10}
\mathbf{C}_1	0.0	0.01475	0.04437
nC_4	0.01475	0.0	0.00845
nC_{10}	0.04437	0.00845	0.0

S _W	k _{rw}	k _{row}	Sg	k_{rg}	k_{rog}
0.0001	0	1	0.0001	0	1
0.0417625	0.041667	0.958333	0.0416625	0.041667	0.958333
0.083425	0.083333	0.916667	0.083325	0.083333	0.916667
0.1250875	0.125	0.875	0.1249875	0.125	0.875
0.16675	0.166667	0.833333	0.16665	0.166667	0.833333
0.2084125	0.208333	0.791667	0.2083125	0.208333	0.791667
0.250075	0.25	0.75	0.249975	0.25	0.75
0.2917375	0.291667	0.708333	0.2916375	0.291667	0.708333
0.3334	0.333333	0.666667	0.3333	0.333333	0.666667
0.3750625	0.375	0.625	0.3749625	0.375	0.625
0.416725	0.416667	0.583333	0.416625	0.416667	0.583333
0.4583875	0.458333	0.5416677	0.4582875	0.458333	0.541667
0.50005	0.5	0.5	0.49995	0.5	0.5
0.5417125	0.541667	0.458333	0.5416125	0.541667	0.458333
0.583375	0.583333	0.416667	0.583275	0.583333	0.416667
0.6250375	0.625	0.375	0.6249375	0.625	0.375
0.6667	0.666667	0.333333	0.6666	0.666667	0.333333
0.7083625	0.708333	0.291667	0.7082625	0.708333	0.291667
0.750025	0.75	0.25	0.749925	0.75	0.25
0.7916875	0.791667	0.208333	0.7915875	0.791667	0.208333
0.83335	0.833333	0.166667	0.83325	0.833333	0.166667
0.8750125	0.875	0.125	0.8749125	0.875	0.125
0.916675	0.916667	0.083333	0.916575	0.916667	0.083333
0.9583375	0.958333	0.041667	0.9582375	0.958333	0.041667
1	1	0	0.9999	1	0

Table 6-11 Relative permeability used in the one-dimensional methane injection process

Dimensions (ft)	
Length ×Width ×Thickness	2639.7×2639.7×160
Grid Number	
$n_x \times n_y \times n_z$	9×9×4
Grid Size (ft)	
dx dy dz (layer 1:4)	293 293 (50,50,30,30)
Datum, ft	7500
Relative Permeability Model	Stone II
Porosity	0.13
Rock Compressibility (psi ⁻¹)	4.0
Initial Temperature (°F)	200
Initial Pressure (psia)	3550
Initial Oil Composition	
$C_1 \ C_2 \ C_3 \ C_4 \ C_5$	$0.6793 \ 0.0990 \ 0.0591 \ 0.0517 \ 0.0269$
$C_6 \ C_{79} \ C_{1011} \ C_{1214} \ C_{15\text{+}}$	0.0181 0.0399 0.0122 0.0080 0.0058
Injected Composition	Cycling
Intertion Data (and MSCE/day)	4700 ($t \le 10$ years)
injection Rate (gas MSCF/day)	0 (t > 10 years)
Production Rate (gas MSCF/day)	6200
Final Time (year)	15

Layer	Horizontal Permeability (md) K_x, K_y	Vertical permeability (md) K_z
1	150	15
2	20	2
3	40	4
4	130	13

	p_c (psia)	T_c (°F)	v_c (ft ³ /lbmol)	mw	ω
C_1	587.838	-109.667	1.585855	16.043	0.013
C_2	708.3447	90.104	2.370773	30.07	0.0986
C ₃	617.3768	206.15	3.203748	44.097	0.1524
C_4	550.6572	305.69	4.084778	58.124	0.201
C ₅	489.5221	385.61	4.981828	72.151	0.2539
C_6	439.7028	454.55	5.894896	86.178	0.3007
C ₇₋₉	385.8127	572.54	7.459926	114.43	0.3613
C ₁₀₋₁₁	340.7109	688.352	9.12107	144.83	0.4501
C ₁₂₋₁₄	293.7279	774.68	11.05453	177.78	0.5339
C ₁₅₊	184.4988	887.3258	15.45488	253.63	0.7244

 Table 6-13 Component properties for the third SPE comparative project

 $C_{1/}\,C_{15+} \qquad \qquad 0.2466$

All others are 0.0

 Table 6-14 Separator conditions for the third SPE comparative project

Stage	Temperature (°F)	Pressure (psia)
1	80	815
2	80	65
3	60	14.7

S _W	k _{rw}	k _{row}	p _{cow} (psi)	Sg	k_{rg}	k _{rog}	p _{cog} (psi)
0.16	0.0	0.8	50.0	0.0	0.0	0.8	0.0
0.2	0.002	0.65	32.0	0.04	0.005	0.62	0.0
0.24	0.01	0.513	21.0	0.08	0.013	0.513	0.0
0.28	0.02	0.4	15.5	0.12	0.026	0.4	0.0
0.32	0.033	0.315	12.0	0.16	0.04	0.315	0.0
0.36	0.049	0.25	9.2	0.2	0.058	0.25	0.0
0.4	0.066	0.196	7.0	0.14	0.078	0.196	0.0
0.44	0.09	0.15	5.3	0.28	0.10	0.150	0.0
0.48	0.119	0.112	4.2	0.32	0.126	0.112	0.0
0.52	0.15	0.082	3.4	0.36	0.156	0.086	0.0
0.56	0.186	0.06	2.7	0.4	0.187	0.06	0.0
0.60	0.227	0.04	2.1	0.44	0.222	0.04	0.0
0.64	0.277	0.024	1.7	0.48	0.26	0.024	0.0
0.68	0.33	0.012	1.3	0.52	0.3	0.012	0.0
0.72	0.39	0.05	1.0	0.56	0.348	0.005	0.0
0.76	0.462	0.0	0.7	0.6	0.4	0.0	0.0
0.80	0.54	0.0	0.5	0.64	0.45	0.0	0.0
0.84	0.62	0.0	0.4	0.68	0.505	0.0	0.0
0.88	0.71	0.0	0.3	0.72	0.562	0.0	0.0
0.92	0.8	0.0	0.2	0.76	0.62	0.0	0.0
0.96	0.9	0.0	0.1	0.8	0.68	0.0	0.0
1.00	1.0	0.0	0.0	0.84	0.74	0.0	0.0

Table 6-15 Relative permeability and capillary pressure used in the third SPE comparative project



Figure 6-1 Calculated phase mole fraction vs pressure for the five-component CO₂hydrocarbon-water mixture from this work



Figure 6-2 Calculated phase mole fraction vs pressure for the five-component CO₂hydrocarbon-water mixture from WinProp



Figure 6-3 Comparison of water-in and water-free multiphase equilibrium calculation results for the five-component CO₂-hydrocarbon-water mixture



Figure 6-4 Calculated phase mole fraction vs pressure for the sixteen-component CO₂hydrocarbon-water mixture from this work



Figure 6-5 Calculated phase mole fraction vs pressure for the sixteen-component CO₂hydrocarbon-water mixture from WinProp



Figure 6-6 Comparison of water-in and water-free multiphase equilibrium calculation results for the sixteen-component CO₂-hydrocarbon-water Mixture



Figure 6-7 Discretized gridblocks for the one-dimensional methane injection process



Figure 6-8 Comparison of saturation profiles at 0.6 PVI for the one-dimensional methane injection process



Figure 6-9 Comparison of saturation profiles at 1.2 PVI for the one-dimensional methane injection process



Figure 6-10 Comparison of gas production rate and cumulative gas production at standard condition for the one-dimensional methane injection process



Figure 6-11 Comparison of oil production rate and cumulative oil production at standard condition for the one-dimensional methane injection process



Figure 6-12 Comparison of gas-oil ratio at standard condition for the one-dimensional methane injection process



Figure 6-13 Discretized gridblocks and well locations for the third SPE comparative project



Figure 6-14 Comparison of oil production rate and cumulative oil production at standard condition for the third SPE comparative project



Figure 6-15 Comparison of oil Saturation in gridblock (7,3,1) for the third SPE comparative project

Chapter Seven: Simulation Results and Discussion

The four-phase compositional model developed in this work is used to simulate complex phase behaviors and flow mechanisms in the CO_2 injection processes. Simulation results of onedimensional and two-dimensional problems are presented to demonstrate the computational capability of this model and illustrate the phase-behavior on fluid properties and displacement efficiency.

7.1 One-dimensional Slim-tube Displacement of Wasson Oil

7.1.1 Displacement by CO₂

Simulations of one-dimensional CO₂ flooding are performed in a slim tube with the size of $60{\times}0.025{\times}0.025~{\rm ft}^3$ for two recombined oils (deal oil + 312 SCF/BBL and dead oil + 602 SCF/BBL) from the Wasson field originally reported by Orr and Jensen (1984). According to the fluid characterization results obtained by Nghiem and Li (1986), a 10-hydrocarbon-component system is used in the simulations because they are adequate to predict the important features of experimental phase diagrams. Table 7-1 gives the compositions of the two recombined oils as well as the compositions of the gas and dead oil used in the recombination. Component properties are presented in Table 7-2. Input data for reservoir properties are listed in Table 7-3. The slim tube is discretized into 80 equal sized gridblocks. Initial water saturation is 0.2 and the amount of water is converted into overall composition of the water component. It is assumed that a maximum of four equilibrium phases can coexist and flow together. The Peng-Robinson EOS is used to compute the densities and fugacity coefficients of all phases. Phase relative permeabilities are calculated using Corey's model with parameters measured by Dria et al. (1990). These parameters are given in Table 7-3. Even though the aqueous phase is immobile since it exists at the residual saturation, the effect of water-hydrocarbon mutual solubility is taken into account. Gravity and capillary pressures are assumed negligible. Pure CO₂ is injected

into one end of the slim tube at a constant injection rate of 0.001125 ft³ (equivalent to 0.1 pore volume or 0.125 hydrocarbon pore volume) per day and the reservoir fluid is produced from the other end at a pressure equal to the initial pressure. The simulations are carried out at a constant temperature of 90°F and five different initial pressures that cover typical regions of oil-gas-aqueous, oil-2nd liquid-gas-aqueous and oil-2nd liquid-aqueous in the phase diagram.

Fig. 7-1 shows recovery factors for the displacement of the 312 SCF/BBL recombined Wasson oil at different pressures. The displacement at 700 psia recovers 73.64% oil in the end of the process when 1.5 hydrocarbon pore volume of CO₂ is injected. The recovery factor is improved significantly when the initial pressure is increased to 1,100 psia which yields 91.96% oil recovery at 1.5 hydrocarbon pore volume injected (HCPVI). As shown in Fig. 7-2 for the comparison of oil recovery factors at different HCPVI versus pressure, a further raise in pressure contributes very little to the ultimate recovery. Only 2% extra oil is recovered at 1.5 HCPVI when the pressure is increased from 1,100 psia to 1,500 psia.

Figs. 7-3, 7-4 and 7-5 show the simulated saturation profiles at 0.8 HCPVI for the displacements of the 312 SCF/BBL recombined Wasson oil at 900, 1,100 and 1,300 psia, respectively. For the displacement at 900 psia, the mass density profiles shown in Fig. 7-6 indicate that the CO₂-rich phase is a gas phase and a CO₂-rich liquid phase is not detected. The gas phase has already broken through and the injected CO₂ increases the mass densities of both the oil and gas phases behind the gas bank. Three-phase oil-gas-aqueous equilibrium exists in the entire slim tube while the effect of dissolved CO₂ on the aqueous density is negligible. The water content in the oil and gas phases results in a tiny drop of water saturation in the injection end of the slim tube. Four-phase equilibrium occurs during the displacement at 1,100 psia. A gas phase appears at the displacement front where oil-gas-aqueous equilibrium is observed. Following the

gas phase, a narrow four-phase region exists in four gridblocks. These four phases can be clearly distinguished from each other based on their mass density profiles shown in Fig. 7-7. Behind the four-phase zone, there is a trailing CO₂-rich liquid phase and the reservoir mixture exhibits oil-2nd liquid-aqueous equilibrium in this area. An increase in the mass density of the CO₂-rich liquid phase close to the displacement front is caused by the heavy hydrocarbon components extracted from the oil phase. The drop of water saturation in the injection is more substantial than that at lower pressures because more water content dissolves in the oil phase and evaporates into the gas phase as pressure increases. The displacement at 1,300 psia shows three-phase regions only. A three-phase oil-gas-aqueous region located at the displacement front is followed by a three-phase oil-2nd liquid-aqueous region. A four-phase oil-gas-2nd liquid-aqueous region is not detected in between. The leading gas phase has just broken through. In Fig. 7-8, it is seen that an inversion of mass densities of the oil and second liquid happens in the injection block. The mass density of the CO_2 -rich liquid phase is slightly greater than that of the oil phase in this gridblock. Using the mass density alone as a criterion to identify the phases may cause phase swapping in this case.

The appearance of a CO₂-rich liquid phase at 1,100 psia significantly increases ultimate oil recovery but the increment becomes little at higher pressures once the CO₂-rich liquid phase is formed. In contrast, the gas phase itself at low pressures does not efficiently displace the oil. To understand the high displacement efficiency resulting from the CO₂-rich liquid phase, we calculate component molar distribution $C_{m\alpha}$ which represents the fraction of the total amount of component *m* that presents in phase α using

$$C_{m\alpha} = \frac{L_{\alpha} x_{m\alpha}}{z_m}$$
 7-1

for $m = 1, ..., n_c$ and $\alpha = o, g, l, w$. Figs. 7-9, 7-10 and 7-11 give the molar distributions of intermediate and heavy components (C₅, C₆, C₇₋₁₃, C₁₄₋₂₀, C₂₁₋₂₈ and C₂₉₊) at 0.8 HCPVI for the displacements at 900, 1,100 and 1,300 psia, respectively. The molar distribution of hydrocarbon components in water is barely visible due to extremely low solubility predicted by the Peng-Robinson EOS. The extraction of intermediate and heavy components by the gas phase is trivial. At 900 psia, the gas phase is capable of extracting small amounts of C₅ and C₆. Nearly all C₇₋₁₃ and heavier components remain in the oil phase, leaving the high oil saturation behind the displacement front. For the displacement at 1,100 psia, substantial amounts of C₅, C₆ and C₇₋₁₃ are extracted by the CO₂-rich liquid phase and the extraction becomes less efficient for heavier components. It is also observed that the CO₂-rich liquid phase extracts components more efficiently as pressure increases; however, the increment in the extraction is small. This explains that the oil recovery is improved marginally by an increase in pressure once the CO₂-rich liquid phase is generated.

Runs using 40 and 160 gridblocks for the one-dimensional displacement of the 312 SCF/BBL recombined Wasson oil by CO₂ are also performed to investigate the effect of grid size on the simulation results. Figs. 7-12 through 7-14 compare the calculated saturation profiles at 0.6 HCPVI for the displacements at 900, 1,100 and 1,300 psia. The results of simulations with different numbers of gridblocks are consistent with each other. At all pressures, numerical dispersion has been observed on the rate of advance of the displacement front. The effect of numerical dispersion at 1,100 psia is more considerable than that at 900 and 1,300 psia. Phase saturations in the trailing multiphase zone are less sensitive to the grid size. The ultimate recovery at 1.5 HCPVI slightly increases as more gridblocks are used in the simulation. At 900 psia, the 40-block run predicts 78.7% oil recovery compared with 79.07% for the 80-block run

and 79.34% for the 160-block run. At 1,100 psia, the 40-block run results in 90.4% oil recovery compared with 91.96% for the 80-block run and 93.19% for the 160-block run. At 1,300 psia, the 40-block run yields 91.88% oil recovery compared with 92.62% for the 80-block run and 93.33% for the 160-block run.

For the 602 SCF/BBL recombined Wasson oil, more gas is added to the dead oil in the recombination and results in higher contents of light hydrocarbon components (C_1 to C_4). Recovery factors for the displacement at different pressures are shown in Fig. 7-15. The displacement pressure of 700 psia results in 71.03% oil recovery at 1.5 HCPVI and higher recovery is achieved as pressure increases. However, the small slope in the recovery curves in Fig. 7-16 for pressures higher than 1,100 psia indicates that an increase in pressure improves little the displacement efficiency after a CO₂-rich liquid phase appears. At the same pressure, the displacement efficiency of the 602 SCF/BBL recombined Wasson oil is slightly higher than that of the run case using the 312 SCF/BBL recombined Wasson oil.

Figs. 7-17, 7-18 and 7-19 show the simulated saturation profiles at 0.8 HCPVI for the displacements of the 602 SCF/BBL recombined Wasson oil at 900, 1,100 and 1,300 psia, respectively. The simulated density profiles are given in Figs. 7-20, 7-21 and 7-22 for different pressures. It is seen that phase behaviors and density profiles of the 602 SCF/BBL recombined Wasson oil during the displacements are similar to those of the 312 SCF/BBL Wasson oil. A four-phase region is present in six gridblocks for the displacement at 1,100 psia. It occurs between a leading gas phase and a trailing CO₂-rich liquid phase. At lower pressures, a CO₂-rich liquid phase is not generated and three-phase oil-gas-aqueous equilibrium exists throughout the slim tube. For the displacements at 1,300 psia, a three-phase oil-gas-aqueous region travels ahead of a three-phase oil-2nd liquid-aqueous region. However, there is no four-phase region between

them. Even though the aqueous phase is immobile, a drop in water saturation in the injection blocks occurs at all pressures. As pressure increases, the drop becomes larger because more water transports to hydrocarbon phases. The phase identifications discussed above are confirmed by the mass density profiles in Figs. 7-20 through 7-22. An inversion of mass densities of the oil and second liquid phases is also observed in the injection block at 1,300 psia. Figs. 7-23, 7-24 and 7-25 show the molar distribution of intermediate and heavy components (C_5 , C_6 , C_{7-13} , C_{14-20} , C_{21-28} and C_{29+}) at 0.8 HCPVI the displacements at 900, 1,100 and 1,300 psia, respectively. The CO₂-rich liquid provides improved displacement efficiency by efficiently extracting significant amounts of C_5 , C_6 and C_{7-13} .

7.1.2 Displacement by Water-alternating-gas Injection

To demonstrate four-phase flow, the displacements of the two recombined Wasson oil by CO_2 at 1,100 psia studied in the last section are modified to water-alternating-gas (WAG) flooding. The same reservoir properties and relative permeabilites are used in the simulations but a different injection pattern is applied. Instead of pure CO_2 , water and CO_2 slugs are injected alternately into the slim tube at a constant injection rate of 0.001125 ft³ (equivalent to 0.1 pore volume or 0.125 hydrocarbon pore volume) per day for three cycles. Each cycle contains a period of two-day CO_2 injection followed by a period of two-day water injection. In this case, four phases, oil, gas, 2^{nd} liquid and water are flowing simultaneously.

Fig. 7-26 compares the oil recoveries of the one-dimensional displacements of the 312 SCF/BBL Wasson oil at 1,100 psia by pure CO_2 and WAG. Because water is less compressible than the CO_2 -rich liquid, the injected water in the WAG flooding induces a larger pressure gradient which leads to earlier breakthrough. Consequently, the WAG flooding recovers a bit more oil than CO_2 flooding does before 1.1 HCPVI. However, the ultimate oil recoveries of both

processes are the same because the sweep efficiency of one-dimensional simulations is not affected by the water injection.

Fig. 7-27 shows the saturation profiles for the displacement of the 312 SCF/BBL recombined Wasson oil at 0.5 HCPVI which corresponds to the end of the first cycle. The injected CO₂ slug develops a leading gas bank at the displacement front and a narrow four-phase oil-gas- 2^{nd} liquid-water region behind it. The four-phase occurs in four gridblocks and is followed by a water slug flowing together with the oil and CO₂-rich liquid phases. As the second cycle starts, another slug of CO₂ is injected into the slim tube, causing an increase in the saturation of the CO₂-rich liquid phase. The water slug is then pushed forward and travels ahead of the gas bank. As shown in Fig. 7-28 for the saturation profiles at the second slug of CO₂ injected (0.75 HCPVI), a water-oil region exists at the displacement front and the water is about to break through. Behind the water front, the flow patterns remain the same. By the end of the second cycle, all the phases have broken through. The four-phase region moves towards the production block. Following the four-phase region, slugs of the CO₂-rich liquid and water can be clearly seen in Fig. 7-29.

The simulation of the displacement of the 602 SCF/BBL recombined Wasson oil by WAG is also carried out. Fig. 7-30 presents the oil recoveries of the CO₂-flooding and WAG flooding. Both processes yield the same ultimate displacement efficiency. Figs. 7-31, 7-32, 7-33 show the saturation profiles at 0.5, 0.75 and 1.0 HCPVI, respectively. Phase behaviors during the displacement are similar to those of the 312 SCF/BBL recombined Wasson oil but a larger leading gas bank is observed.

7.2 Two-Dimensional Cross-Sectional Displacement of Bob Slaughter Block Oil

Two-dimensional x-z cross-sectional simulations are performed for displacements of the Bob Slaughter Block (BSB) oil by CO₂ injection. A seven-component fluid characterization provided by Khan et al. (1992) is used to represent the reservoir oil. Component properties and the initial overall composition are given in Table 7-4. Phase densities and phase behaviors are modelled by the Peng-Robinson EOS. Input data for reservoir properties are presented in Table 7-5. The initial reservoir temperature is 105°F at which the CO₂/BSB oil mixture exhibits threehydrocarbon-phase equilibrium in a small pressure range above 1,100 psia. The reservoir is discretized into $30 \times 1 \times 10$ equal gridblocks with the size of $20 \times 20 \times 2$ ft³ as shown in Fig. 7-34. Corey's model is used to calculate phase relative permeabilities, with the parameters provided by Dria et al. (1990). The gravity effect is taken into account in this case and reservoir pressure is initialized using the method described in Section 5.2. Pure CO₂ is injected at a constant surface rate of 5×10^4 SCF/day. A bottomhole pressure equal to the initial reservoir pressure is maintained in the producing well. Both the injector and the producer are multilayer wells parallel to the z-direction and Fig. 7-34 shows the location and completion of each well. The amount of CO₂ injected into each layer is determined by the mobility allocation method.

Fig. 7-35 shows the oil recoveries for the displacements at two different pressures 700 and 1,100 psia. The displacement pressure of 1,100 psia results in a high recovery factor of 74.22% at 1.2 HCPVI while the displacement at 700 psia recovers 62.71% oil at the same pore volume of CO_2 injected.

Figs. 7-36 through 7-39 show the pressure profiles and saturation profiles of the oil, gas, and 2^{nd} liquid phases at 0.3, 0.6 and 1.2 HCPVI for the displacement at 700 psia. A gas phase is developed as a result of the injected CO₂ behind the displacement front. At 0.3 HCPVI, a CO₂-

rich liquid phase is generated and coexists with the oil, gas and water phases at equilibrium because of initial pressure built-up. As production continues, the reservoir pressure gradually drops out of the three-hydrocarbon-phase region. Consequently, the CO₂-rich liquid phase vanishes and three-phase oil-gas-water equilibrium is observed at 0.6 HCPVI. Because the gas is less dense than the oil it is displacing, gravity override occurs and leaves the high oil saturation in the bottom of the formation. Molar distributions of intermediate and heavy components (C₄₋₆, C₇₋₁₅, C₁₆₋₂₇ and C₂₈₊) at 0.6 HCPVI are shown in Fig. 7-40. It is seen that only a small amount of C₄₋₆ presents in the gas phase while C₇₋₁₅ and heavier components mainly stay in the oil phase.

For the displacement at 1,100 psia, Figs. 7-41 through 7-44 show the simulated pressure profiles and saturation profiles of the oil, gas, and 2^{nd} liquid phases at 0.3, 0.6 and 1.2 HCPVI. A four-phase oil- 2^{nd} liquid-gas-water region is detected in a few gridblocks between a leading gas phase at the displacement front and a trailing CO₂-rich liquid phase. A late breakthrough is obtained compared to the displacement at 700 psia. Gravity override is also observed but the dense CO₂-rich liquid phase improves vertical sweep efficiency and makes the bypassed zone smaller. Fig. 7-45 gives molar distributions of C₄₋₆, C₇₋₁₅, C₁₆₋₂₇ and C₂₈₊ at 0.6 HCPVI. The CO₂-rich liquid phase extracts these components more efficiently than the gas phase does. The extraction successfully reduces the residual oil saturation and contributes to the oil recovery.

The two-dimensional simulation results of CO_2 -flooding demonstrate that the formation of a CO_2 -rich liquid phase at 1,100 psia significantly increases the recovery factor by efficiently extracting oil components, improving vertical sweep efficiency and leading late breakthrough. Even though a CO_2 -rich liquid phase is also observed at 700 pisa at an early stage, the reservoir pressure is not maintained high enough to keep the phase in place throughout production.

	Gas	Dead Oil	Dead Oil + 312 SCF/BBL	Dead Oil + 602 SCF/BBL
C_1	0.5736	-	0.2151	0.3080
C_2	0.1989	-	0.0746	0.1068
C ₃	0.1629	-	0.0611	0.0875
C_4	0.0646	-	0.0242	0.0347
C_5	-	0.0548	0.0343	0.0254
C_6	-	0.0537	0.0360	0.0249
C ₇₋₁₃	-	0.4805	0.3000	0.2224
C14-20	-	0.1704	0.1066	0.0788
C ₂₁₋₂₈	-	0.0884	0.0552	0.0410
C ₂₉₊	_	0.1522	0.0953	0.0705

 Table 7-1 Wasson oil composition (Nghiem and Li, 1986)

	p_c (psia)	T_c (°F)	v_c (ft ³ /lbmol)	mw	ω
C1	667.1960	-116.59	1.585855	16.043	0.008
C_2	708.3447	90.05	2.370773	30.07	0.098
C ₃	615.7603	205.97	3.251803	44.097	0.152
C_4	551.0981	305.69	4.084778	58.124	0.193
C ₅	489.3751	385.61	4.869696	72.151	0.251
C_6	477.0305	453.83	5.510445	86.178	0.2637
C ₇₋₁₃	384.5930	632.03	7.833163	125.96	0.3912
C14-20	248.2146	872.33	13.64796	227.86	0.63
C ₂₁₋₂₈	181.3480	1022.81	18.91813	325.56	0.8804
C ₂₉₊	116.9798	1206.95	28.22501	484.7	1.2457
CO_2	1069.865	87.89	1.505761	44.01	0.2250
H_2O	3197.84	705.47	0.8971	18.015	0.344

 Table 7-2 Component properties for the one-dimensional Wasson oil displacement

	C_1	C_2	C ₃	C_4	C ₅	C_6	C ₇₋₁₃	C ₁₄₋₂₀	C ₂₁₋₂₈	C ₂₉₊	CO_2	H ₂ O
C ₁	0.0	0.003	0.009	0.015	0.021	0.025	0.041	0.073	0.095	0.125	0.103	0.491
C_2	0.003	0.0	0.002	0.005	0.009	0.012	0.023	0.049	0.068	0.095	0.13	0.491
C ₃	0.009	0.002	0.0	0.001	0.003	0.005	0.013	0.033	0.05	0.073	0.135	0.547
C_4	0.015	0.005	0.001	0.0	0.001	0.001	0.007	0.024	0.038	0.059	0.13	0.508
C5	0.021	0.009	0.003	0.001	0.0	0.0	0.004	0.017	0.03	0.049	0.125	0.5
C ₆	0.025	0.012	0.005	0.001	0.0	0.0	0.002	0.014	0.025	0.043	0.125	0.45
C ₇₋₁₃	0.041	0.023	0.013	0.07	0.004	0.002	0.0	0.005	0.013	0.027	0.13	0.45
C14-20	0.073	0.049	0.033	0.024	0.017	0.014	0.005	0.0	0.002	0.009	0.13	0.45
C21-28	0.095	0.068	0.05	0.038	0.03	0.025	0.013	0.002	0.0	0.003	0.13	0.45
C ₂₉₊	0.125	0.095	0.073	0.059	0.049	0.043	0.027	0.009	0.003	0.0	0.13	0.45
$\rm CO_2$	0.103	0.13	0.135	0.13	0.125	0.125	0.13	0.13	0.13	0.13	0.0	0.2
H_2O	0.491	0.491	0.547	0.508	0.5	0.45	0.45	0.45	0.45	0.45	0.2	0.0

Dimensions (ft)				
Length ×Width ×Thickness	60×0.025×0.025			
Grid Number				
$n_x \times n_y \times n_z$	80×1×1			
Grid Size (ft)				
dx dy dz	0.75 0.025 0.025			
Permeability (md)	1000			
Relative Permeability Model	Corey			
Endpoint $k_{ro}^o k_{rg}^o k_{rl}^o k_{rw}^o$	0.574 0.278 0.278 0.365			
Residual saturation $s_{or} s_{gr} s_{lr} s_{wr}$	0.16 0.0 0.0 0.2			
Exponent $e_o e_g e_l e_w$	3.0 6.89 6.89 2.7			
Porosity	0.3			
Rock Compressibility (psi ⁻¹)	0.0			
Initial Temperature (°F)	90			
Initial Pressure (psia)	700, 900,1100,1300,1500			
Injected Composition				
$C_1 C_2 C_3 C_4 C_5 C_6$	$0.0 \ 0.0 \ 0.0 \ 0.0 \ 0.0 \ 0.0$			
$C_{713} C_{1420} C_{2128} C_{29\text{+}} CO_2$	$0.0 \ 0.0 \ 0.0 \ 0.0 \ 1.0$			
Injection Rate (ft ³ /day)	0.001125			
Production Pressure (psia)	Initial pressure			
Final Time (day)	12			

Table 7-3 Summary of reservoir properties for the one-dimensional Wasson oil displacement

	p_c (psia)	T_c (°F)	v_c (ft ³ /lbmol)	mw	ω	Z _m
CO ₂	1069.8651	87.8900	1.5057	44.0100	0.225	0.0337
C_1	667.1961	-171.6700	1.5858	16.0430	0.008	0.0861
C ₂₋₃	652.5573	159.8985	2.9016	37.2002	0.1305	0.1531
C ₄₋₆	493.0660	374.1298	4.9137	69.4984	0.2404	0.1671
C7-15	315.4380	630.6844	9.0000	140.9560	0.6177	0.3304
C ₁₆₋₂₇	239.8969	892.1640	17.1000	280.9914	0.9566	0.1661
C_{28+}	238.1210	1236.7920	32.5000	519.6219	1.2683	0.0713
H ₂ O	3197.84	705.47	0.8971	18.015	0.344	

Table 7-4 Component properties for the two-dimensional BSB Oil displacement (Khan
et al., 1992)

	CO ₂	C_1	C ₂₋₃	C4-6	C7-15	C16-27	C ₂₈₊	H ₂ O
CO ₂	0.0	0.055	0.055	0.055	0.105	0.105	0.105	0.2
\mathbf{C}_1	0.055	0.0	0.0	0.0	0.0	0.0	0.0	0.491
C ₂₋₃	0.055	0.0	0.0	0.0	0.0	0.0	0.0	0.547
C ₄₋₆	0.055	0.0	0.0	0.0	0.0	0.0	0.0	0.5
C ₇₋₁₅	0.105	0.0	0.0	0.0	0.0	0.0	0.0	0.45
C ₁₆₋₂₇	0.105	0.0	0.0	0.0	0.0	0.0	0.0	0.45
C ₂₈₊	0.105	0.0	0.0	0.0	0.0	0.0	0.0	0.45
H ₂ O	0.2	0.491	0.547	0.5	0.45	0.45	0.45	0.0

Dimensions (ft)			
Length×Width×Thickness 60			
Grid Number			
$n_x \times n_y \times n_z$	30×1×10		
Grid Size (ft)			
dx dy dz	20 20 2		
Datum (ft)	975		
Permeability (md)			
$K_x K_y K_z$	500 500 100		
Relative Permeability Model	Corey		
Endpoint k_{ro}^{o} k_{rg}^{o} k_{rl}^{o} k_{rw}^{o}	0.574 0.278 0.278 0.365		
Residual saturation $s_{or} s_{gr} s_{lr} s_{wr}$	0.16 0.0 0.0 0.2		
Exponent $e_o e_g e_l e_w$	3.0 6.89 6.89 2.7		
Porosity	0.3		
Rock Compressibility (psi ⁻¹)	5×10 ⁻⁶		
Initial Temperature (°F)	105		
Initial Pressure (psia)	700,1100		
Initial Water Saturation	0.2		
Injected Composition			
CO ₂ C ₁ C ₂₋₃ C ₄₋₆ C ₇₋₁₅	1.0 0.0 0.0 0.0 0.0		
C ₁₆₋₂₇ C ₂₈₊	0.0 0.0		
Injection Rate (SCF/day)	5×10 ⁴		
Production Pressure (psia)	Initial pressure		
Final Time (day)	200		

Table 7-5 Summary of reservoir properties for the two-dimensional BSB oil displacement



Figure 7-1 Comparison of recovery factors at different initial pressures for the onedimensional 312 SCF/BBL recombined Wasson oil displacement by CO₂



Figure 7-2 Comparison of recovery factors at different HCPVI for the one-dimensional 312 SCF/BBL recombined Wasson oil displacement by CO₂



Figure 7-3 Saturation profiles at 0.8 HCPVI and 900 psia for the one-dimensional 312 SCF/BBL recombined Wasson oil displacement by CO₂



Figure 7-4 Saturation profiles at 0.8 HCPVI and 1,100 psia for the one-dimensional 312 SCF/BBL recombined Wasson oil displacement by CO₂



Figure 7-5 Saturation profiles at 0.8 HCPVI and 1,300 psia for the one-dimensional 312 SCF/BBL recombined Wasson oil displacement by CO₂



Figure 7-6 Mass density profiles at 0.8 HCPVI and 900 psia for the one-dimensional 312 SCF/BBL recombined Wasson oil displacement by CO₂



Figure 7-7 Mass density profiles at 0.8 HCPVI and 1,100 psia for the one-dimensional 312 SCF/BBL recombined Wasson oil displacement by CO₂



Figure 7-8 Mass density profiles at 0.8 HCPVI and 1,300 psia for the one-dimensional 312 SCF/BBL recombined Wasson oil displacement by CO₂



Figure 7-9a C₅ distribution at 0.8 HCPVI and 900 psia for the one-dimensional 312 SCF/BBL recombined Wasson oil displacement by CO₂



Figure 7-9b C₆ distribution at 0.8 HCPVI and 900 psia for the one-dimensional 312 SCF/BBL recombined Wasson oil displacement by CO₂



Figure 7-9c C₇₋₁₃ distribution at 0.8 HCPVI and 900 psia for the one-dimensional 312 SCF/BBL recombined Wasson oil displacement by CO₂



Figure 7-9d C₁₄₋₂₀ distribution at 0.8 HCPVI and 900 psia for the one-dimensional 312 SCF/BBL recombined Wasson oil displacement by CO₂



Figure 7-9e C₂₁₋₂₈ distribution at 0.8 HCPVI and 900 psia for the one-dimensional 312 SCF/BBL recombined Wasson oil displacement by CO₂



Figure 7-9f C₂₉₊ distribution at 0.8 HCPVI and 900 psia for the one-dimensional 312 SCF/BBL recombined Wasson oil displacement by CO₂


Figure 7-10a C₅ distribution at 0.8 HCPVI and 1,100 psia for the one-dimensional 312 SCF/BBL recombined Wasson oil displacement by CO₂



Figure 7-10b C₆ distribution at 0.8 HCPVI and 1,100 psia for the one-dimensional 312 SCF/BBL recombined Wasson oil displacement by CO₂



Figure 7-10c C₇₋₁₃ distribution at 0.8 HCPVI and 1,100 psia for the one-dimensional 312 SCF/BBL recombined Wasson oil displacement by CO₂



Figure 7-10d C₁₄₋₂₀ distribution at 0.8 HCPVI and 1,100 psia for the one-dimensional 312 SCF/BBL recombined Wasson oil displacement by CO₂



Figure 7-10e C₂₁₋₂₈ distribution at 0.8 HCPVI and 1,100 psia for the one-dimensional 312 SCF/BBL recombined Wasson oil displacement by CO₂



Figure 7-10f C₂₉₊ distribution at 0.8 HCPVI and 1,100 psia for the one-dimensional 312 SCF/BBL recombined Wasson oil displacement by CO₂



Figure 7-11a C₅ distribution at 0.8 HCPVI and 1,300 psia for the one-dimensional 312 SCF/BBL recombined Wasson oil displacement by CO₂



Figure 7-11b C₆ distribution at 0.8 HCPVI and 1,300 psia for the one-dimensional 312 SCF/BBL recombined Wasson oil displacement by CO₂



Figure 7-11c C₇₋₁₃ distribution at 0.8 HCPVI and 1,300 psia for the one-dimensional 312 SCF/BBL recombined Wasson oil displacement by CO₂



Figure 7-11d C₁₄₋₂₀ distribution at 0.8 HCPVI and 1,300 psia for the one-dimensional 312 SCF/BBL recombined Wasson oil displacement by CO₂



Figure 7-11e C₂₁₋₂₈ distribution at 0.8 HCPVI and 1,300 psia for the one-dimensional 312 SCF/BBL recombined Wasson oil displacement by CO₂



Figure 7-11f C₂₉₊ distribution at 0.8 HCPVI and 1,300 psia for the one-dimensional 312 SCF/BBL recombined Wasson oil displacement by CO₂



Figure 7-12 Comparison of saturation profiles calculated using different number of grid blocks at 0.6 HCPVI and 900 psia for the one-dimensional 312 SCF/BBL recombined Wasson oil displacement by CO₂



Figure 7-13 Comparison of saturation profiles calculated using different number of grid blocks at 0.6 HCPVI and 1,100 psia for the one-dimensional 312 SCF/BBL recombined Wasson oil displacement by CO₂



Figure 7-14 Comparison of saturation profiles calculated using different number of grid blocks at 0.6 HCPVI and 1,300 psia for the one-dimensional 312 SCF/BBL recombined Wasson oil displacement by CO₂



Figure 7-15 Comparison of recovery factors at different initial pressures for the onedimensional 602 SCF/BBL recombined Wasson oil displacement by CO₂



Figure 7-16 Comparison of recovery factors at different HCPVI for the one-dimensional 602 SCF/BBL recombined Wasson oil displacement by CO₂



Figure 7-17 Saturation profiles at 0.8 HCPVI and 900 psia for the one-dimensional 602 SCF/BBL recombined Wasson oil displacement by CO₂



Figure 7-18 Saturation profiles at 0.8 HCPVI and 1,100 psia for the one-dimensional 602 SCF/BBL recombined Wasson oil displacement by CO₂



Figure 7-19 Saturation profiles at 0.8 HCPVI and 1,300 psia for the one-dimensional 602 SCF/BBL recombined Wasson oil displacement by CO₂



Figure 7-20 Mass density profiles at 0.8 HCPVI and 900 psia for the one-dimensional 602 SCF/BBL recombined Wasson oil displacement by CO₂



Figure 7-21 Mass density profiles at 0.8 HCPVI and 1,100 psia for the one-dimensional 602 SCF/BBL recombined Wasson oil displacement by CO₂



Figure 7-22 Mass density profiles at 0.8 HCPVI and 1,300 psia for the one-dimensional 602 SCF/BBL recombined Wasson oil displacement by CO₂



Figure 7-23a C₅ distribution at 0.8 HCPVI and 900 psia for the one-dimensional 602 SCF/BBL recombined Wasson oil displacement by CO₂



Figure 7-23b C₆ distribution at 0.8 HCPVI and 900 psia for the one-dimensional 602 SCF/BBL recombined Wasson oil displacement by CO₂



Figure 7-23c C₇₋₁₃ distribution at 0.8 HCPVI and 900 psia for the one-dimensional 602 SCF/BBL recombined Wasson oil displacement by CO₂



Figure 7-23d C₁₄₋₂₀ distribution at 0.8 HCPVI and 900 psia for the one-dimensional 602 SCF/BBL recombined Wasson oil displacement by CO₂



Figure 7-23e C₂₁₋₂₈ distribution at 0.8 HCPVI and 900 psia for the one-dimensional 602 SCF/BBL recombined Wasson oil displacement by CO₂



Figure 7-23f C₂₉₊ distribution at 0.8 HCPVI and 900 psia for the one-dimensional 602 SCF/BBL recombined Wasson oil displacement by CO₂



Figure 7-24a C₅ distribution at 0.8 HCPVI and 1,100 psia for the one-dimensional 602 SCF/BBL recombined Wasson oil displacement by CO₂



Figure 7-24b C₆ distribution at 0.8 HCPVI and 1,100 psia for the one-dimensional 602 SCF/BBL recombined Wasson oil displacement by CO₂



Figure 7-24c C₇₋₁₃ distribution at 0.8 HCPVI and 1,100 psia for the one-dimensional 602 SCF/BBL recombined Wasson oil displacement by CO₂



Figure 7-24d C₁₄₋₂₀ distribution at 0.8 HCPVI and 1,100 psia for the one-dimensional 602 SCF/BBL recombined Wasson oil displacement by CO₂



Figure 7-24e C₂₁₋₂₈ distribution at 0.8 HCPVI and 1,100 psia for the one-dimensional 602 SCF/BBL recombined Wasson oil displacement by CO₂



Figure 7-24f C₂₉₊ distribution at 0.8 HCPVI and 1,100 psia for the one-dimensional 602 SCF/BBL recombined Wasson oil displacement by CO₂



Figure 7-25a C₅ distribution at 0.8 HCPVI and 1,300 psia for the one-dimensional 602 SCF/BBL recombined Wasson oil displacement by CO₂



Figure 7-25b C₆ distribution at 0.8 HCPVI and 1,300 psia for the one-dimensional 602 SCF/BBL recombined Wasson oil displacement by CO₂



Figure 7-25c C₇₋₁₃ distribution at 0.8 HCPVI and 1,300 psia for the one-dimensional 602 SCF/BBL recombined Wasson oil displacement by CO₂



Figure 7-25d C₁₄₋₂₀ distribution at 0.8 HCPVI and 1,300 psia for the one-dimensional 602 SCF/BBL recombined Wasson oil displacement by CO₂



Figure 7-25e C₂₁₋₂₈ distribution at 0.8 HCPVI and 1,300 psia for the one-dimensional 602 SCF/BBL recombined Wasson oil displacement by CO₂



Figure 7-25f C₂₉₊ distribution at 0.8 HCPVI and 1,300 psia for the one-dimensional 602 SCF/BBL recombined Wasson oil displacement by CO₂



Figure 7-26 Oil recovery for the one-dimensional 312 SCF/BBL recombined Wasson oil displacement by WAG



Figure 7-27 Saturation profiles at 0.5 HCPVI and 1,100 psia for the one-dimensional 312 SCF/BBL recombined Wasson oil displacement by WAG



Figure 7-28 Saturation profiles at 0.75 HCPVI and 1,100 psia for the one-dimensional 312 SCF/BBL recombined Wasson oil displacement by WAG



Figure 7-29 Saturation profiles at 1.0 HCPVI and 1,100 psia for the one-dimensional 312 SCF/BBL recombined Wasson oil displacement by WAG



Figure 7-30 Oil recovery for the one-dimensional 602 SCF/BBL recombined Wasson oil displacement by WAG



Figure 7-31 Saturation profiles at 0.5 HCPVI and 1,100 psia for the one-dimensional 602 SCF/BBL recombined Wasson oil displacement by WAG



Figure 7-32 Saturation profiles at 0.75 HCPVI and 1,100 psia for the one-dimensional 602 SCF/BBL recombined Wasson oil displacement by WAG



Figure 7-33 Saturation profiles at 1.0 HCPVI and 1,100 psia for the one-dimensional 602 SCF/BBL recombined Wasson oil displacement by WAG



Figure 7-34 Discretized gridblocks and well locations for for the two-dimensional BSB oil displacement by CO₂



Figure 7-35 Oil recovery for the two-dimensional BSB oil displacement







Figure 7-37 Oil saturation profiles for the two-dimensional BSB oil displacement by CO₂ at 700 psia



Figure 7-38 Gas saturation profiles for the two-dimensional BSB oil displacement by CO₂ at 700 psia



Figure 7-39 The 2nd Liquid saturation profiles for the two-dimensional BSB oil displacement by CO₂ at 700 psia



Figure 7-40a C₄₋₆ distribution at 0.6 HCPVI for the two-dimensional BSB oil displacement by CO₂ at 700 psia



Figure 7-40b C₇₋₁₅ distribution at 0.6 HCPVI for the two-dimensional BSB oil displacement by CO₂ at 700 psia



Figure 7-40c C₁₆₋₂₇ distribution at 0.6 HCPVI for the two-dimensional BSB oil displacement by CO₂ at 700 psia



Figure 7-40d C₂₈₊ distribution at 0.6 HCPVI for the two-dimensional BSB oil displacement by CO₂ at 700 psia



Figure 7-41 Pressure profiles for the two-dimensional BSB oil displacement by CO₂ at 1,100 psia


Figure 7-42 Oil saturation profiles for the two-dimensional BSB oil displacement by CO₂ at 1,100 psia



Figure 7-43 Gas saturation profiles for the two-dimensional BSB oil displacement by CO₂ at 1,100 psia



Figure 7-44 The 2nd Liquid saturation profiles for the two-dimensional BSB oil displacement by CO₂ at 1,100 psia



Figure 7-45a C₄₋₆ distribution at 0.6 HCPVI for the two-dimensional BSB oil displacement by CO₂ at 1,100 psia



Figure 7-45b C₇₋₁₅ distribution at 0.6 HCPVI for the two-dimensional BSB oil displacement by CO₂ at 1,100 psia



Figure 7-45c C₁₆₋₂₇ distribution at 0.6 HCPVI for the two-dimensional BSB oil displacement by CO₂ at 1,100 psia



Figure 7-45d C₂₈₊ distribution at 0.6 HCPVI for the two-dimensional BSB oil displacement by CO₂ at 1,100 psia

Chapter Eight: Conclusions and Recommendations

In this chapter, the conclusions drawn from this work and recommendation for future studies are presented.

8.1 Conclusions

In this work, a new three-dimensional equation-of-state isothermal compositional reservoir simulator has been developed on the basis of a generalized mathematical formulation derived from the law of mass conservation and the second law of thermodynamics. The simulator is incorporated with a robust multiphase equilibrium calculation routine that sequentially applies a stability analysis and phase split calculation. Both the simulator and the phase equilibrium calculation routine are designed to solve problems of multiphase flow and complex phase behaviors for CO₂ and rich-gas injection processes. A maximum of four phases (oil, gas, 2nd liquid and water) that commonly occurs in the recovery processes of interest is assumed. In the formulations of compositional flow and phase equilibrium, water is considered as a component rather than an independent phase and components are allowed to partition into all phases existing in the system as far as the thermodynamic equilibrium conditions are satisfied. Either the Peng-Robinson EOS or the Soave-Redlich-Kwong EOS can be selected to model the phase behaviors and densities of all the phases.

The multiphase equilibrium calculation routine has been validated with CMG WinProp and excellent agreements have been obtained for different mixtures and various types of phase equilibrium including, but not limited to oil-gas-water, oil-gas-2nd liquid-water and oil-2nd liquid-water. It is also seen that in addition to forming an aqueous phase, the introduction of water to the system in multiphase equilibrium calculation not only shifts the multiple hydrocarbon phase region to lower pressures but also expands the multiple hydrocarbon phase region to a wider

pressure range for certain mixtures. Simulations of slim tube methane injection and the SPE Third Comparative Solution Project have been carried out to verify the four-phase simulator developed for one-dimensional and three-dimensional problems with two hydrocarbon phases at equilibrium. Both saturation profiles and production data obtained from this work are compared with those of CMG-GEM. Our simulator presents a satisfactory range of accuracy agreeable with CMG-GEM in the simulation results.

The simulator has been used to investigate complex phase behaviors and flow mechanisms in CO_2 injection processes. One-dimensional displacements of the two recombined Wasson oil and two-dimensional displacements of the Bob Slaughter Block oil are studied. Different types of phase equilibria and flow conditions have been observed in the simulation results. Waterhydrocarbon mutual solubilities and the effect of the water component on phase behavior are taken into account in the simulations. High displacement efficiency is obtained as a result of the formation of a CO_2 -rich liquid phase that efficiently extracts hydrocarbon components from the reservoir oil. The extraction becomes more efficient as pressure increases. The dense CO2-rich liquid phase also improves sweep efficiency of the process and leads late breakthrough. These aspects also contribute to the high recovery factor attained. Therefore, in order to achieve high oil recovery of CO_2 injection processes, reservoir pressure should be maintained at a certain level that keeps the CO_2 -rich liquid phase in place throughout production.

8.2 Recommendations

1. Due to the stability issues of the IMPES solution scheme, the time step is required to satisfy the CFL condition; otherwise, the simulation will produce incorrect results. To enable the usage of a large time step during simulations, a more stable solution scheme such as fully implicit or adaptive-implicit should be implemented. Implicit treatments of well models are also recommended.

- 2. In order to simulate thermal processes, an energy balance equation should be formulated and solved together with component flow equations to allow temperature variance in a reservoir.
- 3. More accurate thermodynamic models, such as Henry's law constants and the cubic-plusassociation (CPA) equation of state, should be incorporated to calculate the solubility of solutes in the aqueous phase. Modification and tuning of EOS parameters should be performed to match experimental data.
- 4. The formation and deposition of solid-like asphaltene is an important problem in production. To model the asphaltene precipitation, additional equations that describe asphaltene deposition and plugging in reservoirs and thermodynamic models for the solid phase behavior should be introduced to the system (Nghiem, 1999).
- 5. To enhance the computational efficiency, parallel computation can be applied to phase equilibrium and physical properties calculation. Development and implementation of more efficient algorithms for multiphase equilibrium calculation are also desirable.
- 6. Further research on four-phase relative permeabilities should be conducted.

Appendix A: Derivatives of Fugacity and Compressibility Factor

When solving phase equilibrium equations and component flow equations by the Newton-Raphson method, it is required to construct a Jacobian matrix which involves the calculation of partial derivatives of the component fugacities and compressibility factors of each phase. In this appendix, the analytical expressions of the required partial derivatives with respect to pressure and composition are presented. The partial derivatives with respect to the component mole number in the phase per unit bulk volume can be calculated using

$$\frac{\partial}{\partial n_{m\alpha}} = \sum_{n=1}^{n_c} \frac{\partial x_{n\alpha}}{\partial n_{m\alpha}} \frac{\partial}{\partial x_{n\alpha}}$$
 A-1

where

$$x_{n\alpha} = \frac{n_{n\alpha}}{n_{\alpha}} = \frac{n_{n\alpha}}{\sum_{i=1}^{n_c} n_{i\alpha}}$$

and

$$\frac{\partial x_{n\alpha}}{\partial n_{m\alpha}} = \frac{\delta_{nm} - x_{n\alpha}}{n_{\alpha}}$$
 A-2

In Chapter Four, the Soave-Redlich-Kwong (SRK) EOS and the Peng-Robinson (PR) EOS are described for the representation of volumetric, thermodynamic, and phase equilibrium properties. Both EOSs can be written in terms of the compressibility factor as the following general expression:

$$Z_{\alpha}^{3} + c_{2}Z_{\alpha}^{2} + c_{1}Z_{\alpha} + c_{0} = 0$$
 A-3

where α is the phase index and c_0 , c_1 and c_2 are the cubic equation coefficients related to the EOS parameters A_{α} and B_{α} . For the SRK EOS

$$\begin{cases} c_0 = -A_\alpha B_\alpha \\ c_1 = (A_\alpha - B_\alpha + B_\alpha^2) \\ c_2 = -1 \end{cases}$$

and for the PR EOS

$$\begin{cases} c_0 = -(A_{\alpha}B_{\alpha} - B_{\alpha}^2 - B_{\alpha}^3) \\ c_1 = (A_{\alpha} - 2B_{\alpha} - 3B_{\alpha}^2) \\ c_2 = -(1 - B_{\alpha}) \end{cases}$$

To simplify the notation, the subscript α is dropped from the following equations.

A.1 Derivatives of Equation of State Parameters

- Partial derivatives of the attraction parameter *a*
 - with respect to pressure

$$\frac{\partial a}{\partial p} = 0$$
 A-4

- with respect to phase composition

$$\frac{\partial a}{\partial x_m} = 2\sqrt{a_m} \sum_{n=1}^{n_c} x_n (1 - \kappa_{mn}) \sqrt{a_n}$$
 A-5

- Partial derivatives of the co-volume parameter *b*
 - with respect to pressure

$$\frac{\partial b}{\partial p} = 0$$
 A-6

- with respect to phase composition

$$\frac{\partial b}{\partial x_m} = b_m \tag{A-7}$$

- Partial derivatives of the EOS parameter *A*
 - with respect to pressure

$$\frac{\partial A}{\partial p} = \frac{a}{R^2 T^2}$$
 A-8

- with respect to phase composition

$$\frac{\partial A}{\partial x_m} = \frac{p}{R^2 T^2} \frac{\partial a}{\partial x_m}$$
 A-9

- Partial derivatives of the EOS parameter *B*
 - with respect to pressure

$$\frac{\partial B}{\partial p} = \frac{b}{RT}$$
 A-10

- with respect to phase composition

$$\frac{\partial B}{\partial x_m} = \frac{p}{RT} \frac{\partial b}{\partial x_m}$$
A-11

A.2 Derivatives of Compressibility Factor

Based on the derivatives of EOS parameters, the derivatives of compressibility are obtained using implicit differentiation

$$\frac{\partial Z}{\partial p} = -\frac{\frac{\partial c_2}{\partial p}Z^2 + \frac{\partial c_1}{\partial p}Z + \frac{\partial c_0}{\partial p}}{3Z^2 + 2c_2Z + c_1}$$
 A-12

and

$$\frac{\partial Z}{\partial x_m} = -\frac{\frac{\partial c_2}{\partial x_m} Z^2 + \frac{\partial c_1}{\partial x_m} Z + \frac{\partial c_0}{\partial x_m}}{3Z^2 + 2c_2 Z + c_1}$$
A-13

A.3 Derivatives of Component Fugacity

The partial derivatives of the fugacity of component m are given by

$$\frac{\partial f_m}{\partial p} = x_m \varphi_m + x_m p \frac{\partial \varphi_m}{\partial p}$$
 A-14

and

$$\frac{\partial f_m}{\partial x_n} = \delta_{mn} p \varphi_m + x_m p \frac{\partial \varphi_m}{\partial x_n}$$
 A-15

In Eqs. A-14 and A-15, the partial derivatives of the fugacity coefficient of component m with respect to pressure and composition for the SRK EOS can be evaluated from the following equations:

$$\frac{1}{\varphi_m} \frac{\partial \varphi_m}{\partial p} = \frac{b_m}{b} \frac{\partial Z}{\partial p} - \frac{1}{Z - B} \left(\frac{\partial Z}{\partial p} - \frac{\partial B}{\partial p} \right)$$

$$- \left(\frac{1}{a} \frac{\partial a}{\partial x_m} - \frac{b_m}{b} \right) \left[\left(\frac{1}{B} \frac{\partial A}{\partial p} - \frac{A}{B^2} \frac{\partial B}{\partial p} \right) \ln \left(1 + \frac{B_\alpha}{Z_\alpha} \right) + \frac{A}{B} \left(\frac{\frac{\partial Z}{\partial p} + \frac{\partial B}{\partial p}}{Z + B} - \frac{\frac{\partial Z}{\partial p}}{Z} \right) \right]$$
A-16

and

$$\frac{1}{\varphi_m} \frac{\partial \varphi_m}{\partial x_n} = \left[\frac{b_m}{b} \frac{\partial Z}{\partial x_n} - \frac{b_m}{b^2} (Z - 1) \frac{\partial b}{\partial x_n}\right] - \frac{1}{Z - B} \left(\frac{\partial Z}{\partial x_n} - \frac{\partial B}{\partial x_n}\right)$$
$$- \frac{1}{2\sqrt{2}} \left(\frac{1}{a} \frac{\partial a}{\partial x_m} - \frac{b_m}{b}\right) \left[\left(\frac{1}{B} \frac{\partial A}{\partial x_n} - \frac{A}{B^2} \frac{\partial B}{\partial x_n}\right) \ln \left(\frac{Z + (1 + \sqrt{2})B}{Z + (1 - \sqrt{2})B}\right) + \frac{A}{B} \left(\frac{\frac{\partial Z}{\partial p} + \frac{\partial B}{\partial p}}{Z + B} - \frac{\frac{\partial Z}{\partial p}}{Z}\right) \right] \quad A-17$$
$$- \frac{A}{2\sqrt{2}B} \ln \left(1 + \frac{B_a}{Z_a}\right) \left[-\frac{1}{a^2} \frac{\partial a}{\partial x_m} \frac{\partial a}{\partial x_n} + \frac{2}{a} (1 - \kappa_{mn}) \sqrt{a_m a_n} - \frac{b_m}{b^2} \frac{\partial b}{\partial x_n} \right]$$

For the PR EOS, the partial derivatives of the fugacity coefficient of component m with respect to pressure and composition can be calculated using

$$\frac{1}{\varphi_m} \frac{\partial \varphi_m}{\partial p} = \frac{b_m}{b} \frac{\partial Z}{\partial p} - \frac{1}{Z - B} \left(\frac{\partial Z}{\partial p} - \frac{\partial B}{\partial p} \right)$$
$$- \frac{1}{2\sqrt{2}} \left(\frac{1}{a} \frac{\partial a}{\partial x_m} - \frac{b_m}{b} \right) \left[\left(\frac{1}{B} \frac{\partial A}{\partial p} - \frac{A}{B^2} \frac{\partial B}{\partial p} \right) \ln \left(\frac{Z + (1 + \sqrt{2})B}{Z + (1 - \sqrt{2})B} \right) + \frac{A}{B} \left(\frac{\partial Z/\partial p + (1 - \sqrt{2}) \partial B/\partial p}{Z + (1 + \sqrt{2})B} - \frac{\partial Z/\partial p + (1 + \sqrt{2}) \partial B/\partial p}{Z + (1 - \sqrt{2})B} \right) \right]$$

and

$$\frac{1}{\varphi_m} \frac{\partial \varphi_m}{\partial x_n} = \left[\frac{b_m}{b} \frac{\partial Z}{\partial x_n} - \frac{b_m}{b^2} (Z - 1) \frac{\partial b}{\partial x_n}\right] - \frac{1}{Z - B} \left(\frac{\partial Z}{\partial x_n} - \frac{\partial B}{\partial x_n}\right) - \frac{1}{2\sqrt{2}} \left(\frac{1}{a} \frac{\partial a}{\partial x_m} - \frac{b_m}{b}\right) \left[\left(\frac{1}{B} \frac{\partial A}{\partial x_n} - \frac{A}{B^2} \frac{\partial B}{\partial x_n}\right) \ln \left(\frac{Z + (1 + \sqrt{2})B}{Z + (1 - \sqrt{2})B}\right) + \frac{A}{B} \left(\frac{\partial Z/\partial x_n + (1 - \sqrt{2}) \frac{\partial B}{\partial x_n}}{Z + (1 + \sqrt{2})B} - \frac{\partial Z/\partial x_n + (1 + \sqrt{2}) \frac{\partial B}{\partial x_n}}{Z + (1 - \sqrt{2})B}\right) \right] - \frac{A}{2\sqrt{2B}} \ln \left(\frac{Z_a + (1 + \sqrt{2})B_a}{Z_a + (1 - \sqrt{2})B_a}\right) \left[-\frac{1}{a^2} \frac{\partial a}{\partial x_m} \frac{\partial a}{\partial x_n} + \frac{2}{a} (1 - \kappa_{mn}) \sqrt{a_m a_n} - \frac{b_m}{b^2} \frac{\partial b}{\partial x_n} \right]$$

Nomenclature

a(T)	attraction parameter in the EOS
a_m	attraction parameter of component m
Α	equation of state parameter
ACC _m	molar accumulation of component <i>m</i>
\mathcal{A}_{ξ}	perpendicular cross-sectional area between two gridblocks in ξ -direction
b	co-volume parameter in the EOS
b_m	co-volume parameter of component m
В	equation of state parameter
C _m	molar volume translation constant of component m
$C_{m\alpha}$	molar distribution of component m in phase α
C _{SW}	salt concentration
C_R	rock compressibility
cnt	number of connected gridblocks
D	depth
e_{lpha}	exponent of relative permeability function of phase α in modified Corey's Model
$f_{m\alpha}$	fugacity of component m in phase α
\vec{F}_p	primary equation set
\vec{F}_{S}	secondary equation set
$Flux_m$	molar flux of component m
Flux _{ma}	molar flux of component m carried by phase α
g	gravitational acceleration

G	molar Gibbs free energy
G_m^0	molar Gibbs free energy of component m in the standard state
J	Jacobian matrix
k _{rα}	relative permeability of phase α
$k_{r\alpha}^{o}$	endpoint relative permeability of phase α in modified Corey's Model
$k_{rlphaeta}$	relative permeability of phase α in the presence of phase β
K_{ξ}	absolute permeability in ξ -direction
K _{mα}	K-value of component m in phase α
L_{lpha}	mole fraction of phase α
mw_m	molecular weight of component m
mw_{lpha}	molecular weight of phase α
n_b	number of gridblocks
n _c	number of components
n _{hc}	number of non-water components
n_p	number of phases
n_m	total number of moles of component m per unit bulk volume
$n_{m\alpha}$	number of moles of component m in phase α per unit bulk volume
n_T	total number of moles in the system per unit bulk volume
n_x	number of gridblocks in <i>x</i> -direction
n_y	number of gridblocks in y-direction
n _z	number of gridblocks in z-direction
n_{lpha}	number of moles of phase α per unit bulk volume
p	pressure

p_c	critical pressure
p_{cm}	critical pressure of component m
$p_{clphaeta}$	capillary pressure between phase α and phase β
p_{ref}	reference pressure
p_{wf}	well bottomhole pressure
$_{p}p_{c\alpha}$	pseudo critical pressure of phase α
q_m	molar flow rate of injection/production of component m
\overline{q}_m	sink/source of component m
q_t	total molar flow rate of injection/production
Q_t	total volumetric flow rate
Q_{α}	volumetric flow rate of phase α
r _e	equivalent radius
r_w	wellbore radius
\vec{r}	residual vector
R	gas constant
Ŕ	residual vector
S	skin factor
S _{wc}	connate water saturation
s_{α}	saturation of phase α
S _{αe}	effective saturation of phase α in modified Corey's Model
s _{αr}	residual saturation of phase α
t	time
Т	temperature

T_c	critical temperature
T_{cm}	critical temperature of component m
$T^L_{c\alpha}$	estimated critical temperature of phase α using Li's mixing rule
T_{α}	transmissibility of phase α
$T_{m\alpha}$	transmissibility of component m in phase α
T_{rm}	reduced temperature of component m
$_{p}T_{c\alpha}$	pseudo critical temperature of phase α
$ec{u}_{lpha}$	Darcy velocity of phase α
ν	molar volume
v ^{corr}	corrected molar volume
v _c	critical molar volume
v _{cm}	critical molar volume of component m
V_b	bulk volume
$_{p}V_{c\alpha}$	pseudo critical volume of phase α
WI	well index
x_m	composition of component m
$x_{m\alpha}$	composition of component m in phase α
<i>x_{mr}</i>	composition of component m in the reference phase
\vec{x}_p	primary variable set
\vec{x}_s	secondary variable set
x _{tm}	composition of component m in the trial phase
X_{tm}	independent variables interpreted as mole number
Z _{m,inj}	injection fluid composition

Z _m	overall composition of component <i>m</i>
Z_{α}	compressibility factor of phase α

Greek Symbols

α_m	temperature dependent parameter of component m in the EOS
γ_{lpha}	specific weight of phase α
γ_F	total specific weight
δ_{mn}	Kronecker delta
ϵ_{conv}	convergence tolerance
ϵ_{switch}	switch tolerance
κ _{mn}	binary interaction parameter between components m and n
λ_m	acentric factor dependent parameter of component m
$\lambda^{(k)}$	acceleration parameter
μ_{lpha}	viscosity of phase α
μ^*_lpha	dilute gas viscosity of phase α at the standard atmosphere pressure
μ_m	chemical potential of component m
μ_m^{ig}	chemical potential of component m for an ideal gas mixture
ξ_m	viscosity-reducing parameter of component m
ξα	viscosity-reducing parameter of phase α
$ ho_F$	total molar density
$ ho_{rlpha}$	reduced density of phase α
$ ho_{lpha}$	molar density of phase α
$ ilde{ ho}_{lpha}$	mass density of phase α

$_{p} ho_{clpha}$	pseudo critical molar density of phase α
$\tau_m(T)$	integration constant of component m
$arphi_{mlpha}$	fugacity coefficient of component m in phase α
ϕ	porosity
ϕ_0	porosity at the reference pressure
Φ_{α}	potential of phase α
ω_m	acentric factor of component m

Subscripts

С	critical property
g	gas phase
i	component index
i	gridblock index in <i>x</i> -direction
iwl	well layer index
j	gridblock index in y-direction
jwl	well layer index
k	gridblock index in z-direction
l	the 2 nd liquid phase
т	component index
М	gridblock index
n	component index
Ν	gridblock index

0	oil phase
r	reference phase
W	aqueous/water phase
x	<i>x</i> -direction
У	y-direction
Ζ	z-direction
α	phase index
β	phase index
ξ	direction index

Superscripts

l	Newton-Raphson iteration level
k	phase split calculation iteration level
n	time level
Т	transpose

Operators

d	differential Operator
д	differential Operator
Δ	change
$ abla \cdot abla$	divergence operator

Accents

→	vector
=	matrix
~	element that have been modified during partial elimination

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