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Equation-of-State, Compositional, One-Dimensional Radial Flow Method to Simulate Invasion and Fluid Withdrawal in the Presence of Oil- or Water-Base Muds

by

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Equation-of-State, Compositional, One-Dimensional Radial Flow Method to Simulate Invasion and Fluid Withdrawal in the Presence of Oil- or Water-Base Muds

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To my parents
Abolfazl and Fatemeh
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I develop and successfully test a one-dimensional (1D) radial, isothermal, equation-of-state (EOS) compositional method to simulate invasion and fluid withdrawal in the presence of oil- or water-base muds. The method can simulate simultaneous flow of a maximum of three fluid phases (water, oil and gas); it is also capable of tracking salt concentration and simulating both water- or oil-base mud-filtrate invasion.

The simulation procedure is based on the assumption of axial-symmetric fluid flow, where phase behavior has a large effect on the results. I model hydrocarbon components and fluid phases based on Peng-Robinson's equation of state. The simulations are based on the method of implicit pressure and explicit concentration (IMPEC) to solve the partial differential equation arising from the discretization of the fluid-flow equation.

Verification of the 1D radial fluid flow simulation method is performed for the cases of injection and production of different fluid types against two commercial reservoir simula-
tors (CMG\textsuperscript{1}-GEM\textsuperscript{2} and CMG-STARS\textsuperscript{3}). Comparison of results against those obtained with commercial reservoir simulators indicates a good agreement.

I use the developed simulator to study and quantify the effect of mud-filtrate invasion on invasion flow rate and on the radial distributions of pressure, fluid saturation, and salt concentration. Comparison of simulations with and without mudcake indicates that mudcake growth has a significant effect on the radial distributions of pressure, fluid saturation, and salt concentration.

\begin{itemize}
  \item \textsuperscript{1}CMG: Computer Modeling Group
  \item \textsuperscript{2}GEM: Generalized Equation-of-State Model Compositional Reservoir Simulator
  \item \textsuperscript{3}STARS: Steam, Thermal, and Advanced Processes Reservoir Simulator
\end{itemize}
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Chapter 1

Introduction

In this chapter, I describe the problem and the motivation for developing a compositional simulator. I present a review of relevant literature for the formulation of compositional simulators and mud-filtrate invasion, a list of objectives for the research and, finally, a brief review of all chapters included in the thesis.

1.1 Problem Statement

Oil-base mud is increasingly being used to enhance speed and efficiency of drilling, decrease washouts and, therefore, achieving better hole control, as well as to minimize the swelling of shales [19,37]. The composition of hydrocarbon components in the injected mud filtrate is usually different from the composition of formation fluid. Miscibility of fluids causes changes in composition of phases which leads to changes of fluid viscosity, compressibility, molar mass density, gas-oil ratio, etc. Therefore, these changes in physical properties should be considered in simulations of mud-filtrate invasion.

In a compositional model, at each grid block, mass conservation equations together with equations for thermodynamic equilibrium of phases are solved to calculate pressure of oil (or any other reference fluid pressure), concentration of components, composition of phases, and saturations.

Developing a compositional simulator requires using a reliable model for characterizing components and using relations to accurately calculate properties of phases such as
GOR, viscosity, molar density, etc.

There have been numerous published papers that described the development of compositional simulators for different applications. For example, Thele [35,36] includes a thorough literature review for compositional simulators using the K-value approach. The formulation of equation-of-state compositional simulators is divided into the following categories:

- Fully-implicit formulations:

  Coats [7] developed a fully-implicit, three-dimensional (3D), three-phase simulator, which included relative permeability and capillary pressure in the modeling but discarded physical dispersion. For computing properties of hydrocarbon phases, Coats used a modified version of the Redlich-Kwong equation of state [28] and used Newton-Raphson’s method to simultaneously compute pressure, saturation, and phase compositions.

  Chien et al. [4] developed a fully-implicit formulation, selecting different primary variables from Coats. In their formulation, the aqueous phase consisted of only water whereas hydrocarbon components existed in non-aqueous phases. They implemented the Peng-Robinson [25] equation-of-state to model hydrocarbon phase behavior.

- IMPES-type formulations:

  In Nghiem et al.’s [22] and Nghiem’s [21] formulation, hydrocarbon components were allowed to enter the aqueous phase. However, water was limited to remain in the aqueous phase only. They used Peng-Robinson’s equation-of-state [25] to calculate properties of hydrocarbon phases and Henry’s law to calculate concentration of the hydrocarbon components in the aqueous phase.

  Acs et al. [1] developed an IMPES-type formulation which was similar to Nghiem et al.’s [22] formulation. However, they considered the composition-dependent terms in the pressure equation. Their pressure equation was derived based on the premise that pore volume should be filled with the total volume of the fluid.

  Chang et al. [2] and Chang [3] used a similar algorithm to Acs et al.’s but implemented a more efficient formulation for constructing the pressure matrix and included the case of four-phase flow.
Mayank et al. [20] developed a new compositional simulator for near-wellbore problems using a similar approach to Chang et al.’s [2]. They designed the simulator assuming azimuthal symmetry in formation properties with respect to a vertical axis. The developed simulator was designed with the assumption of first-contact fluid miscibility.

- Sequential implicit compositional formulation:
  Watts [38] expanded Acs et al.’s formulation to solve the pressure equation implicitly and developed a sequential semi-implicit algorithm for solving saturation at ensuing times. In Watts’ formulation, both capillary pressure and relative permeability were calculated implicitly.

- Adaptive-implicit formulation:
  Collins et al. [8] developed a compositional simulator with the idea that only a few grid blocks needed to be solved implicitly and the rest could be solved explicitly. Based on changes of fluid saturation and overall fluid composition, they switched grid blocks into implicit or explicit groups. They used Newton-Raphson’s method to calculate pressure and overall composition. Subsequently, phase composition was computed using flash calculations.

Mud-filtrate invasion is another part of the study considered in this thesis. Overbalance pressure, due to the difference between hydrostatic pressure at the wellbore and reservoir fluid pressure, results in mud-filtrate invasion into the formation. With time, thickness of mudcake increases until it reaches a maximum limit [5]. Porosity and permeability of mudcake decrease with time [11]. The effect of mudcake was studied using a black-oil model by Wu [40], Lee [16], and Salazar [30]. Salazar [30] also studied mudcake growth for the case of oil-base mud. However, mudcake properties for the case of oil-based mud have not been investigated thoroughly for compositional simulations.

1.2 Research Objectives

Development of a 1D radial compositional simulator is the main objective of this thesis. The simulator is specifically targeted for near-wellbore problems, and is based on the following assumptions:
• equation of state,
• 1D radial fluid flow,
• multiple components in different fluid phases.

The method is capable of:

• Simulating oil-water, gas-water, gas-oil and gas-oil-water fluid flow,
• tracking variations of salt concentration,
• Applying different boundary conditions at the well during injection and fluid production,
• Taking into account the effect of mud-filtrate invasion.

Using the developed simulator, I study the effect of mud-filtrate invasion on pressure, saturation, and salt concentration profiles along the radial distance. In addition, I investigate the effect of reference properties of mudcake on the growth of mudcake thickness and rate of fluid flow.

1.3 Review of Chapters

I develop and validate a 1D radial compositional simulator to model invasion and fluid withdrawal in the presence of oil- or water-base muds. I use Peng-Robinson’s equation-of-state [25] to model phase behavior of hydrocarbon mixtures. Likewise I implement an experimental model for mudcake growth to simulate mud-filtrate invasion.

In Chapter 2, I describe the mathematical formulation of the models used in the simulator including assumptions, mass conservation and constitutive equations, the pressure equation, models for physical properties, and phase behavior.

Chapter 3 discusses the discretization of the pressure equation, molar mass equations, definition of well and boundary conditions, computation of saturation, and automatic time-step control. Phase behavior for the developed simulator is discussed in Chapter 4.

I test several case studies in Chapter 5 to validate the developed simulator against two commercial reservoir simulators (CMG-STARS and CMG-GEM). These simulation
cases cover validations for gas-water, oil-water, and gas-oil-water flow, as well as radial
distribution of salt concentration after water-base mud-filtrate invasion. The effect of mud-
cake growth is discussed in Chapter 6. Chapter 7 summarizes the conclusions of the
thesis and recommendations for future work.
Chapter 2

Mathematical Models

2.1 Introduction

In this chapter, I describe the mathematical formulation for multi-phase, multi-component fluid flow for the problem under consideration. In addition, I introduce the partial differential equation along with boundary and initial conditions for the problem. Assumptions for the mathematical formulation are listed below:

1. Reservoir is isothermal,
2. Reservoir is impermeable at infinite radial distance,
3. There is no chemical reaction or precipitation between fluid and rock,
4. Formation is slightly compressible,
5. Darcy’s law for multi-phase flow is valid,
6. Physical dispersion is negligible.

The developed simulator assumes variations of properties only in the radial direction and models three-phase flow problems, including water, gas, and oil.
2.2 Mass Conservation and Constitutive Equations

This section describes the mathematical equations for multi-phase, multi-component systems in an isothermal porous medium. For component $i$, the general mass balance equation can be written as

$$\frac{\partial W_i}{\partial t} + \nabla \cdot \vec{F}_i - R_i = 0,$$

(2.1)

where $W_i$, $\vec{F}_i$ and $R_i$ are the accumulation, flux, and source term, respectively. In the above equation the accumulation term for the pore space, $W_i$, can be expressed as

$$W_i = \phi \sum_{j=1}^{n_p} \xi_j S_j x_{ij},$$

(2.2)

where $\phi$ is porosity, $n_p$ is the number of phases, $x_{ij}$ is the mole fraction of component $i$ in phase $j$, $\xi_j$ is the molar density of phase $j$, and $S_j$ is the saturation of phase $j$.

I assume that there is no mass transfer between the hydrocarbon components and the aqueous phase, and that the aqueous phase consists of only the water component. Moreover, the water component does not affect phase behavior. Based on this last assumption, Equation (2.2) can be modified to

$$W_i = \phi \sum_{j=2}^{n_p} \xi_j S_j x_{ij}$$

for hydrocarbon components and

$$W_{nc+1} = \phi \xi_1 S_1,$$

(2.3)

(2.4)

for water. In this modeling, $i = 1$ is for aqueous, $i = 2$ for oil, and $i = 3$ is for gas phase. In equation (2.1), the flux term, $\vec{F}_i$, can be expressed as

$$\vec{F}_i = \sum_{j=1}^{n_p} \xi_j x_{ij} \vec{u}_j - \phi \xi_j \overline{K}_{ij} \nabla x_{ij},$$

(2.5)

where $\vec{u}_j$ is the superficial velocity of phase $j$ and $\overline{K}_{ij}$ is the dispersion tensor. Applying
Darcy’s multi-phase relation for superficial velocity, I obtain

\[ \overrightarrow{u}_j = \overline{k}_{ij} \lambda_{rj} (\nabla P_j - \gamma_j \nabla D), \]

(2.6)

where \( \overline{k}_{ij} \) is permeability tensor, \( \gamma_j \) is specific weight of phase \( j \), \( D \) is depth, and \( \lambda_{rj} \) is mobility with respect to the reference phase (in this case, the oil phase), which can be expressed in terms of relative permeability, \( k_{ij} \), and viscosity, \( \mu_j \), as

\[ \lambda_{rj} = \frac{k_{rj}}{\mu_j}. \]

(2.7)

In the above model, I neglect the dispersion term in Equation (2.5). In that equation, the source term is correlated with the well condition as follows.

\[ R_i = \frac{q_i}{V_b} \quad \forall \quad i = 1, \ldots, n_c, n_c + 1, \]

(2.8)

where \( q_i \) is molar flow rate of each component, here considered positive whenever injecting to the well and negative whenever producing from the well. Only for the first grid block \( q_i \) may be nonzero. After substituting Equations (2.2),(2.5) and (2.8) into Equation (2.1), I obtain

\[ \frac{\partial}{\partial t} \left( \phi \sum_{j=1}^{n_p} \xi_j S_j x_{ij} + \overrightarrow{n} \cdot \sum_{j=1}^{n_p} \xi_j x_{ij} \overrightarrow{u}_j \right) - \frac{q_i}{V_b} = 0 \quad \forall \quad i = 1, \ldots, n_c, n_c + 1. \]

(2.9)

Equation (2.9) is a set of coupled partial differential equations which are nonlinear with respect to concentration of components and pressure. In Equation (2.9), there are \( n_c n_p + 6n_p + 2 \) variables which are listed in Table (2.1).

### 2.3 Auxiliary Relations

In Equation (2.9), there are \( n_c n_p + 6n_p + 2 \) variables. In order to determine the unknown parameters, I use the following equations to uniquely define the variables.
2.3.1 Saturation Constraint

The sum of saturations in each grid block must be equal to one, i.e.,

$$\sum_{j=1}^{n_p} S_j = 1.$$  \hfill (2.10)

2.3.2 Porosity Dependency on Pressure

Formation porosity is a function of pressure, namely,

$$\phi = \phi(P).$$  \hfill (2.11)

2.3.3 Phase Molar Density

Molar density of each hydrocarbon phase at a given temperature is a function of the pressure and composition of each phase, to wit,

$$\xi_j = \xi_j(P, \overrightarrow{X}_j) \quad \forall \quad j = 2 \ldots, n_p.$$  \hfill (2.12)

However, molar density of the aqueous phase is a function of the pressure, i.e.,

$$\xi_1 = \xi_1(P).$$  \hfill (2.13)

<table>
<thead>
<tr>
<th>Variables</th>
<th>Number of Variables</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\phi$</td>
<td>1</td>
</tr>
<tr>
<td>$S_j$</td>
<td>$n_p$</td>
</tr>
<tr>
<td>$\xi_j$</td>
<td>$n_p$</td>
</tr>
<tr>
<td>$x_{ij}$</td>
<td>$n_c(n_p - 1)$</td>
</tr>
<tr>
<td>$k_{rj}$</td>
<td>$n_p$</td>
</tr>
<tr>
<td>$\mu_j$</td>
<td>$n_p$</td>
</tr>
<tr>
<td>$P_j$</td>
<td>$n_p$</td>
</tr>
<tr>
<td>$\gamma_j$</td>
<td>$n_p$</td>
</tr>
<tr>
<td>$q_i$</td>
<td>$n_c + 1$</td>
</tr>
</tbody>
</table>

$$\sum_{j=1}^{n_p} \# \quad n_c n_p + 6 n_p + 2$$

Table 2.1: List of variables included in Equation (2.9)
2.3.4 Phase Composition Constraint

The sum of mole fractions of the components in each fluid phase should be equal to one, namely,

$$\sum_{i=1}^{n} x_{ij} = 1. \quad (2.14)$$

2.3.5 Flow Rate

Flow rate of each component is a function of the pressure difference between sand face and reservoir, saturation of phases, and composition of fluid phases, i.e.,

$$q_i = q_i(P, \overrightarrow{S}, \overrightarrow{X}) \quad (2.15)$$

where $\overrightarrow{S}$ is saturation of all fluid phases and $\overrightarrow{X}$ is the molar fraction of components.

2.3.6 Phase Pressure

Pressure of each fluid phase can be related to the reference pressure with its corresponding capillary pressure between those phases, to wit,

$$P_j = P_r + P_{crj} \quad \forall \quad j = 1, \ldots, n_p \quad (j \neq r) \quad (2.16)$$

where $P_j$ is the pressure of fluid phase $j$, $P_r$ is the pressure of the reference fluid phase, and $P_{crj}$ is the capillary pressure between fluid phase $j$ and pressure of the reference fluid phase. In the above equation, the capillary pressure is a function of phase saturation and composition, i.e.,

$$P_{crj} = P_{crj}(\overrightarrow{S}, \overrightarrow{X}) \quad \forall \quad j = 1, \ldots, n_p \quad (j \neq r), \quad (2.17)$$

where $\overrightarrow{S}$ is saturation of all fluid phases and $\overrightarrow{X}$ is the molar fraction of components.
2.3.7 Phase Mass Density

Mass density of each hydrocarbon phase at a given temperature is a function of the pressure and composition of that phase, i.e.,

\[ \gamma_j = \gamma_j(P_j, X_j) \quad \forall \quad j = 2, \ldots, n_p. \quad (2.18) \]

The mass density of the aqueous phase is only a function of the pressure, namely,

\[ \gamma_1 = \gamma_1(P_1). \quad (2.19) \]

2.3.8 Phase Viscosity

Viscosity of each hydrocarbon phase at a given temperature is a function of pressure and composition of that phase, namely,

\[ \mu_j = \mu_j(P_j, X_j) \quad \forall \quad j = 2, \ldots, n_p. \quad (2.20) \]

For the aqueous phase the change of viscosity is negligible and is set to a constant value, i.e.,

\[ \mu_1 = \text{constant}. \quad (2.21) \]

2.3.9 Relative Permeability

Relative permeability can be expressed as a function of saturation, to wit,

\[ k_{rj} = k_{rj}(S). \quad (2.22) \]

2.3.10 Phase Equilibrium

The assumption of thermodynamic equilibrium in each grid block yields the following relations for hydrocarbon phases [31]:

\[ f_{ij} = f_{ir} \quad \forall \quad i = 1, \ldots, n_c \quad & \quad j = 2, \ldots, n_p \quad (j \neq r), \quad (2.23) \]
in which, the fugacity of each component in each phase, $f_{ij}$, is obtained from an equation of state.

### 2.4 Pressure Equation

The method for the compositional simulation is similar to that of UTCOMP [3], which is called IMPEC. In the IMPEC method, the pressure equation is solved implicitly whereas moles of components are calculated explicitly. Saturations of fluid phases are also explicitly related to moles of components. A maximum of three fluid phases are considered in the simulations. The fundamental equation for pressure is based on the assumption that pore volume contains the total volume of the fluid, that is,

$$V_i(P, \overrightarrow{N}_t) = V_p(P), \quad (2.24)$$

where $V_i$ is the total fluid volume, which is a function of pressure and total number of moles of hydrocarbons, $\overrightarrow{N}_t$, in the pore volume, $V_p$. Differentiating both sides of Equation (2.24) with respect to time, and using the chain rule yields

$$\left( \frac{\partial V_i}{\partial P} \right)_{N_t} \left( \frac{\partial P}{\partial t} \right) + \sum_{i=1}^{n_c+1} \left( \frac{\partial V_i}{\partial N_{i}} \right)_{P,N_{k},(i \neq k)} \left( \frac{\partial N_{i}}{\partial t} \right) = \left( \frac{dV_p}{dP} \right) \left( \frac{\partial P}{\partial t} \right). \quad (2.25)$$

In the following sections, I describe various components of Equation (2.25) as functions of some known parameters.

1. Relation for $dV_p/dP$.

   From the slightly compressibility assumption for the formation, one can write the following equation for porosity,

   $$\phi = \phi_0 [1 + c_f (P - P^0)], \quad (2.26)$$

   in which $\phi_0$ is porosity at reference reservoir pressure, $P^0$, and $c_f$ is compressibility of the formation. The definition of pore volume indicates that,

   $$V_p = V_b \phi \quad (2.27)$$
Differentiating both sides of equation (2.27) gives

\[ \frac{dV_p}{dP} = V_p^0 c_f, \quad (2.28) \]

where \( V_p^0 \) is the pore volume at the reference pressure.

2. Relation for \( \frac{\partial N_i}{\partial t} \):

The total moles of each component at each grid block, \( N_i \), is equal to the accumulation in that grid, \( V_b W_i \). Using the relation in Equation (2.2) yields

\[ N_i = V_p \sum_{j=1}^{n_p} \xi_j S_j x_{ij}. \quad (2.29) \]

From Equations (2.29) and (2.9), I obtain a differential equation for moles of each component, namely,

\[ \frac{\partial N_i}{\partial t} = -V_b \nabla \cdot \left( \sum_{j=1}^{n_p} \xi_j x_{ij} \overrightarrow{u}_j \right) + q_i \quad \forall \quad i = 1, \ldots, n_c, n_c + 1, \quad (2.30) \]

where \( n_p \) is the number of coexisting fluid phases, \( q_i \) is the molar rate of component \( i \), \( \xi_j \) is the molar density of fluid phase \( j \), \( \overrightarrow{u}_j \) is the velocity of fluid phase \( j \), and \( x_{ij} \) is the molar fraction of component \( i \) in fluid phase \( j \).

3. Relation for \( \left( \frac{\partial V_i}{\partial N_i} \right)_{P,N \neq k(x)} \):

A partial molar volume can be defined for each component as suggested in [3], namely,

\[ \nabla_{ti} = \left( \frac{\partial V_i}{\partial N_i} \right)_{P,N \neq k(x)}, \quad (2.31) \]

Substituting Equations (2.28), (2.30), and (2.31) into Equation (2.25) yields:

\[ \left( \frac{\partial V_i}{\partial P} \right)_{N_i} \frac{\partial P}{\partial t} - V_b \sum_{i=1}^{n_c+1} \nabla_{ti} \cdot \left( \sum_{j=1}^{n_p} \xi_j x_{ij} \overrightarrow{u}_j \right) + \sum_{i=1}^{n_c+1} \nabla_{ti} q_i = V_p^0 c_f \frac{\partial P}{\partial t}. \quad (2.32) \]
In the above equation, I have used oil pressure as the reference equation; all other fluid pressures are related to that with the corresponding capillary pressure equation\(^\text{(1)}\), to wit,

\[ P_j = P + P_{c2j}, \]  

where \( P \) is the pressure of oil phase, \( P_{c2j} \) is the capillary pressure of fluid phase \( j \) with respect to oil phase, and \( P_j \) is the pressure of fluid phase \( j \). Substituting Equations (2.33), and (2.6) into Equation (2.32) yields

\[
(V_0^0 c_f - (\frac{\partial V_t}{\partial P}) \frac{\partial P}{\partial t}) - V_b \sum_{i=1}^{n_c+1} \nabla t_i \cdot \sum_{j=1}^{n_p} \sum_{i=1}^{n_c+1} \xi_j x_{ij} \nabla P = V_b \sum_{i=1}^{n_c+1} \nabla t_i \cdot \sum_{j=1}^{n_p} \sum_{i=1}^{n_c+1} \xi_j x_{ij} \nabla P_{c2j}) + \sum_{i=1}^{n_c+1} \nabla t_i q_i. \quad (2.34)
\]

In this model, I assume variation of pressure and concentration only in the radial direction. Thus, I do not include a gravity term in Equation (2.34). Equation (2.34) can thus be written as

\[
(V_0^0 c_f - (\frac{\partial V_t}{\partial P}) \frac{\partial P}{\partial t}) - V_b \sum_{i=1}^{n_c+1} \nabla t_i \cdot \sum_{j=1}^{n_p} \sum_{i=1}^{n_c+1} \xi_j x_{ij} \nabla P = V_b \sum_{i=1}^{n_c+1} \nabla t_i \cdot \sum_{j=1}^{n_p} \sum_{i=1}^{n_c+1} \xi_j x_{ij} \nabla P_{c2j}) + \sum_{i=1}^{n_c+1} \nabla t_i q_i. \quad (2.35)
\]

### 2.5 Moles of Components

After solving the pressure equation, (2.35), I find moles of each component at the current pressure using Equation (2.30), namely,

\[
\frac{\partial N_i}{\partial t} = V_b \nabla \cdot \xi_j x_{ij} (k \lambda_j \nabla P_j) + q_i \quad \forall \quad i = 1, \ldots, n_c, n_c + 1, \quad (2.36)
\]

where \( N_i \) is the total moles of component \( i \) in the grid block, \( V_b \) is the bulk volume, \( n_p \) is the number of coexisting fluid phases, \( \xi_j \) is the molar density of fluid phase \( j \), \( x_{ij} \) is the mole

\(^1\)The capillary pressure has negative value compared to conventional water-oil capillary pressure.
fraction of component $i$ in fluid phase $j$, $k$ is the permeability of rock, $\lambda_j$ is the mobility of fluid phase $j$, $P_j$ is the pressure of fluid phase $j$, $q_i$ is the molar rate of component $i$, and $n_c$ is the number of component

## 2.6 Modeling Physical Properties

In this section I briefly explain the models I have used for viscosity, relative-permeability, capillary pressure, as well as interfacial tension.

### 2.6.1 Viscosity

In this model, viscosity of the aqueous phase is assumed constant, and is inputed by the user. I use one the following relations for the calculation of hydrocarbon-phase viscosity: (1) Lohrenz et al. [18], (2) quarter-power mixing rule [3], and (3) linear mixing rule [3].

**Lohrenz et al. correlation**

Lohrenz et al. [18] combined several correlations to calculate hydrocarbon-phase viscosity. The procedure for the calculation of hydrocarbon-phase viscosity is as follows:

**Step 1:** Using the Stiel and Thodos correlation [33], I compute the low pressure, pure component viscosity as

$$
\tilde{\mu}_i = 3.4 \times 10^{-4} \frac{T_{ri}^{0.94}}{\zeta_i} \quad \text{for} \quad T_{ri} \leq 1.5,
$$

(2.37)

or

$$
\tilde{\mu}_i = 1.776 \times 10^{-4} \frac{(4.58 \times T_{ri} - 1.67)^{5/8}}{\zeta_i} \quad \text{for} \quad T_{ri} > 1.5,
$$

(2.38)

where $\tilde{\mu}_i$ is the low-pressure viscosity of component $i$, $T_{ri}$ is the reduced temperature of component $i$, and $\zeta_i$ is the viscosity parameter of component $i$ and is calculated using the following equation.

$$
\zeta_i = 5.44 \frac{T_{ci}^{1/6}}{W_{ci}^{1/2} P_{ci}^{2/3}},
$$

(2.39)
where $W_{ti}$ is molecular weight of component $i$, and $P_{ci}$ is the critical pressure of component $i$.

Step 2: Using Herning and Zipperer’s equation [13], I find the low-pressure viscosity, namely,

$$\mu_j^* = \frac{\sum_{i=1}^{n_c} x_{ij} \tilde{\mu}_i \sqrt{W_{ti}}}{\sum_{i=1}^{n_c} x_{ij} \sqrt{W_{ti}}}.$$  \hspace{1cm} (2.40)

where $\mu_j^*$ is the low-pressure viscosity of hydrocarbon-phase $j$, $x_{ij}$ is the mole fraction of component $i$ in phase $j$, and $n_c$ is the number of hydrocarbon components in hydrocarbon-phase $j$.

Step 3: I compute the reduced phase molar density, $\xi_{jr}$, as

$$\xi_{jr} = \xi_j \sum_{i=1}^{n_c} x_{ij} V_{ci},$$  \hspace{1cm} (2.41)

where $\xi_j$ is the molar density of hydrocarbon-phase $j$. Moreover, I calculate the mixture viscosity parameter, $\eta_j$, from

$$\eta_j = 5.44 \frac{(\sum_{i=1}^{n_c} x_{ij} T_{ci})^{1/6}}{(\sum_{i=1}^{n_c} x_{ij} W_{ti})^{1/2} (\sum_{i=1}^{n_c} x_{ij} P_{ci})^{2/3}}.$$  \hspace{1cm} (2.42)

Step 4: Using Jossi et al.’s correlation [15], I calculate hydrocarbon-phase viscosity at the phase pressure with

$$\mu_j = \mu^* + 2.05 \times \frac{\xi_{jr}}{\eta_j} \quad \text{if} \quad \xi_{jr} \leq 0.18,$$  \hspace{1cm} (2.43)

or

$$\mu_j = \frac{\mu^* + \chi_j^4 - 1}{10^4 \times \eta_j} \quad \text{if} \quad \xi_{jr} > 0.18,$$  \hspace{1cm} (2.44)
where $\chi_j$ is the viscosity parameter defined by

$$
\chi_j = 1.023 \xi_{jr} + 0.23364 \xi_{jr}^2 + 0.58533 \xi_{jr}^3 - 0.40758 \xi_{jr}^3 + 0.093324 \xi_{jr}.
$$

(2.45)

### Quarter-Power Mixing rule

The quarter-power mixing rule [3] for viscosity of each hydrocarbon phase is formulated as

$$
\mu_j = \left( \sum_{i=1}^{n_p} x_{ij} \tilde{\mu}_i^{1/4} \right)^{-4} \text{ for } j = 2, \ldots, n_p,
$$

(2.46)

where $\tilde{\mu}_i$ is the viscosity of the pure component.

### Linear Mixing rule

The linear mixing rule [3] for hydrocarbon-phase viscosity is given by

$$
\mu_j = \sum_{i=1}^{n_p} x_{ij} \tilde{\mu}_i \text{ for } j = 1, \ldots, n_p,
$$

(2.47)

where $\tilde{\mu}_i$ is the viscosity of the pure component.

### 2.6.2 Relative-Permeability Models

There are several relative-permeability models which are currently used in simulators. Stone’s model 2 [34], Baker’s model (Delshad and Pope [10]), Pope’s model [10], and Corey’s model [9] are a few examples of models for relative permeability. These models are described in Chang’s dissertation [3]. In this simulator, I implemented Stone’s model 2. The simulator can also read in input table for relative permeability and estimate three-phase relative-permeability based on Stone’s model 2.

#### Stone’s Model 2

In this simulator, oil-water two-phase relative permeability is calculated using Corey’s model, namely,

$$
k_{r21} = k_{r21}^{0} \left( \frac{1 - S_1 - S_{2r1}}{1 - S_{1r} - S_{2r1}} \right)^{e_{r21}},
$$

(2.48)
whereas oil-gas two-phase relative permeability is calculated with Corey’s model, given by

\[ k_{r23} = k_{r2}^0 \left( \frac{1 - S_3 - S_{2r3}}{1 - S_{1r} - S_{2r3} - S_{3r}} \right)^{e_{23}}, \]  

(2.49)

where

- \( k_{r21} \) is relative permeability of the aqueous phase, 1, flowing with oil phase, 2,
- \( k_{r23} \) is relative permeability of gas phase, 3, flowing with oil phase, 2,
- \( k_{r2}^0 \) is endpoint relative permeability of oil phase, 2,
- \( S_1 \) is saturation of the aqueous phase, 1,
- \( S_{2r1} \) is residual saturation of oil phase, 2, flowing with the aqueous phase, 1,
- \( S_{2r3} \) is residual saturation of oil phase, 2, flowing with gas phase, 3,
- \( S_{1r} \) is residual saturation of the aqueous phase,
- \( S_{3r} \) is residual saturation of gas phase,
- \( e_{21} \) is exponent of relative permeability function of oil phase, 2, flowing with the aqueous phase, 1, and
- \( e_{23} \) is exponent of relative permeability function of oil phase, 2, flowing with gas phase, 3.

Relative permeability of water and gas are similarly calculated with Corey’s model, given by

\[ k_{r1} = k_{r1}^0 \left( \frac{S_1 - S_{1r}}{1 - S_{1r} - S_{2r1}} \right)^{e_1}, \]  

(2.50)

and

\[ k_{r3} = k_{r3}^0 \left( \frac{S_3 - S_{3r}}{1 - S_{1r} - S_{2r3} - S_{3r}} \right)^{e_3}, \]  

(2.51)

where

- \( k_{r1} \) is relative permeability of the aqueous phase, 1,
- \( k_{r3} \) is relative permeability of gas phase, 3,
• $k_{r1}^0$ is endpoint relative permeability of the aqueous phase, 1,

• $k_{r3}^0$ is endpoint relative permeability of gas phase, 3,

• $e_1$ is exponent of relative permeability function of the aqueous phase, 1, and

• $e_3$ is exponent of relative permeability function of gas phase, 3.

Finally, the relative permeability of oil for three-phase flow is calculated as

$$k_{r2} = k_{r2}^0 \left[ \left( \frac{k_{r21}}{k_{r2}} + k_{r1} \right) \left( \frac{k_{r23}}{k_{r2}} + k_{r3} \right) - k_{r1} - k_{r3} \right]. \tag{2.52}$$

Table-Lookup for Relative Permeability

The relative permeabilities of water and gas are found from linear interpolation. For two-phase gas-oil and oil-water, relative permeability of oil is calculated from linear interpolation of the input table. Relative permeability of oil in three-phase flow is computed from Stone’s model 2, Equation (2.52).

### 2.6.3 Capillary Pressure

Capillary pressure is a function of other parameters, such as interfacial tension, permeability, porosity and saturation [17]. For three-phase water-oil-gas flow, capillary pressure is given by [3]

$$P_{c21} = -C_{pc}\sigma_{12}\sqrt{\frac{\phi}{k_r}}(1 - S_1)^{E_{pc}}, \tag{2.53}$$

and

$$P_{c23} = C_{pc}\sigma_{23}\sqrt{\frac{\phi}{k_y}}\left( \frac{S_1}{S_2 + S_3} \right)^{E_{pc}}, \tag{2.54}$$

where

• $P_{c21}$ is capillary pressure of oil phase, 2, and the aqueous phase, 1,

• $P_{c23}$ is capillary pressure of oil phase, 2, and gas phase, 3,

• $C_{pc}$ is the constant of capillary function,

• $\sigma_{12}$ is interfacial tension of the aqueous phase, 1, and oil phase, 2,
• $\sigma_{32}$ is interfacial tension of gas phase, 3, and oil phase, 2,

• $\phi$ is porosity,

• $k_r$ is permeability,

• $E_{pc}$ is the exponent of the capillary pressure function, and

• $S_{\bar{j}}$ is normalized saturation defined by

$$S_{\bar{1}} = \frac{S_1 - S_{1r}}{1 - S_{1r} - S_{2r}^{\circ} - S_{3r}}, \quad (2.55)$$

$$S_{\bar{2}} = \frac{1 - S_1 - S_{2r}^{\circ} - S_{3r}}{1 - S_{1r} - S_{2r}^{\circ} - S_{3r}}, \quad (2.56)$$

and

$$S_{\bar{3}} = \frac{S_3 - S_{3r}}{1 - S_{1r} - S_{2r}^{\circ} - S_{3r}}, \quad (2.57)$$

where equivalent residual saturation of oil phase, $S_{2r}^{\circ}$, is defined by [3]

$$S_{2r}^{\circ} = bS_{2r1} + (1 - b)S_{2r3}, \quad (2.58)$$

with

$$b = 1 - \frac{S_3}{1 - S_{1r} - S_{2r3}}. \quad (2.59)$$

These parameters are determined from curve matching of laboratory experiments of water-oil capillary pressure.

### 2.6.4 Interfacial Tension

The interfacial tension between water and hydrocarbon phases is assumed to be constant. Macleod-Sudgen [29] introduced an equation for the interfacial tension between hydrocarbon phases, which relates interfacial tension to molar density, $\xi_j$, phase composition, $x_{ij}$, and parachor of components, $\Psi_i$, given by

$$\sigma_{jr} = \left(0.016018 \sum_{i=1}^{n} \Psi_i (\xi_j x_{ij} - \xi_j x_{ir})\right)^4. \quad (2.60)$$
2.7 Phase Behavior

In this thesis hydrocarbon phase behavior is modeled using Peng-Robinson’s equation of state (PR-EOS) [25].

2.7.1 Peng-Robinson Equation-of-State

Peng and Robinson modified Van der Waals’s equation of state as

\[ P + \frac{\alpha(T)}{v(v+b)+b(v-b)}(v-b) = RT, \]  

(2.61)

where \( v \) is the molar volume, \( P \) is the pressure, \( T \) is the temperature, \( R \) is the universal gas constant, and \( \alpha \) and \( b \) are constants of equation of state calculated by

\[ \alpha(T) = \Omega_a \frac{\alpha(RT_c)^2}{P_c}, \]  

(2.62)

and

\[ b = \Omega_b \frac{RT_c}{P_c}, \]  

(2.63)

where

\[ \Omega_a = 0.45724, \]  

(2.64)

\[ \Omega_b = 0.0778, \]  

(2.65)

and

\[ \alpha = [1 + m(1 - \sqrt{\frac{T}{T_c}})]^2, \]  

(2.66)

where

\[ m = 0.37464 + 1.54226\omega - 0.26992\omega^2. \]  

(2.67)

In the above equations, \( T_c \) is the temperature at the critical point, \( P_c \) is the pressure at the critical point, and \( \omega \) is the accentric factor of hydrocarbon component. Keeping simplicity, this equation is more reliable than any other equation-of-state, since the prediction of liquid-phase densities are closer to the experimental data [12, 24]. The universal critical compressibility factor for pure components obtained with Equation (2.61) is 0.307, whereas
that obtained with SRK\(^2\) is 0.333 but both are larger than experimental data [24]. Compressibility factor of hydrocarbon phase, \(Z\), is defined as

\[
Z = \frac{P_v}{RT}.
\]  

(2.68)

I can express PR-EOS in the form of a cubic equation of fluid phase compressibility, \(Z\), as

\[
Z^3 - (1 - B)Z^2 + (A - 3B^2 - 2B)Z - (AB - B^2 - B^3) = 0,
\]  

(2.69)

where

\[
A = \frac{aP}{(RT)^2},
\]  

(2.70)

and

\[
B = \frac{bP}{RT},
\]  

(2.71)

where \(a\) and \(b\) are the constants of equation of state for hydrocarbon fluid phase and are calculated as

\[
a = \sum_{i=1}^{n_c} \sum_{k=1}^{n_c} x_i x_k a_{ik},
\]  

(2.72)

where \(a_{ik}\) is calculated as

\[
a_{ik} = (1 - \delta_{ik}) \sqrt{a_i a_k},
\]  

(2.73)

and

\[
b = \sum_{i=1}^{n_c} x_i b_i.
\]  

(2.74)

In the above equations, \(\delta_{ik}\) is the binary interaction between components \(i\) and \(k\), and \(x_i\) is the mole fraction of component \(i\) in the fluid phase.

\(^2\text{SRK: Soave-Redlich-Kwong equation-of-state [12, 24]}\)
Fugacity of Components

The fugacity of component \( i \) in a mixture can be computed from the following equation [12]:

\[
\ln \frac{f_i}{x_i P} = \frac{b_i}{b}(Z - 1) - \ln(Z - B) - \frac{A}{2\sqrt{2}B} \left( \sum_{k=1}^{n_c} x_k a_{ik} - \frac{b_k}{b} \right) \times \ln\left( \frac{Z + (1 + \sqrt{2})B}{Z + (1 - \sqrt{2})B} \right),
\]

(2.75)

where

- \( f_i \) is fugacity of component \( i \),
- \( x_i \) is the mole fraction of component \( i \) in fluid phase,
- \( P \) is the pressure of the fluid phase,
- \( b_i \) and \( a_{ik} \) are constants of equation of state,
- \( A, B, a, \) and \( b \) are constants of equation of state for fluid phase,
- \( Z \) is the compressibility of fluid phase.

2.7.2 Molar Density

From the equation of state, I compute the compressibility factor, \( Z \), of each hydrocarbon phase. The molar density of hydrocarbon phase \( j \), \( \xi_j \), is given by

\[
\xi_j = 1 = \frac{1}{v_j} = \frac{P}{Z_j RT},
\]

(2.76)

where \( P \) is the fluid phase pressure, \( Z_j \) is the compressibility of the fluid phase, \( R \) is the universal gas constant, and \( T \) is temperature. In this model, I assume that water is slightly compressible. Consequently, the molar density is written as

\[
\xi_1 = \xi_1^0 \left[ 1 + c_1 (P - P_1^0) \right],
\]

(2.77)

where \( \xi_1^0 \) is the water molar density at the reference pressure, \( c_1 \) is the compressibility of water at reference pressure, \( P_1^0 \), and \( \xi_1 \) is the compressibility of water at pressure \( P \).
2.7.3 Derivatives of the Pressure Equation

Analytical computation of partial derivatives of total fluid volume is needed to solve the pressure equation, \((2.35)\). Accordingly, I briefly formulate the derivatives in the following section, and refer to Chang’s Dissertation [3] for detailed derivation.

Derivative of Total Volume of Fluid with respect to Moles of Components

The partial derivative of total fluid volume with respect to moles of component was introduced in equation \((2.31)\), which is defined as

\[
\nabla_{t_i} = \left( \frac{\partial V_t}{\partial N_i} \right)_{P,N_{r(e\neq i)}} = \frac{\partial}{\partial N_i} \left( \sum_{j=1}^{n_p} n_j v_j \right) \quad \forall \quad i = 1, \ldots, n_c, n_c + 1, \quad (2.78)
\]

where \(\nabla_{t_i}\) is the partial molar volume of component \(i\), \(V_t\) is the total fluid volume, \(N_i\) is the total moles of component \(i\), \(n_j\) is the total moles of components in fluid phase \(j\), \(v_j\) is the molar volume of fluid phase \(j\), \(n_c\) is the number of components, and \(n_p\) is the number of fluid phases. To begin with, the partial molar volume of water component becomes

\[
\nabla_{t_{(n_c+1)}} = v_1, \quad (2.79)
\]

where \(v_1\) is the molar volume of water at grid pressure. For the case of hydrocarbon components the partial molar volume, \(\nabla_{t_i}\), is given by

\[
\nabla_{t_i} = \sum_{j=2}^{n_p} \sum_{i=1}^{n_c} [v_j + n_j \frac{\partial v_j}{\partial n_{kj}}] \left( \frac{\partial n_{kj}}{\partial N_i} \right)_{P,N_{r(e\neq i)}} , \quad (2.80)
\]

where \(v_j\) is the molar volume of fluid phase \(j\), \(n_j\) is the total moles of all components in hydrocarbon phase \(j\), and \(n_{kj}\) is moles of component \(k\) in hydrocarbon phase \(j\).

Using the equation of state, I compute the partial molar volume derivative as

\[
\frac{\partial v_j}{\partial n_{kj}} = \frac{R T}{P} \left( \frac{\partial Z_j}{\partial n_{kj}} \right) \quad \text{for} \quad j = 2, \ldots, n_p \quad \& \quad k = 1, \ldots, n_c , \quad (2.81)
\]

where \(R\) is the universal gas constant, \(T\) is temperature, \(P\) is pressure, and \(Z_j\) is compressibility of hydrocarbon phase \(j\).
For the case of two hydrocarbon phases, $\frac{\partial n_{k2}}{\partial N_i}$ is computed by solving the following set of equations:

$$\sum_{k=1}^{n_c} \left[ \frac{\partial \ln f_{s2}}{\partial n_{k2}} + \frac{\partial \ln f_{s3}}{\partial n_{k3}} \right] \left( \frac{\partial n_{k2}}{\partial n_{k3}} \right) = \left( \frac{\partial \ln f_{s3}}{\partial n_{k3}} \right),$$

for $s = 1, \ldots, n_c$ and $i = 1, \ldots, n_c$. \hspace{1cm} (2.82)

where $f_{sj}$ is the fugacity of component $s$ in hydrocarbon phase $j$, and $n_{ij}$ is the moles of component $i$ in hydrocarbon phase $j$.

**Derivative of Total Volume of Fluid with respect to Pressure**

The derivative of total fluid volume with respect to pressure is given by

$$\left( \frac{\partial V_t}{\partial P} \right)_{N_i} = \left( \frac{\partial V_1}{\partial P} \right)_{N_i} + \sum_{j=2}^{n_p} \left( \frac{\partial V_j}{\partial P} \right)_{N_i},$$

where $V_t$ is total fluid volume, $P$ is pressure, $V_1$ is volume of the aqueous phase, and $V_j$ is volume of the hydrocarbon phase $j$.

For the aqueous phase, with the assumption of being slightly compressible, the derivative can be expressed as

$$\left( \frac{\partial V_1}{\partial P} \right)_{N_i} = -\frac{n_1 \xi_0 c_1}{\xi_1^2},$$

where $\xi_0$ is molar density of water at reference pressure, $\xi_1$ is molar density of water at the grid’s pressure, $n_1$ is moles of water component, and $c_1$ is the compressibility of water.

For hydrocarbon phases, the corresponding derivative is calculated from the equation of state with

$$\left( \frac{\partial V_j}{\partial P} \right)_{N_i} = \sum_{k=1}^{n_c} \left[ v_j + n_j \left( \frac{\partial v_j}{\partial n_{kj}} \right) \right] \left( \frac{\partial n_{kj}}{\partial n_{k2}} \right)_{N_i} + n_j \left( \frac{\partial v_j}{\partial P} \right)_{n_x j}, \hspace{1cm} \text{for } j = 2, \ldots, n_p. \hspace{1cm} (2.85)$$

In the above equation, $V_j$ is volume of fluid phase $j$, $v_j$ is molar volume of phase $j$, $n_j$ is the moles of all components in fluid phase $j$, $n_{kj}$ is the moles of component $k$ in fluid phase $j$, and $N_i$ is the total moles of component $i$.

In equation (2.81), I analytically calculated $\frac{\partial v_j}{\partial n_{k2}}$, where $v_j$ is the molar volume of fluid.
phase \( j \) and \( n_{kj} \) is moles of component \( k \) in fluid phase \( j \). Similarly, I expressed the partial derivative of molar volume with respect to pressure, \( \frac{\partial v_j}{\partial P} \), as

\[
\frac{\partial v_j}{\partial P} = \frac{RT}{P^2} [P(\frac{\partial Z_j}{\partial P}) - Z_j] \quad \text{for } j = 2, \ldots, n_p,
\]

(2.86)

where \( v_j \) is molar volume of fluid phase \( j \), \( P \) is pressure, \( T \) is the temperature, \( R \) is universal gas constant, \( Z_j \) is compressibility of fluid phase \( j \), and \( n_p \) is the number of phases.

For the case of two hydrocarbon phases, I found the partial derivative of moles of component \( k \) in fluid phase 2 with respect to pressure, \( \left( \frac{\partial n_{k2}}{\partial P} \right) \) by solving the following set of equations:

\[
\sum_{k=1}^{n_c} \left[ \frac{\partial \ln f_{s2}}{\partial n_{k2}} + \frac{\partial \ln f_{s3}}{\partial n_{k3}} \right] \left( \frac{\partial n_{k2}}{\partial P} \right) = \left( \frac{\partial \ln f_{s3}}{\partial P} \right)_{n_r3} - \left( \frac{\partial \ln f_{s2}}{\partial P} \right)_{n_r2},
\]

for \( s = 1, \ldots, n_c \) and \( i = 1, \ldots, n_c \),

(2.87)

where \( f_{sj} \) is the fugacity of component \( s \) in fluid phase \( j \), \( n_{kj} \) is the moles of component \( k \) in fluid phase \( j \), \( P \) is pressure, and \( n_c \) is the number of components.

### 2.8 Initial and Boundary Conditions

I initialized the reservoir at the start of the simulation. For hydrocarbon components, molar fraction of each component is given as the initial condition of the reservoir. Pressures, moles of each component, and saturation of phases initialized based on the assumption of thermodynamic equilibrium inside the isothermal reservoir.

In this simulator, the end boundary of the reservoir is assumed to be impermeable, whereupon the normal flux of components is zero, i.e.,

\[
\overrightarrow{n} \cdot \overrightarrow{F}_{ij} = 0,
\]

(2.88)

where \( \overrightarrow{n} \) is the unit normal vector to the boundary, and

\[
\overrightarrow{F}_{ij} = \xi_{ij} x_{ij} \overrightarrow{u}_j,
\]

(2.89)
where $\xi_j$ is molar density of fluid phase $j$, $x_{ij}$ is molar fraction of component $i$ in fluid phase $j$, and $\vec{u}_j$ is velocity of component $i$. At the wellbore, I supported different conditions such as injection or production with controlled flow rate or controlled wellbore pressure.
Chapter 3

Computational Approach

3.1 Introduction

This chapter describes the discretization of the pressure and mass conservation equations using the finite-difference method for 1D radial fluid flow. The simulation algorithm is based on solving the pressure equation in implicit form and updating the compositions explicitly. Following the calculation of overall composition, each fluid phase composition is determined with a phase-behavior module.

3.2 Discretization of the Pressure Equation

From Chapter 2, the pressure equation is given by

\[
(V_0^p c_f - (\frac{\partial V_t}{\partial P})_N_i)(\frac{\partial P}{\partial t}) - V_b \sum_{i=1}^{n_c+1} \nabla_t \cdot (\sum_{j=1}^{n_p} k \lambda_{rj} \xi_j x_{ij} \nabla P) \]

\[
= V_b \sum_{i=1}^{n_c+1} \nabla_t \cdot (\sum_{j=1}^{n_p} k \lambda_{rj} \xi_j x_{ij} (\nabla P_{c2j})) + \sum_{i=1}^{n_c+1} \nabla_t q_i, \quad (3.1)
\]

where

- \( V_0^p \) is pore volume at reference pressure,
• $V_b$ is bulk volume,
• $c_f$ is compressibility of the rock,
• $P$ is pressure,
• $N_i$ is total moles of component $i$,
• $V_{ti}$ is partial molar volume defined in Equation (2.78),
• $\bar{k}$ is permeability tensor,
• $\lambda_{rj}$ is relative mobility of fluid phase $j$,
• $\xi_j$ is molar density of fluid phase $j$,
• $x_{ij}$ is molar fraction of component $i$ in fluid phase $j$,
• $P_{c2j}$ is capillary pressure of fluid phase $j$ and oil phase, and
• $q_i$ is flow rate of component $i$.

Using finite difference method, the time derivative becomes

$$[V^0_p c_f - \left( \frac{\partial V^i_p}{\partial P} \right)_{N_i} \frac{\partial P}{\partial t} = \frac{1}{\Delta t} \left( V^0_p c_f - \frac{\partial V^i_p}{\partial P} \right)_{r\theta z} (P^n_{r\theta z} - P^n_{r\theta z}),]$$

(3.2)

where the subscript $r\theta z$ identifies the spatial coordinates and superscripts $n$ and $n + 1$ are used to indicate time levels. The spatial derivative in the second term on the left-hand side of Equation (3.1) can be expressed as

$$\nabla \cdot \bar{k}\lambda_{rj}\xi_j x_{ij} \nabla P = \frac{1}{r} \frac{\partial}{\partial r} (k\lambda_{rj}\xi_j x_{ij} r \frac{\partial P}{\partial r})$$

(3.3)

Substituting $\epsilon = r^2$ and rearranging Equation (3.3), we obtain

$$\frac{1}{r} \frac{\partial}{\partial r} (k\lambda_{rj}\xi_j x_{ij} r \frac{\partial P}{\partial r}) = 4 \frac{\partial}{\partial \epsilon} (k\lambda_{rj}\xi_j x_{ij} \frac{\partial P}{\partial \epsilon}).$$

(3.4)
We then discretize Equation (3.4) to obtain

\[
\frac{4}{\epsilon_{m+1/2} - \epsilon_{m-1/2}} \left[ (\epsilon k \lambda r_j \xi_j x_{ij})_{(m+1/2)} \frac{P_{m+1} - P_m}{\epsilon_{m+1} - \epsilon_m} - (\epsilon k \lambda r_j \xi_j x_{ij})_{(m-1/2)} \frac{P_m - P_{m-1}}{\epsilon_{m-1} - \epsilon_m} \right], \tag{3.5}
\]

where subscripts \( m - 1/2, m, \) and \( m + 1/2 \) indicate the left, center, and right side of the element \( m \), respectively. After substituting the finite-difference expressions, we express Equation (3.1) as

\[
(V^0_p c_f - \frac{\partial V_t}{\partial P})_{xy z} P_{m+1}^{n+1} - (\Delta_r A \Delta_r P^{n+1}) \]

\[
= (V_t - V_p)_{r \theta z}^n + (V^0_p c_f - \frac{\partial V_t}{\partial P})_{r \theta z}^n + \Delta t \sum_{i=1}^{n_e+1} (\nabla_{ti})_{r \theta z}^n q_i + \Delta t (B_{cap})_{r \theta z}^n, \tag{3.6}
\]

where \((V_t - V_p)_{r \theta z}^n\) is the difference between fluid volume and pore volume at the previous time step. This difference arises because of numerical errors in the calculation of pressure and saturation from the previous time step [32] [1]. In Equation (3.6), \((\Delta_r A \Delta_r P)\) is given by

\[
(\Delta_r A \Delta_r P) = A_{r+1/2}(P_{r+1} - P_r) - A_{r-1/2}(P_r - P_{r-1}), \tag{3.7}
\]

and

\[
A_{m \pm 1/2} = \Delta t \sum_{i=1}^{n_e+1} (\nabla_{ti})_{m}^n \sum_{j=1}^{n_p} (x_{ij} T_j)_{m \pm 1/2}^n \text{ for } m = r, \tag{3.8}
\]

where \( T_j \) is the transmissibility corresponding to the \( j \) – \( th \) fluid phase.

### 3.2.1 Upstream Weighting

In Equation (3.5), we have used one-point upstream weighting to approximate molar density, \((\xi_j)_{m \pm 1/2}\), phase composition, \((x_{ij})_{m \pm 1/2}\), and relative mobility, \((\lambda_{rj})_{m \pm 1/2}\). For example, upstreaming for molar density is given by

\[
(\xi_j)_{(m-1/2)}^n = (\xi_j)_{(m-1)}^n \text{ if } (\Phi_j)_{m} > (\Phi_j)_{m-1}, \tag{3.9}
\]

\[
(\xi_j)_{(m+1/2)}^n = (\xi_j)_{(m)}^n \text{ if } (\Phi_j)_{m} > (\Phi_j)_{m+1}. \tag{3.10}
\]
and

\[
(\xi_j)^n_{m-1/2} = (\xi_j)^n_m \quad \text{if} \quad (\Phi_j)m < (\Phi_j)m,
\]

\[
(\xi_j)^n_{m+1/2} = (\xi_j)^n_{m+1} \quad \text{if} \quad (\Phi_j)m < (\Phi_j)m+1.
\]

(3.11)

(3.12)

where \((\Phi_j)m\) is the potential of the \(j\)-th fluid phase at the \(m\)-th element. This term specifically in radial direction is equal to the sum of capillary pressure and the pressure of grid, namely,

\[
(\Phi_j)m = P_m + (P_{c2j})_m.
\]

(3.13)

### 3.2.2 Transmissibility

The transmissibility terms in Equation (3.8) are defined as [3]

\[
(T_j)^n_{m\pm1/2} = (\lambda_{rj}\xi_j)^n_{m\pm1/2} T_{m\pm1/2}
\]

\[
= (\frac{k_{rj}\xi_j}{\mu_j})^n_{m\pm1/2} T_{m\pm1/2},
\]

(3.14)

where \(k_{rj}\), \(\xi_j\), and \(\mu_j\) are relative permeability, molar density, and viscosity of fluid phase \(j\), respectively. In the above equation, \(T_{m\pm1/2}\) is calculated from [23]

\[
T_{m\pm1/2} = \frac{2\pi h}{\ln \frac{r_{m\pm1/2}}{r_m} + \ln \frac{r_{m\pm1/2}}{K_{m+1}} + \frac{K_{m+1}}{K_m}}.
\]

(3.15)

where \(K_m\) and \(K_{m+1}\) are corresponding permeabilities of elements \(m\) and \(m+1\).

### 3.2.3 Capillary-Pressure Term

The capillary term \(B_{cap}\) in Equation (3.6) is defined as

\[
B_{cap} = \sum_{i=1}^{n_z+1} (\nabla\tau)^n_{i\theta} \sum_{j=1}^{n_p} \Delta_r(x_{ij} T_j)^n \Delta_r(P_{c2j}^n),
\]

(3.16)
where $\nabla V_i$ is the partial derivative of total fluid volume with respect to component $i$, and

$$
\Delta_r(x_{ij} T_j)^n \Delta_r (P_{c2j})^n =
(x_{ij} T_j)^{n+1} [(P_{c2j})_{r+1} - (P_{c2j})_r]^n - (x_{ij} T_j)^n [(P_{c2j})_r - (P_{c2j})_{r-1}]^n,
$$

where $x_{ij}$ is the mole fraction of the $i$-th component in the $j$-th fluid phase, $P_{c2j}$ is the capillary pressure of fluid phase $j$ and oil phase, $n$ is the time level, and $r$, $r + 1/2$, and $r - 1/2$, are the radial coordinates of center, right boundary, and left boundary of the corresponding grid block.

### 3.3 Discretization of the Molar Mass Equation

The moles of each component is calculated explicitly after calculating pressure of each grid block. Previously, we expressed the mass conservation equation in the form of Equation (2.36) (page 14). In this section, we discretize and rearrange Equation (2.36) as

$$
N_i^{n+1} = N_i^n + \Delta t \left\{ \sum_{j=1}^{n_p} \Delta_r (x_{ij} T_j)^n \Delta_r (P^{n+1} + P_{c2j}) + q_i \right\}, \quad \text{for } i = 1, \ldots, n_c, n_c + 1,
$$

where $N_i$ is the moles of component $i$, $x_{ij}$ is the mole fraction of component $i$ in the fluid phase $j$, $P_{c2j}$ is capillary pressure of fluid phase $j$ and oil phase, and $q_i$ is flow rate of component $i$. The convection term in Equation (3.18) is elaborated as

$$
\Delta_r(x_{ij} T_j)^n \Delta_r (P^{n+1} + P_{c2j})^n = (x_{ij} T_j)^{n+1} [(P^{n+1} + P_{c2j})_{r+1} - (P^{n+1} + P_{c2j})_r]^n
-(x_{ij} T_j)^n [(P^{n+1} + P_{c2j})_r - (P^{n+1} + P_{c2j})_{r-1}]^n.
$$

### 3.4 Boundary and Well Conditions

In this section, I describe different boundary conditions for the wells such as injection with constant volume rate, injection with constant bottomhole pressure, production with constant volumetric rate, and production with constant bottomhole pressure.
3.4.1 Boundary Conditions

The no-flow condition is given by
\[ \vec{n} \cdot \vec{u}_j = 0, \]
(3.20)
where \( \vec{n} \) is the unit normal vector along the no-flow boundary. In this model, I impose Equation (3.20) by setting the transmissibility, \( T_{m \pm 1/2} \), in Equation (3.14), equal to zero. For inflow boundaries, the total injection rate of each component is specified and depends on the specific well condition.

3.4.2 Well Models

In this model, the sink or source term in the mass conservation equations is representative of wells in the reservoir. Wells are constrained with one of the following boundary condition constraints.

1. Flow rate, and
2. Bottomhole pressure.

Volumetric flow rate and bottomhole pressure of the well are related through the productivity index, namely,
\[ Q_j = PI_j (P_{wf} - P_j), \]
(3.21)
where \( PI_j \) is productivity index, \( Q_j \) is volumetric flow rate \([\text{ft}^3/\text{D}]\), \( P_{wf} \) is bottomhole pressure, and \( P_j \) is pressure of fluid phase \( j \). For one-dimensional radial direction, the phase productivity index can be written as
\[ PI_j = \frac{k_r \Delta z \lambda_{rj}}{25.14872 \ln \frac{r_2}{r_w}}, \]
(3.22)
where \( k \) is permeability in the radial direction, \( \Delta z \) is grid thickness, \( \lambda_{rj} \) is relative mobility of fluid phase \( j \), and \( r_w \) and \( r_o \) are the radii of wellbore and center of first grid, respectively.
Injection with Constant Volume Rate

Total volumetric flow rate, $Q_t$, and total molar flow rate of hydrocarbon components, $(q_t)_{hyd}$, are related by the total molar volume of injected hydrocarbon components, $([v_t]_{hyd})_{inj}$, i.e.,

$$(q_t)_{hyd} = \frac{Q_t}{[v_t]_{hyd}}_{inj}, \quad (3.23)$$

where total molar volume of the hydrocarbon components of injected fluid, $([v_t]_{hyd})_{inj}$, is calculated by

$$(v_t)_{hyd} = (1 - f_v)_{inj} + \left(\frac{f_v}{\xi_2}\right)_{inj}, \quad (3.24)$$

where $f_v$ is molar fraction of vapor phase in the injected fluid, and $\xi_2$ and $\xi_3$ are, respectively, molar densities of oil, and vapor phase in the injected fluid. Furthermore, the flow rate of each component is given by

$$q_i = (z_i)_{inj} (q_t)_{hyd}, \quad (3.25)$$

where $z_i$ is mole fraction of component $i$ in the injected fluid. On the other hand, molar flow rate of the water component is given by

$$(q_t)_{n_{c+1}} = (Q_t)_{aqu} (\xi_1)_{inj}, \quad (3.26)$$

where $\xi_1$ is molar density of water in the injected fluid. Moreover, values of $(\xi_j)_{inj}$ and $(f_v)_{inj}$ are determined by flash calculations for the injected fluid. The bottomhole pressure is determined using the following equation

$$P_{wf} = P + \frac{Q_t}{PI_t}, \quad (3.27)$$

where

$$PI_t = \sum_{j=1}^{n_p} PI_j \quad (3.28)$$

and $P$ is the pressure of the grid adjacent to the wellbore.
Injection with Constant Bottomhole Pressure

In this type of well constraint, injected fluid is described by the bottomhole pressure, $P_{wf}$, molar fraction of water, $(f_1)_{inj}$, and the composition of hydrocarbon components, $(z_i)_{inj}$. Specifically, in this single-layer model, I compute flow rate of each component with the equation

$$q_i = [1 - (f_1)_{inj}](z_i)_{inj}q_t,$$

(3.29)

where $(f_1)_{inj}$ is molar fraction of water, $(z_i)_{inj}$ is mole fraction of component $i$ in the injected fluid, and $q_t$ is total molar volume rate. For the case of the water component,

$$q_{n_c + 1} = (f_1)_{inj}q_t.$$  

(3.30)

The total molar volume rate, $q_t$, and total volume rate, $Q_t$, are related by

$$q_t = \frac{Q_t}{(v_t)_{inj}}.$$  

(3.31)

where

$$Q_t = \sum_{j=1}^{n_p} PI_j [P_{wf} - P_j],$$

(3.32)

and

$$(v_t)_{inj} = (f_1)_{inj} + (1 - (f_1)_{inj})[\frac{1 - f_v}{\xi_2} + \frac{f_v}{\xi_3}],$$

(3.33)

where $f_v$ is molar fraction of the vapor phase, and $\xi_2$ and $\xi_3$ are the molar densities of the oil and gas phase, respectively. Replacing the well term in the pressure equation, Equation (3.6), with Equations (3.29) and (3.30), I obtain a new pressure equation at the new time level. Afterward, I calculate the flow rate of each component using Equations (3.29) and (3.30).

Production with Constant Volumetric Rate

In this type of well, the total volumetric production rate, $Q_t$, is specified. The production rate for every component is calculated with

$$q_i = \frac{(q_t) \sum_{j=1}^{n_p} \xi_j x_{ij} PI_j}{\sum_{j=1}^{n_p} \xi_j PI_j} \quad \text{for} \quad i = 1, \ldots, n_c,$$

(3.34)

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and

\[ q_i = \frac{(q_t) \xi_i P I_i}{\sum_{j=1}^{n_p} \xi_j P I_j}, \]  

(3.35)

where total molar rate of production is calculated with

\[ q_t = \frac{Q_t \sum_{j=1}^{n_p} \xi_j P I_j}{P I_t}, \]  

(3.36)

and \( \xi_j \) is molar density of fluid phase \( j \), \( x_{ij} \) is molar fraction of component \( i \) in the fluid phase \( j \), \( P I_j \) is productivity index of fluid phase \( j \), and \( P I_t \) is total productivity index.

**Production with Constant Bottomhole Pressure**

For this type of well condition, the production rate for each component is obtained from

\[ (q_i) = \sum_{j=2}^{n_p} (\xi_j x_{ij} P I_j)(P_{wf} - P_j) \quad \text{for} \quad i = 1, \ldots, n_c, \]  

(3.37)

and

\[ (q_{n_c+1}) = (\xi_1 P I_1)(P_{wf} - P_1), \]  

(3.38)

where \( \xi_j \) is molar density of fluid phase \( j \), \( P_{wf} \) is bottomhole pressure, and \( n_p \) and \( n_c \) are numbers of fluid phases and components, respectively.

### 3.5 Computation of Saturation

After the calculation of moles of each component in all grid blocks, we calculate the saturation of each phase. In our model, \( S_1 \), \( S_2 \) and \( S_3 \) are, respectively, saturation of aqueous, oil, and gas phase. Saturation of aqueous phase is calculated with

\[ S_1^{n+1} = \frac{N_w^{n+1}}{(V_p \xi_1)^{n+1}}, \]  

(3.39)

where \( (\xi_1)^{n+1} \) is the molar density of water at time level \( n+1 \), \( (V_p)^{n+1} \) is the pore volume at time level \( n+1 \), and \( N_w^{n+1} \) is total moles of water component. On the other hand, saturation
of the gas phase is given by

\[ S_3^{n+1} = \frac{(1 - S_1^{n+1})(F_v^n)^{n+1}}{\sum_{j=2}^{n_p} F_j^n \xi_j^n}, \]  

(3.40)

where \( F_v \) is molar fraction of the vapor phase, \( \xi_j \) is molar density of the fluid phase \( j \), and \( F_j \) is the molar fraction of the phase \( j \). Finally, saturation of oil is calculated with

\[ S_2^{n+1} = 1 - S_1^{n+1} - S_3^{n+1}. \]  

(3.41)

3.6 Material Balance Error

In our model, we have modified equation (3.6) to include the material balance error as \( V_t - V_p \), where \( V_p \) is the pore volume at the current pressure, and \( V_t \) is the total fluid volume, i.e.,

\[ V_t = \sum_{j=1}^{n_p} n_j v_j, \]  

(3.42)

where \( n_j \) is the total moles of all hydrocarbon components in fluid phase \( j \), and \( v_j \) is the molar volume of the fluid phase \( j \).

3.7 Automatic Time Step Control

We implemented the method of relative change ([14] and [3]) to update the time step size. The procedure for updating the time step is as follows

1. Obtain time step bounds

   - Initial time step size, \( \Delta t_{\text{init}} \),
   - Maximum and minimum time step size, \( \Delta t_{\text{max}} \) and \( \Delta t_{\text{min}} \),
   - Maximum relative change of pressure, \( \Delta P_{\text{lim}} \),
   - Maximum relative change of saturation, \( \Delta S_{\text{lim}} \),
   - Maximum relative change of volume error, \( \Delta V_{\text{lim}} \),
   - Maximum relative change of moles of component, \( \Delta N_{\text{lim}} \),
2. Calculate maximum changes in the following variables at times \( n \) and \( n + 1 \) for all elements:

\[
\Delta P_{max} = \max \left( \frac{|P_{m}^{n+1} - P_{m}^{n}|}{P_{m}^{n+1}} \right),
\]

\( (3.43) \)

\[
\Delta S_{max} = \max (|(S_{j})_{m}^{n+1} - (S_{j})_{m}^{n}|),
\]

\( (3.44) \)

\[
\Delta V_{max} = \max \left( \frac{|(V_{i})_{m}^{n+1} - (V_{i})_{m}^{n}|}{(V_{i})_{m}^{n+1}} \right),
\]

\( (3.45) \)

\[
\Delta N_{max} = \max \left( \frac{|(N_{i})_{m}^{n+1} - (N_{i})_{m}^{n}|}{(N_{i})_{m}^{n+1}} \right),
\]

\( (3.46) \)

for \( m = 1, \ldots, NG_{radial} \),

\( j = 1, \ldots, n_{p} \),

and \( i = 1, \ldots, n_{c} + 1 \),

where \( P_{m}^{n} \) is pressure at time level \( n \) in the \( m \)–th element, \( (S_{j})_{m}^{n} \) is saturation of the fluid phase \( j \) at time level \( n \) in the \( m \)–th element, \( (V_{i})_{m}^{n} \) is total fluid volume at time level \( n \) in the \( m \)–th element, \( (N_{i})_{m}^{n} \) is total moles of component \( i \) at time level \( n \) in the \( m \)–th element, and \( NG_{radial} \) is number of elements in the grid in radial direction.

3. Update time step size by

\[
\Delta t_{new} = \min (\Delta t_{P}, \Delta t_{S}, \Delta t_{V}, \Delta t_{N}),
\]

\( (3.47) \)

where

\[
\Delta t_{P} = \Delta t_{old} \frac{\Delta P_{lim}}{\Delta P_{max}},
\]

\( (3.48) \)

\[
\Delta t_{S} = \Delta t_{old} \frac{\Delta S_{lim}}{\Delta S_{max}},
\]

\( (3.49) \)

\[
\Delta t_{V} = \Delta t_{old} \frac{\Delta V_{lim}}{\Delta V_{max}},
\]

\( (3.50) \)
and

\[ \Delta t_N = \Delta t_{\text{old}} \frac{\Delta N_{\text{max}}}{\Delta N_{\text{old}}}, \]  \hspace{1cm} (3.51)

4. Constrain updating the time step size

The updated time step should satisfy the following relation

\[ \Delta t_{\text{min}} \leq \Delta t_{\text{new}} \leq \Delta t_{\text{max}}. \]  \hspace{1cm} (3.52)
Chapter 4

Phase Behavior

4.1 Introduction

Chapter 3 describes the solution of the pressure equation to subsequently calculate the mole quantity of each component. This chapter summarizes the algorithm used to calculate the number of phases and their corresponding compositions. The implemented algorithm for the enforcement of phase equilibrium is similar to that of Chang’s [3] and Perschke’s [26]. In addition, this chapter describes the stability analysis, flash calculation for two-phase equilibrium, and phase identifications.

4.2 Phase Stability

In the phase stability calculation, I search for a trial phase with composition $\mathbf{x}$, which minimizes the following equation [3,12]:

$$
\Delta g(\mathbf{x}) = \sum_{i=1}^{n_c} x_i [\mu_i(\mathbf{x}) - \mu_i(\mathbf{z})],
$$

(4.1)

where $\Delta g$ is the molar Gibbs free energy, $\mu_i$ is the chemical potential of component $i$, $\mathbf{z}$ is the overall hydrocarbon composition, and $x_i$ is the molar fraction of component $i$ in the trial phase.
4.2.1 Tangent-Plane Distance Approach

In this method, I solve the following set of nonlinear equations for the independent variable for phase stability, $X_i$, defined by the equation

$$\ln X_i + \ln \varphi_i(\vec{x}) - \ln z_i - \ln \varphi_i(\vec{z}) = 0, \quad i = 1, \ldots, n_c, \quad (4.2)$$

where mole fraction, $x_i$, is related to independent variable of phase stability, $X_i$, by

$$x_i = \frac{X_i}{\sum_{p=1}^{n_c} X_p}, \quad i = 1, \ldots, n_c. \quad (4.3)$$

In addition, I have used the method of successive substitution to solve Equation (4.2)([12]). In this method, at each step, the independent variable of phase stability, $X_i$, is updated by

$$X_i^{\text{new}} = \exp[(\ln z_i + \ln \varphi_i(\vec{x})) - \ln \varphi_i(\vec{z})], \quad i = 1, \ldots, n_c, \quad (4.4)$$

and then $x_i$ is updated with Equation (4.3). Depending upon the assumption for feed composition (i.e., assuming liquid or vapor for feed composition), I choose one of the following values as initial guess for $X_i$:

- **Liquid phase**
  $$X_i = z_i K_i, \quad i = 1, \ldots, n_c, \quad \text{and} \quad (4.5)$$

- **Vapor phase**
  $$X_i = \frac{z_i}{K_i}, \quad i = 1, \ldots, n_c, \quad (4.6)$$

where the $K_i$ values are estimated from Wilson’s correlation [39], namely,

$$K_i = \frac{P_{ci}}{T} \exp[5.37(1 + \omega_i)(1 - \frac{T_{ci}}{T})], \quad i = 1, \ldots, n_c, \quad (4.7)$$

in which $P_{ci}$ and $T_{ci}$ are, respectively, the critical pressure and temperature of component $i$. 
4.2.2 Flash Calculation

Stability analysis indicates whether an specific composition of hydrocarbon components at the desired pressure and temperature is stable or not. In the event that mixture is found unstable, the mixture will split into more than one phase. I have assumed that the mixture splits into two phases, liquid and gas. Flash calculation computes the amount and also composition of each hydrocarbon phase. Equations for two-phase flash are [12]:

- Equality of chemical potential or fugacity at equilibrium, namely,
  \[ f^L_i(T, P, \bar{x}) = f^V_i(T, P, \bar{x}), \]  
  \[ (4.8) \]
  where \( f^L_i \) and \( f^V_i \) are the fugacities of component \( i \) in the liquid, and component \( i \) in the gas, respectively.

- Material balance for components, to wit,
  \[ z_i = F_v y_i + (1 - F_v) x_i, \]  
  \[ (4.9) \]
  where \( x_i \) is the mole fraction of liquid, \( y_i \) is the mole fraction of vapor, and \( F_v \) is the mole fraction of vapor, defined as
  \[ F_v = \frac{n_v}{n_v + n_L}. \]  
  \[ (4.10) \]

- Sum of mole fractions of all phases is equal to one, i.e.,
  \[ \sum_{i=1}^{n_c} x_i = 1, \]  
  \[ (4.11) \]
  and
  \[ \sum_{i=1}^{n_c} y_i = 1. \]  
  \[ (4.12) \]
Successive Substitution Method

In this method, I search for a solution of vapor mole fraction, $F_v$, in an iterative manner. For this purpose, I define the equilibrium ratio, $K_i$, as

$$K_i = \frac{y_i}{x_i}. \quad (4.13)$$

By combining Equations (4.9), (4.11), (4.12), and (4.13), I obtain

$$x_i = \frac{z_i}{1 + F_v(K_i - 1)}, \quad (4.14)$$
$$y_i = K_i x_i, \quad (4.15)$$

and

$$h(F_v) = \sum_{i=1}^{n_c} \frac{z_i(K_i - 1)}{1 + F_v(K_i - 1)} = 0, \quad (4.16)$$

where the last equation is Rachford-Rice’s expression [27]. The fugacity of each component, Equation (4.8), can be related to the equilibrium ratio in Equation (4.13) to give

$$K_i = \frac{y_i}{x_i} = \frac{\psi_L^i}{\psi_v^i}. \quad (4.17)$$

The procedure used to find the composition of each phase, $\mathbf{X}$ and $\mathbf{Y}$, is as follows:

1. Guess the initial values of $K_i$. I used the values estimated from Wilson’s correlation (4.7) as initial guess.
2. Solve Rachford-Rice’s expression, Equation (4.16). I used Newton’s method to solve Rachford-Rice’s expression.
3. Calculate the composition of gas and liquid phases from Equation (4.14) and (4.15).
4. Update $K_i$. I update the equilibrium ratio using $K_i^{\text{new}} = K_i^{\text{old}} \frac{F_v}{F_{vi}}$.

Newton’s Method

Equations (4.8), (4.9), (4.11), and (4.12) define the two-phase flash calculation. I solve $2n_c + 1$ equations using Newton’s method to find $2n_c + 1$ unknowns, $F_v$, $\mathbf{X}$, and $\mathbf{Y}$. This
method is explained in detail in Firoozabadi [12].

Combination of the Successive Substitution Method and Newton’s Method

In this simulator, I use the successive substitution method to obtain the composition of the phases with a tolerance of $10^{-4}$, then I apply Newton’s method to obtain the composition of the phases with a smaller tolerance ($10^{-8}$).

4.3 Phase Identification

This simulator handles three coexisting phases: aqueous, oil, and gas. The aqueous phase is tracked separately. When there are two hydrocarbon phases, the one with greater molar density is labeled as oil and the remaining one as gas. If single-phase hydrocarbon is found to be stable, depending on whether

$$\sum_{i=1}^{n_r} \frac{z_i}{K_i} > \sum_{i=1}^{n_r} z_i K_i,$$

(4.18)

is true or not, then the phase is labeled as gas or liquid.
Chapter 5

Validation of the Simulator

For validation purpose, I compare results obtained with the developed simulator against two commercial reservoir simulators developed by the Computer Modeling Group, CMG. The developed simulator, called UTFECS, is an equation-of-state compositional simulator, thence I chose the Generalized Equation-of-State Model Compositional Reservoir Simulator, GEM for validation. In addition, I use CMG - WinProp to calculate input data for Steam, Thermal, and Advanced Processes Reservoir Simulator, STARS, which enabled me to validate results obtained for aqueous salt concentration. I describe the validation of the simulator for different flow regimes, gas-water, oil-water, and gas-oil-water flow taking place in different rock types.

5.1 Description of Case Studies

The following sections list the reservoir properties, rock types along with the components and their properties.

5.1.1 Reservoir

For all validation exercises, I assume the reservoir properties listed in Table 5.1.
### Table 5.1: List of parameters assumed in the description of the reservoir

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Unit</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Wellbore radius</td>
<td>ft</td>
<td>0.477</td>
</tr>
<tr>
<td>Wellbore outer radius</td>
<td>ft</td>
<td>2000</td>
</tr>
<tr>
<td>Rock compressibility</td>
<td>1/psi</td>
<td>4 × 10⁻⁷</td>
</tr>
<tr>
<td>Reservoir temperature</td>
<td>°F</td>
<td>200</td>
</tr>
<tr>
<td>Logarithmic gridding elements</td>
<td></td>
<td>50</td>
</tr>
</tbody>
</table>

Figure 5.1: Water-oil capillary pressure and relative permeability curves of rock types studied in this thesis. Variables \( k_{ro} \) and \( k_{rw} \) are relative permeability of oil and water, respectively.

#### 5.1.2 Rock Types

I have tested the developed simulator using three rock types. Figure 5.1 shows the assumed capillary pressure and relative permeability curves for these rock types. Table 5.2 lists the remaining properties, such as absolute permeability and porosity assumed for the description of rock types.

### Table 5.2: Absolute permeability, porosity, irreducible water saturation, and irreducible oil saturation assumed for the selected rock types

<table>
<thead>
<tr>
<th></th>
<th>Unit</th>
<th>Rock 1</th>
<th>Rock 2</th>
<th>Rock 3</th>
</tr>
</thead>
<tbody>
<tr>
<td>Absolute Permeability</td>
<td>md</td>
<td>10</td>
<td>100</td>
<td>500</td>
</tr>
<tr>
<td>Porosity</td>
<td>-</td>
<td>0.16</td>
<td>0.25</td>
<td>0.32</td>
</tr>
<tr>
<td>( S_{wir} )</td>
<td>-</td>
<td>0.16</td>
<td>0.11</td>
<td>0.07</td>
</tr>
<tr>
<td>( S_{oir} )</td>
<td>-</td>
<td>0.12</td>
<td>0.12</td>
<td>0.12</td>
</tr>
<tr>
<td>Name</td>
<td>(P_{\text{crit}}) [atm]</td>
<td>(T_{\text{crit}}) [°K]</td>
<td>(\omega)</td>
<td>Mw</td>
</tr>
<tr>
<td>------</td>
<td>----------------</td>
<td>----------------</td>
<td>-------</td>
<td>-------</td>
</tr>
<tr>
<td>C1</td>
<td>45.4</td>
<td>191</td>
<td>0.01</td>
<td>16</td>
</tr>
<tr>
<td>C2</td>
<td>48.2</td>
<td>305</td>
<td>0.1</td>
<td>30.1</td>
</tr>
<tr>
<td>C3</td>
<td>41.9</td>
<td>370</td>
<td>0.15</td>
<td>44.1</td>
</tr>
<tr>
<td>IC4</td>
<td>36</td>
<td>408</td>
<td>0.18</td>
<td>58.1</td>
</tr>
<tr>
<td>IC5</td>
<td>33.4</td>
<td>460</td>
<td>0.23</td>
<td>72.2</td>
</tr>
<tr>
<td>FC6</td>
<td>32.5</td>
<td>508</td>
<td>0.28</td>
<td>86</td>
</tr>
<tr>
<td>FC7</td>
<td>31</td>
<td>543</td>
<td>0.31</td>
<td>96</td>
</tr>
<tr>
<td>FC8</td>
<td>29.1</td>
<td>571</td>
<td>0.35</td>
<td>107</td>
</tr>
<tr>
<td>FC9</td>
<td>26.9</td>
<td>599</td>
<td>0.39</td>
<td>121</td>
</tr>
<tr>
<td>FC10</td>
<td>25</td>
<td>622</td>
<td>0.44</td>
<td>134</td>
</tr>
</tbody>
</table>

Table 5.3: Properties of hydrocarbon components assumed in validation of this simulator. \(P_{\text{crit}}\), \(T_{\text{crit}}\), \(\omega\), Mw, and \(V_{\text{crit}}\) are, respectively, critical pressure, critical temperature, acentric factor, molecular weight, and critical volume of the components. IC4, IC5, and FC6 through FC10 are pseudo components. (Source: CMG-WinProp)

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Unit</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Water compressibility</td>
<td>1/psi</td>
<td>(3.6 \times 10^{-6})</td>
</tr>
<tr>
<td>Viscosity</td>
<td>cp</td>
<td>1.0</td>
</tr>
<tr>
<td>Density</td>
<td>lb/ft³</td>
<td>62.4278</td>
</tr>
</tbody>
</table>

Table 5.4: Assumed properties of the water component

### 5.1.3 Components

For validating my simulator, I select several hydrocarbon components and their corresponding properties from CMG-WinProp. Table 5.3 lists the characteristic properties of these components. Also, I assume properties listed in Table 5.4 for the water component.

### 5.2 Two-Phase Simulations

In this section, I validate results for two-phase flow regimes, i.e. gas-water and oil-water. Initially, I study simulations for single component, and afterwards I test the simulator for cases of multi-components in hydrocarbon phases.
<table>
<thead>
<tr>
<th>Property</th>
<th>Unit</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pressure</td>
<td>psi</td>
<td>1500</td>
</tr>
<tr>
<td>Salt concentration</td>
<td>ppm</td>
<td>168,000</td>
</tr>
<tr>
<td>Sw</td>
<td>-</td>
<td>0.25</td>
</tr>
</tbody>
</table>

Table 5.5: Assumed initial reservoir properties for gas and water.

<table>
<thead>
<tr>
<th>Property</th>
<th>Unit</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pressure</td>
<td>psi</td>
<td>3500</td>
</tr>
<tr>
<td>Salt concentration</td>
<td>ppm</td>
<td>168,000</td>
</tr>
<tr>
<td>Sw</td>
<td>-</td>
<td>0.25</td>
</tr>
</tbody>
</table>

Table 5.6: Summary of initial condition assumed for the reservoir containing oil and water.

5.2.1 Single Component

Depending on the component, I may have gas or oil as the hydrocarbon phase. I have selected C1 and FC7 as two hydrocarbon components which correspondingly yield gas- and oil-phase in the specified reservoir condition. Table 5.3 lists the properties of these components.

Gas-Water Simulation

In simulations of gas-water flow for all rock types, I consider a reservoir with the same initial conditions described in Table 5.5. Moreover, the reservoir contains hydrocarbon component C1 and water. The well constraint is injection of water with a rate of 10 [bbl/day], which has a salinity of 3000 [ppm]. Figures 5.2 through 5.7 compare results obtained with the developed simulator and CMG simulators, GEM and STARS, for the selected rock types at different injection times. These figures indicate that the results obtained with UTFECS agree well with those of the commercial simulator for gas-water flow.

Oil-Water Simulation

For the simulations of oil-water flow in all rock types, I consider a reservoir with initial conditions as summarized in Table 5.6. For this type of flow, I assume that the reservoir contains the hydrocarbon component FC6 and water. The well constraints are injection of water with a bottomhole pressure of 3800 [bbl/day] for 1 day, and then bottomhole fluid
Figure 5.2: **Rock Type 1**: Comparison of calculated (a) pressure and (b) water saturation with CMG-GEM and UTFECS along the radial direction at three different times after the onset of injection.

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Figure 5.3: **Rock Type 1**: Comparison of result for (a) salt concentration and (b) calculated resistivity with CMG-STARS and UTFECS along the radial direction at three different times after the onset of injection.
Figure 5.4: **Rock Type 2**: Comparison of calculated (a) pressure and (b) water saturation with CMG-GEM and UTCFECS along the radial direction at three different times after the onset of injection.
Figure 5.5: **Rock Type 2**: Comparison of result for (a) salt concentration and (b) calculated resistivity with CMG-STARS and UTFECS along the radial direction at three different times after the onset of injection.
Figure 5.6: **Rock Type 3**: Comparison of calculated (a) pressure and (b) water saturation with CMG-GEM and UTFECS along the radial direction at three different times after the onset of injection.
Figure 5.7: **Rock Type 3:** Comparison of result for (a) salt concentration and (b) calculated resistivity with CMG-STARS and UTFECS along the radial direction at three different times after the onset of injection.
production with a rate of 2 [bbl/day]. Figures 5.8 through 5.13 compare results obtained with the developed simulator and those obtained with CMG simulators, GEM and STARS, for the selected rock types at different times after the onset of injection. Comparisons indicate that the results obtained with UTFECS agree with those obtained with the commercial simulator.

5.3 Case Studies for Multi Components

In this section, I describe simulations of fluid flow in which the hydrocarbon phase has multi-components. Similar to the one of single component, different components with different compositions will constitute oil or gas as the hydrocarbon phase for a given value of each pressure and temperature.

Gas-Water Simulation

I consider a reservoir with the initial conditions as described in Table 5.6. Moreover, the reservoir contains hydrocarbon components C1, C2, and C3 with those properties described in Table 5.3. In this case, the well constraint is 1 day of water injection (salt concentration = 3000 [ppm]) at standard conditions with a rate of STW=10 [bbl/day]. Figures 5.2 through 5.7 compare results obtained with the UTFECS and CMG simulators, GEM and STARS, for the selected rock types at different times after the onset of water injection.

Oil-Water Simulation

For simulations of oil-water fluid flow, I assume a reservoir with initial conditions as described in Table 5.6.

In addition, the reservoir includes hydrocarbon components FC10 and FC18 with an initial composition of 0.7 and 0.3 molar fraction, respectively. The well constraint is injection of oil with composition (0.1 0.9) at a bottomhole pressure of 3800 [bbl/day] for 1 day, and then a bottomhole fluid production with a rate of 5 [bbl/day]. Figures 5.16 and 5.17 compare results obtained with the UTFECS and CMG simulators, GEM and STARS, for the selected rock types at different times after the onset of injection. Results obtained with
Figure 5.8: Rock Type 1: Comparison of calculated (a) pressure and (b) water saturation with CMG-GEM and UTFECS along the radial direction at three different times after the onset of injection. The boundary condition is 1 day injection of oil with a bottomhole pressure of 3800 [psi], followed by 1 day of bottomhole fluid production with a rate of 2 [bbl/day].
Figure 5.9: **Rock Type 1:** Comparison of result for (a) oil saturation and (b) calculated resistivity with CMG-STS and UTFECS along the radial direction at three different times after the onset of injection. The boundary condition is 1 day injection of oil with a bottomhole pressure of 3800 [psi], followed by 1 day a bottomhole fluid production with a rate of 2 [bbl/day].
Figure 5.10: **Rock Type 2:** Comparison of calculated (a) pressure and (b) water saturation with CMG-GEM and UTFECS along the radial direction at three different times after the onset of injection. The boundary condition is 1 day injection of oil with a bottomhole pressure of 3800 [psi], followed by 1 day a bottomhole fluid production with a rate of 2 [bbl/day].
Figure 5.11: **Rock Type 2:** Comparison of result for (a) oil saturation and (b) calculated resistivity with CMG-STARS and UTFECS along the radial direction at three different times after the onset of injection. The boundary condition is 1 day injection of oil with a bottomhole pressure of 3800 [psi], followed by 1 day a bottomhole fluid production with a rate of 2 [bbl/day].
Figure 5.12: **Rock Type 3:** Comparison of calculated (a) pressure and (b) water saturation with CMG-GEM and UTFECS along the radial direction at three different times after the onset of injection. The boundary condition is 1 day injection of oil with a bottomhole pressure of 3800 [psi], followed by 1 day a bottomhole fluid production with a rate of 2 [bbl/day].
Figure 5.13: **Rock Type 3**: Comparison of result for (a) oil saturation and (b) calculated resistivity with CMG-STARS and UTFECS along the radial direction at three different times after the onset of injection. The boundary condition is 1 day injection of oil with a bottomhole pressure of 3800 [psi], followed by 1 day a bottomhole fluid production with a rate of 2 [bbl/day].
Figure 5.14: **Rock Type 1**: Comparison of calculated (a) pressure and (b) water saturation with CMG-GEM and UTFECS along the radial direction at three different times after the onset of injection. Initial Pressure = 1500 [psi], initial water saturation=0.25, and composition (0.3, 0.6, and 0.1) of components C1, C2, C3. The maximum time of water injection is 1 day with surface rate of 10 [bbl/day].
Figure 5.15: **Rock-type 1**: Comparison of result for (a) salt concentration and (b) calculated resistivity with CMG-STARS and UT-FECS along the radial direction at three different times after the onset of injection. Initial Pressure = 1500 [psi], Initial water saturation = 0.25, and composition (0.3, 0.6, and 0.1) of components C1, C2, C3. The maximum time of water injection is 1 day with surface rate of 10 [bbl/day].
UTFECS closely match the results obtained with the commercial simulator whenever I have multiple components in the oil phase.

5.4 Three-Phase Simulations

In this section, I compare simulation results obtained for the case of three-phase fluid flow.

- **3 hydrocarbon components:**
  
  For the first case, I have 3 hydrocarbon components: C1, C3, and FC7 and assume an initial composition of (0.4, 0.3, 0.3) in the reservoir. In order to enforce three-phase flow, I have selected a pressure of 800 [psi] and a temperature of 200 [°F] in the phase envelope so that the composition has three coexisting phases. Initial water saturation was assumed equal to 0.25. Other parameters necessary for the description of the reservoir are the same as those described in previous simulations. The boundary condition is 1 day of injection of oil with a composition (0.1, 0.3, 0.6) of C1, C3, and FC7 at a bottomhole pressure constraint of 1300 [psi]. Figures 5.18 and 5.19 compare results obtained with the UTFECS and CMG-GEM. Results obtained with UTFECS coincide with those obtained with the commercial simulator for three-phase flow.

- **4 hydrocarbon components:**
  
  For the first case, I have 4 hydrocarbon components, namely, C1, C2, FC6, and FC7 with an initial composition (0.55, 0.35, 0.05, 0.05) in the reservoir. In order to enforce three-phase flow, I selected a pressure 800 [psi] and a temperature 200 [°F] in the phase envelope for this composition (shown in Figure 5.20). Initial water saturation was assumed equal to 0.25. Remaining parameters necessary for the description of the reservoir are the same as those described in previous simulations. The boundary condition is 1 day of injection of oil with a composition (0.15, 0.15, 0.35, 0.35) of C1, C2, FC6, and FC7 at a bottomhole pressure of 1800 [psi]. Figures 5.21 and 5.22 compare results obtained with the developed simulator and CMG-GEM. UTFECS’s results strongly match those obtained with the commercial simulator for three-phase flow.
Figure 5.16: **Rock Type 2**: Comparison of calculated (a) pressure and (b) water saturation with CMG-GEM and UT-FECS along the radial direction at three different times after the onset of injection. The boundary condition is 1 day injection of oil with composition (0.1, 0.9) of FC10 and FC18 with a bottomhole pressure constraint of 3800 [psi], followed by 1 day production of a bottomhole fluid with a rate of 5 [bbl/day].
Figure 5.17: **Rock Type 2**: Comparison of results for (a) oil saturation and (b) calculated resistivity with CMG-STARS and UT-PECS along the radial direction at three different times after the onset of injection. The boundary condition is 1 day injection of oil with composition (0.1, 0.9) of FC10 and FC18 with a bottomhole pressure constraint of 3800 [psi], followed by 1 day production of a bottomhole fluid with a rate of 5 [bbl/day].
Figure 5.18: **Rock Type 3**: Comparison of calculated (a) pressure and (b) water saturation with CMG-GEM and UTFECS along the radial direction at three different times after the onset of injection. The boundary condition is 1 day of injection of oil with a composition (0.1, 0.3, 0.6) of C1, C3, and FC7 a bottomhole pressure of 1300 [psi].
Figure 5.19: **Rock Type 3**: Comparison of calculated (a) oil and (b) gas saturation with CMG-GEM and UT-FECS along the radial direction at three different times after the onset of injection. The boundary condition is 1 day of injection of oil with a composition (0.1, 0.3, 0.6) of C1, C3, and FC7 at a bottomhole pressure of 1300 [psi].
Figure 5.20: Phase envelope for the 4 hydrocarbon components C1, C2, FC6, and FC7 with a composition of (0.55, 0.35, 0.05, 0.05).
Figure 5.21: Rock Type 2: Comparison of calculated (a) pressure and (b) water saturation with CMG-GEM and UT-FECS along the radial direction at three different times after the onset of injection. The boundary condition is 1 day of injection of oil with a composition (0.15, 0.15, 0.35, 0.35) of C1, C2, FC6, and FC7 at a bottomhole pressure of 1800 [psi].
Figure 5.22: Rock type 2: Comparison of calculated (a) oil and (b) gas saturation with CMG-GEM and UT-FECS along the radial direction at three different times after the onset of injection. The boundary condition is 1 day of injection of oil with a composition (0.15, 0.15, 0.35, 0.35) of C1, C2, FC6, and FC7 at a bottomhole pressure of 1800 [psi].
5.5 Variable Flow Rate

For the simulations of time-variable flow rate, I consider a reservoir with initial conditions as summarized in Table 5.6. For this type of flow, I assume that the reservoir contains the hydrocarbon component FC6 and water. Figure 5.23 shows the imposed flow rate at different times after the onset of injection. Figures 5.24 through 5.26 compare results obtained with the developed simulator to those obtained with CMG simulators, GEM and STARS, at different times after the onset of injection. Comparisons indicate that results obtained with UTFECS agree with those obtained with the commercial simulator.
Figure 5.24: **Variable Flow Rate**: Comparison of radial profiles of pressure at different times after the onset of injection. Pressure increases at the beginning of injection corresponding to the flow rate shown in Figure (5.23). Invasion times are = \([0.011, 0.108, 1.088, 10.877, 108.771]\) seconds.

Figure 5.25: **Variable Flow Rate**: Comparison of radial profiles of pressure at different times after the onset of injection. Pressure decreases with time after 0.002 day of injection corresponding to the flow rate shown in Figure (5.23). Invasion times are = \([0.012, 0.126, 1.259]\) days.
Figure 5.26: **Rock type 2:** Comparison of radial profiles of water saturation and salt concentration at different times after the onset of injection. Figure (5.23) shows the imposed flow rate at different times. Radial profiles are shown at the invasion times = [0.011, 0.109, 1.088, 10.877, 108.771, 1087.71, 10877.15, 108771.55] seconds after the onset of injection.
Chapter 6

Simulation of Mud-Filtrate Invasion

This chapter discusses the effect of mud-filtrate invasion on fluid-flow simulations. I implement a mudcake model in the developed 1D radial compositional simulator (UTFECS) as described in previous chapters. The mudcake model allows one to thicken the mudcake and to change the mudcake’s permeability and porosity with time, and is coupled to the assumed formation properties. Simulation results are compared to those obtained with commercial software.

6.1 Formulation

The process of mud-filtrate invasion dynamically couples mud and rock properties. Properties of mud and rock control mudcake growth during mud-filtrate invasion. Dewan and Chenevert [11] performed a laboratory experiment for WBM invasion to study both mudcake buildup and mud-filtrate invasion. They proposed that mudcake permeability and mudcake pressure differential are related by the equation

\[ k_{mc}(t) = \frac{k_{mc0}}{P_{mc(t)}} \]

(6.1)
where $k_{mc0}$ is mudcake reference permeability, $P_{mc}$ is mudcake pressure differential, and $v$ is a compressibility exponent which is in the range of 0.4 to 0.9. Moreover, Dewan and Chenevert [11] introduced an expression for the time evolution of mudcake porosity, given by

$$
\phi_{mc}(t) = \frac{\phi_{mc0}}{P_{mc}^{\delta}(t)},
$$

where $\phi_{mc0}$ is mudcake reference porosity and $\delta$ is a multiplier for the porosity exponent which is in the range of 0.1 to 0.2.

Chin [6] introduced a relation for the time evolution of mudcake thickness assuming that solid particles in the mud do not enter the formation, given by

$$
r_{mc} \cdot dr_{mc} = f_s (1 - f_s) [1 - \phi_{mc}(t)] \cdot \frac{k_{mc}P_{mc}dt}{\mu_f},
$$

where $f_s$ is mud solid fraction, $r_{mc}$ is mudcake thickness, $dr_{mc}$ is differential mudcake thickness, $dt$ is differential time, and $\mu_f$ is mud-filtrate viscosity.

Wu et al. [40] implemented a mudcake model with a black-oil simulator. In this research I implement an accurate model for mudcake growth with a 1D radial EOS compositional simulator. I assume that at the beginning mudcake has a thickness of $10^{-9}$[inch] and fluid flow in the mudcake grid (first grid) is solely single phase. The procedure for the simulation is as follows:

1. Calculate mudcake pressure differential:
   Mudcake pressure differential is given by
   
   $$
P_{mc} = P_w - P_2,
   $$

   where $P_w$ is the pressure at the sandface and $P_2$ is pressure of the first grid in the radial direction.

2. Update mudcake properties:
   Equations (6.1) and (6.2) update mudcake permeability and mudcake porosity.

3. Calculate mudcake thickness:
Equation (6.3) gives the mudcake thickness at the current mudcake condition.

4. Update transmissibilities:

Transmissibilities of the first and second gridblocks in the radial direction are updated using Equation (3.15), i.e.,

\[
T_{m+1/2} = \frac{2\pi h \ln \frac{r_{m+1}}{r_{m+1/2}}}{K_{m+1}} + \ln \frac{r_{m+1/2}}{r_m} \frac{\ln \frac{r_{m+1/2}}{r_m}}{K_m}
\]

5. Update phase productivity index:

The thickness and permeability of the first grid (mudcake) changes, hence the phase productivity index changes to a new value with Equation (3.22), namely,

\[
PI_j = \frac{k_r \Delta z \lambda_j}{25.14872 \ln \frac{r_r}{r_w}}.
\]

6. Solve the pressure equation.

7. Calculate the flow rate.

8. Update concentrations and all other properties and move to the next time step.

### 6.2 Validation of the Simulations

In this section, I simulate an experiment performed with field Mud 97074 [11]. Physical properties of the mudcake and reservoir are listed in Table 6.1. Figure 6.1 compares the volume of injected filtrate obtained with UTFECS against the experimental data. At \( t = 0 \) there is about 0.433 cm\(^3\) difference between filtrate volume calculated with numerical simulations and experimental data, which may be associated to spurt loss. Figure 6.1 shows an acceptable agreement between numerical simulations and experimental data.

In addition, I validate end-points of the flow rates obtained for the simulation of mud-filtrate invasion. At the beginning of mud-filtrate invasion, flow rate is equal to that without mudcake. Table 6.2 summarizes the assumed parameters for the description of mudcake and the reservoir in the simulations of mud-filtrate invasion. Figures 6.3 and 6.4
<table>
<thead>
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<th>Parameter</th>
<th>Unit</th>
<th>Value</th>
</tr>
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<tr>
<td>Solid fraction, $f_s$</td>
<td>-</td>
<td>0.231</td>
</tr>
<tr>
<td>Mudcake reference permeability, $k_{mc0}$</td>
<td>md</td>
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</tr>
<tr>
<td>Mudcake reference porosity, $\phi_{mc0}$</td>
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<td>0.59</td>
</tr>
<tr>
<td>Compressibility exponent, $v$</td>
<td>-</td>
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</tr>
<tr>
<td>Porosity exponent, $\delta$</td>
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<tr>
<td>Mudcake thickness limit</td>
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</tr>
<tr>
<td>Initial reservoir pressure</td>
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</tr>
<tr>
<td>Pressure at the sandface</td>
<td>psi</td>
<td>4300</td>
</tr>
<tr>
<td>Reservoir thickness</td>
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<tr>
<td>Wellbore radius</td>
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<tr>
<td>Simulation time</td>
<td>minute</td>
<td>36</td>
</tr>
</tbody>
</table>

Table 6.1: Summary of assumed mudcake parameters used in the numerical simulation of mud-filtrate invasion (field Mud 97074) [11,40].

Figure 6.1: Comparison of volume of filtrate obtained with numerical simulations using UTFECS against that measured in the laboratory with field Mud 97074 [11].
Table 6.2: Summary of assumed mudcake parameters in the numerical simulations of mud-filtrate invasion.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Unit</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Solid fraction, ( f_s )</td>
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</tr>
<tr>
<td>Mudcake reference permeability, ( k_{mc0} )</td>
<td>md</td>
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<tr>
<td>Mudcake reference porosity, ( \phi_{mc0} )</td>
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</tr>
<tr>
<td>Compressibility exponent, ( v )</td>
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<tr>
<td>Porosity exponent, ( \delta )</td>
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<td>0.1</td>
</tr>
<tr>
<td>Mudcake thickness limit</td>
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</tr>
<tr>
<td>Initial reservoir pressure</td>
<td>psi</td>
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</tr>
<tr>
<td>Pressure at the sandface</td>
<td>psi</td>
<td>4000</td>
</tr>
<tr>
<td>Simulation time</td>
<td>day</td>
<td>3</td>
</tr>
</tbody>
</table>

compare flow rates obtained with numerical simulations in the presence of mudcake and the one without presence of mudcake. The figures show that the values of flow rate at the onset of invasion are approximately the same.

Overbalance pressure over mudcake reaches a pressure close to the initial pressure difference between reservoir and sandface [40] (Figure 6.2 shows this trend in the time variation of overbalance pressure). I use Darcy’s equation to approximate the final value of flow rate, to wit,

\[
q = \frac{K_{mc} A \mu_f P_{mc}}{\mu_f} \frac{dr}{dr},
\]

(6.5)

where \( K_{mc} \) is the absolute permeability of mudcake, \( A \) is the cross-sectional area, equal to \( 2\pi rh \), \( \mu_f \) is viscosity of filtrate, \( P_{mc} \) is mudcake pressure differential, and \( dr \) is mudcake thickness. For this simulation, flow rate is approximately equal to

\[
q = \frac{0.033 \text{ mmd}}{1 \text{ cp}} \times (2\pi \times 0.5 \text{ ft}) \times 1 \text{ [ft]} \times 350 \text{ [psi]} \times 1.67868 \times 10^{-12} \frac{\text{ ft}^2}{\text{ psi \times day}}
\]

\[
= 0.6013 \frac{\text{ ft}^3}{\text{ day}} = 0.1071 \frac{\text{ bbl}}{\text{ day}},
\]

which is close to the value of late-time flow rate shown in Figures 6.3 and 6.4. Flow rates calculated with the presence of mudcake are always less than those obtained without presence of mudcake.
Figure 6.2: **Rock Type 3**: Time variation of mudcake overbalance pressure.

Figure 6.3: **Rock Type 1**: Time variation of flow rate after the onset of invasion obtained with the following cases: simulation of mud-filtrate invasion and no mudcake.
6.3 Simulations of the Process of Mud-Filtrate Invasion

In this section, I explain the effect of mudcake growth on flow rate, pressure, saturations, salt concentration, and radial resistivity profiles. I compare simulations with and without the presence of mudcake for the cases of two- and three-phase fluid flow.

6.3.1 Two-Phase Flow Case Study

This case study describes the effect of mudcake growth on two-phase, oil-water, fluid flow. The oil phase consists of FC6, whereas the aqueous-phase is composed of water and salt. Table 5.1 summarizes the parameters assumed for the description of the reservoir. Initial reservoir pressure is 3500 [psi], water saturation is 25%, and salt concentration is 168 [kppm]. For the wellbore boundary condition, I assume a bottomhole pressure constraint equal to 3800 [psi], injecting water with a salt concentration of 3000 [kppm]. Figure 6.5 compares mudcake growth for different values of mudcake reference permeability to the corresponding fluid flow rates.

Figures 6.6 and 6.7 show the effect of mudcake growth in mud-filtrate invasion and
compare to results of the case without presence of mudcake. Figure 6.6 indicates that reservoir pressure decreases close to its initial level. Figures 6.6 and 6.7 show that fronts of water saturation and salt concentration obtained with the simulation of mud-filtrate invasion penetrate less than those without presence of mudcake.

6.3.2 Three-phase Flow Case Study

In this section, I illustrate the effect of mudcake growth for the case of three-phase fluid flow simulation. I assume initial composition (0.4, 0.3, 0.3) of hydrocarbon components (C1, C3, FC7) and the aqueous-phase is composed of water and salt. Table 5.1 recapitulates the remaining parameters for the description of the reservoir. Initial reservoir pressure is 500 [psi], water saturation is 25%, and salt concentration is 168 [kppm]. I assume a bottomhole pressure of 1300 [psi], injecting water with a salt concentration of 3000 [kppm]. Figure 6.8 compares mudcake growth for different values of mudcake reference permeability to the corresponding injection fluid flow rates.

Figures 6.9, 6.10, and 6.11 show the effect of taking into account mudcake growth in the simulations of mud-filtrate invasion and compare to results of the case without presence of mudcake.

Figure 6.9 indicates that reservoir pressure decreases to its initial level after about 1 day. Figures 6.9 through 6.11 show that fronts of water, oil, and gas saturation and also salt concentration obtained with the simulation of mud-filtrate invasion do not penetrate as deep as those obtained without presence of mudcake.

6.3.3 Comparison of Oil- and Water-Base Mud-Filtrate

From the definition of productivity index, to wit,

\[ PI_j = \frac{k_r \Delta z \lambda r_j}{25.14872 \ln \frac{r_o}{r_w}}. \]

flow rates for oil- and water-base mud is expected to be different. Inasmuch as flow in the mudcake is assumed to be solely single phase, I assume oils with different viscosities in the simulations to study its corresponding effect on the flow rates of mud-filtrate invasion
Figure 6.5: **Rock Type 1**: Time variation of (a) mudcake thickness and (b) flow rate after the onset of invasion for different values of reference mudcake permeability.
Figure 6.6: Two-phase flow in rock type 1: Comparison of pressure and water saturation profiles at different times after the onset of invasion for two cases: without presence of mudcake and with presence of mudcake. Initial $P=3500$ [psi], $S_w=0.25$. Well constraint is 1 day of invasion with $BHP=3800$ [psi]. Mudcake reference permeability, $K_{mc0}=0.3$, mudcake reference porosity, $\phi_{mc0}=0.3$, and solid fraction, $f_s=0.06$. 
Figure 6.7: **Two-phase flow in rock type 1**: Comparison of salt concentration and calculated water resistivity profiles at different times after the onset of invasion for two cases: without presence of mudcake and with presence of mudcake. Initial $P=3500$ [psi], $S_w = 0.25$. Well constraint is 1 day of invasion with BHP=3800 [psi]. Mudcake reference permeability, $K_{mc0}=0.3$, mudcake reference porosity, $\phi_{mc0}=0.3$, and solid fraction, $f_s=0.06$. 

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Figure 6.8: **Three-phase flow in rock type 3:** Time variation of (a) mudcake thickness and (b) flow rate after the onset of invasion for different values of reference mudcake permeability.
Figure 6.9: **Three-phase flow in rock type 3:** Comparison of pressure and water saturation profiles at different times after the onset of invasion for two cases: without presence of mudcake and with presence of mudcake. Initial $P=500$ [psi], $S_w = 0.25$, Temperature, $T=200$ [$^\circ$F], and hydrocarbon components composition (0.4, 0.3, 0.3) of (C1, C3, FC7). Well constraint is 1 day of water-base mud invasion with BHP=1300 [psi]. Mudcake reference permeability, $K_{mc0}=0.3$, mudcake reference porosity, $\phi_{mc0}=0.3$, and solid fraction, $f_s=0.06$. 
Figure 6.10: Three-phase flow in rock type 3: Comparison of oil and gas saturation profiles at different times after the onset of invasion for two cases: without presence of mudcake and with presence of mudcake. Initial P=500 [psi], $S_w = 0.25$, Temperature, $T=200 \ [\degree F]$, and hydrocarbon components composition (0.4, 0.3, 0.3) of (C1, C3, FC7). Well constraint is 1 day of water-base mud invasion with BHP=1300 [psi]. Mudcake reference permeability, $K_{mco}=0.3$, mudcake reference porosity, $\phi_{mco}=0.3$, and solid fraction, $f_s=0.06$. 

Figure 6.11: **Three-phase flow in rock type 3**: Comparison of salt concentration and calculated resistivity profiles at different times after the onset of invasion for two cases: without presence of mudcake and with presence of mudcake. Initial $P=500$ [psi], $S_w = 0.25$, Temperature, $T=200$ [$^\circ$F], and hydrocarbon components composition (0.4, 0.3, 0.3) of (C1, C3, FC7). Well constraint is 1 day of water-base mud invasion with BHP=1300 [psi]. Mudcake reference permeability, $K_{mco}=0.3$, mudcake reference porosity, $\phi_{mco}=0.3$, and solid fraction, $f_s=0.06$. 
Figure 6.12 compares mudcake growth and the corresponding fluid flow rates for two cases of water-base mud-filtrate invasion and oil-base mud-filtrate invasion. Figure 6.13 compares mudcake growth and the corresponding fluid flow rate for two cases of water-base mud-filtrate invasion and oil-base mud-filtrate invasion and shows that when oil viscosity is greater than water viscosity, fluid flow rate of oil-base mud is less than that of water-base mud.

(relative permeability is equal to one).
Figure 6.12: **Rock Type 3:** Time variation of (a) mudcake thickness and (b) flow rate after the onset of invasion of water-base and oil-base mud ($\mu_o = 0.5$).
Figure 6.13: **Rock Type 3**: Time variation of (a) mudcake thickness and (b) flow rate after the onset of invasion of water-base and oil-base mud \((\mu_o = 2.0)\).
Chapter 7

Conclusions

I developed and successfully validated a one-dimensional (1D) radial, isothermal, equation-of-state (EOS) compositional method to simulate invasion and fluid withdrawal in the presence of oil- or water-base muds. The method can simulate simultaneous fluid flow of a maximum of three fluid phases (water, oil and gas). I derived formulations based on the following assumptions: isothermal reservoir, impermeable reservoir at infinite radial distance, Darcy’s law for fluid flow through porous media is valid, formation is slightly compressible, and dispersion is negligible.

Simulations were based on the method of implicit pressure and explicit concentration (IMPEC) to solve the partial differential equation arising from the discretization of the fluid-flow equation. The fundamental pressure equation is based on the assumption that pore volume contains the total volume of the fluid. I assumed that rock pore volume is only a function of pressure and total fluid volume is a function of pressure and moles of components. Oil pressure was the reference in the pressure equation. I used the general mass balance equation to calculate the moles of each component at the current pressure. The calculations of moles of each component and also the calculation of saturations of fluid phases were done with an explicit method.

I used following auxiliary relations to calculate \( n_c n_p + 6 n_p + 2 \) unknown parameters of the pressure equation and equations of moles of components: saturation constraint, porosity dependency on pressure, phase molar density, phase composition constraint, flow rate, phase
pressure, phase mass density, phase viscosity, relative permeability, and phase equilibrium.

I assumed viscosity of the aqueous phase to be constant and used Lohrenz et al.’s [18] relations for the calculation of hydrocarbon-phase viscosity and implemented Stone’s model 2 to estimate three-phase relative-permeability. I modeled hydrocarbon components and fluid phases based on Peng-Robinson’s equation-of-state.

I assumed that there were no mass transfer between the hydrocarbon components and the aqueous phase, and that the aqueous phase consisted of only the water component. Moreover, the water component did not affect phase behavior. From the equality of fugacities in thermodynamic equilibrium, I obtained analytical expression for partial derivatives of total fluid volume introduced in the pressure equation.

I implemented the tangent-plane distance approach for the calculation of phase stability and the successive substitution method for the flash calculation. Automatic time step control was based on the method of relative change. The code was validated against two commercial simulators: GEM and STARS. I tested the method with simulations for different flow regimes, gas-water, oil-water, and gas-oil-water flow taking place in different rock types. Comparison of results obtained with the developed simulator and commercial reservoir simulator indicated a very good agreement.

I studied the effect of mud-filtrate invasion on the fluid flow simulations by implementing a mudcake model in the developed 1D radial compositional simulator. The mudcake model allowed me to thicken and to change the permeability and porosity of the mudcake with time, and it was coupled to the assumed formation properties.

The developed simulator enabled me to:

- Simulate invasion and fluid withdrawal in the presence of oil- or water-base muds,
- Track aqueous salt concentration in multi-phase flow,
- Constrain the well with different types of boundary conditions, such as
  - Water/oil injection with flow constraints or bottomhole pressure,
  - Bottomhole fluid production,
- Simulate water-base mud or oil-base mud-filtrate invasion.
I implemented Dewan and Chenevert’s mudcake model [11], and Chin’s mudcake model [6] for mudcake growth. I studied water-base mud-filtrate invasion in two-phase and three-phase flow regimes. Comparison of simulations with and without presence of mudcake model, Section 6.3, showed mudcake had a significant effect on the radial profiles of pressure, saturation, and salt concentration.

7.1 Future Work

The developed compositional simulator has a computationally efficient structure. The computational speed of this one-dimensional compositional simulator for two-phase fluid flow is comparable to commercial reservoir simulators. However, due to the IMPEC method stability criteria, the step sizes have smaller values compared to those of fully implicit formulations. Simulations of three-phase flow with the developed simulator are slower than those with commercial simulator. Implementation of a faster flash calculation algorithm can increase the computational speed.

Developing a two-dimensional (radial-azimuthal) compositional simulator will enable one to model fluid flow in different layers in order to track concentrations around a vertical well during invasion and fluid cleanup. Similarly, developing a three-dimensional compositional simulator in cylindrical coordinates will bring the capability necessary to model invasion and fluid withdrawal from probes and point sources. However, because of dependency of step sizes on the grid in IMPEC method, development of a two- or three-dimensional compositional simulator may require implementation of a more efficient method.

Moreover, coupling a two- or three-dimensional reservoir simulator method with a mudcake model not only will result in more stability, but also will enable one to simulate mud-filtrate invasion in deviated and horizontal wells more accurately.
Bibliography


