A MULTI-PHYSICS MODEL FOR ENHANCED OIL RECOVERY
IN LIQUID-RICH UNCONVENTIONAL RESERVOIRS

by

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ABSTRACT

Because most of the hydrocarbon remains trapped in the reservoir, recovery factors for tight oil and shale oil are very low. Recovery factors for these formations typically range from 3 to 7%. Since shale matrix has very low permeability, conventional reservoir simulators often overestimate the mass exchange between shale matrix and fractures. To evaluate the potential of water injection for improving oil recovery, the mass transport in the reservoir at different scales should be modeled properly. These issues have motivated us to conduct this research study to evaluate the potential of water injection enhanced oil recovery in liquid-rich unconventional reservoirs accounting for the effects of salt concentration, fluid type, shale swelling, and wettability alteration.

There are several mechanisms for the imbibition of water into the rock matrix. In pore scale modeling, it was shown in this research that the interfacial tension-induced transport is one of the key mechanisms contributing to the transport of oil trapped in the pores. The change in the interfacial tension and the contact angle results in wettability alteration and can be interpreted as one of the key factors for imbibition of water into the rock matrix, especially in oil-wetted matrix blocks as observed in laboratory experiments. The amount of oil recovery varies for various ion types, indicating an effect of ion type on the oil recovery. This original pore scale modeling study helps us to evaluate the contribution of interfacial tension-induced transport on the imbibition of water into pores. However, upscaling from pore scale to a larger scale requires further studies for a true representation of the reservoir conditions. Hence, while a new pore scale model was introduced in our research study, it is not fully incorporated in the matrix block and reservoir scale models presented in this study.

In a matrix block scale model, a phenomenological model for mass exchange between the rock matrix and the fractures was formulated to compute the mass transfer used in reservoir scale model. This mass transport model was validated using experimental data. A shale
swelling model was also derived to account for the swelling effect on the matrix and fracture permeability and porosity by solving the coupled geomechanics and mass transport models. The coupled fluid flow and geomechanics model was solved for every matrix block within the reservoir scale model to evaluate the overall effect of salt concentration, shale swelling, and wettability alteration on oil recovery.

The matrix block scale simulation results indicate that osmosis is an important force imbibing water into low permeability rock matrix and enhancing the effectiveness of low salinity waterflooding on oil recovery. The imbibition of water into oil-wetted shale matrix is mainly driven by the osmotic transport and wettability alteration. The contribution of osmotic transport continues for a long period of time and contributes to oil production if the membrane efficiency is high and the matrix block size is small. However, the low membrane efficiency of the shale formations, typically less than 10%, considerably reduces the contribution of osmosis on oil recovery. The effect of fluid type on the oil recovery depends on the membrane efficiency and the diffusion coefficient of the ion. Higher membrane efficiency and lower diffusion coefficient of dissolved ions increase the contribution of osmosis on the oil recovery from shale matrix.

Matrix swelling decreases matrix and fracture porosity, forcing the fluid out of the rock matrix and maintaining the pressure in fracture. However, matrix swelling significantly reduces the permeability of the matrix and fractures, reducing oil recovery. Therefore, water injection is not recommended for formations with high swelling potential. Further research on wettability alteration and membrane efficiency variation is recommended for enhanced oil recovery operation in liquid-rich unconventional reservoirs.
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<tr>
<td>$A$</td>
<td>Hamaker constant</td>
</tr>
<tr>
<td>$a_{sf}$</td>
<td>Solute adsorption on the fracture walls</td>
</tr>
<tr>
<td>$C$</td>
<td>Material stiffness tensor</td>
</tr>
<tr>
<td>$c_{fk}$</td>
<td>Fracture permeability proportionality coefficient</td>
</tr>
<tr>
<td>$c_{fp}$</td>
<td>Fracture porosity proportionality coefficient</td>
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<tr>
<td>$c_{mk}$</td>
<td>Matrix permeability proportionality coefficient</td>
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<td>$c_{mp}$</td>
<td>Matrix porosity proportionality coefficient</td>
</tr>
<tr>
<td>$c_{o,f}$</td>
<td>Compressibility of oil in fracture</td>
</tr>
<tr>
<td>$c_{t,f}$</td>
<td>Total compressibility in fracture</td>
</tr>
<tr>
<td>$c_{t,m}$</td>
<td>Total compressibility in matrix</td>
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<td>$c_{s,p}$</td>
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<td>$c_{sw,f}$</td>
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Effective diffusion coefficient \( D_{eff} \)

Bulk diffusion coefficient in fracture \( D_f \)

Diffusion coefficient in free solution \( D_o \)

Pore diameter \( D_{pore} \)

Pore throat diameter \( D_{throat} \)

Young’s modulus of rock \( E \)

Electronic charge \( e \)

External force vector \( \mathbf{F} \)

Fugacity of component \( f_i \)

Gravitational acceleration \( g \)

Shear modulus of rock \( G \)

Mean curvature \( H^{\alpha\gamma} \)

Water fluid level height in fractures and rock matrix \( h_{w,f}, h_{w,m} \)

Plank’s constant \( \hbar \)

Grid cell index \( i, j, k \)

Identity tensor \( \mathbf{I} \)

Mass flux of phase \( i \) \( \mathbf{J}_i \)

Mass flux of phase \( i \) due to chemical \( \mathbf{J}_{i \text{chemical}} \)

Mass flux of phase \( i \) due to gravity \( \mathbf{J}_{i \text{gravity}} \)

Mass flux of phase \( i \) due to pressure \( \mathbf{J}_{i \text{pressure}} \)

Mass flux of phase \( i \) due to thermal \( \mathbf{J}_{i \text{thermal}} \)

Mass flux of oil in rock matrix \( \mathbf{J}_{om} \)
Matrix mass flux of solute .................................................. $J_{sm}$
Mass flux of solute in rock matrix due to diffusion ................. $J'_{sm}$
Mass flux of water in rock matrix ........................................ $J_{w}$
Boltzmann constant ......................................................... $k$
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Fracture effective permeability .......................................... $k_{f,eff}$
Structural constants ....................................................... $K_i, l$
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Fracture water relative permeability ..................................... $k_{rwf}$
Relative permeability of water in the pore .............................. $k_{wp}$
Phenomenological coefficients ............................................ $L_{ij}, L_{ip}$
Molecular weight of component $i$ ......................................... $MW_i$
Current and next time step ................................................. $n, n+1$
Number of components ..................................................... $n_c$
Ion concentration ............................................................ $n_s$
Dimensions of matrix block ............................................... $L_x, L_y, L_z$
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Pressure of water phase in fracture ...................................... $p_{w,f}$
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Pore specific water rate \( \dot{q}_{wp} \)
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Inside radius of annulus \( R_i \)
Outside radius of annulus \( R_o \)
Pore radius \( R_p \)
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Oil saturation in fracture \( S_{o,f} \)
Residual oil saturation in fracture \( S_{orf} \)
Residual water saturation in fracture \( S_{wrf} \)
Water saturation in pore \( S_{wp} \)
Oil saturation in pore \( S_{op} \)
Water saturation in rock matrix \( S_{w,m} \)

Initial water saturation in rock matrix \( S_{w,mi} \)

Oil saturation in rock matrix \( S_{o,m} \)

Residual oil saturation in rock matrix \( S_{orm} \)

Residual water saturation in rock matrix \( S_{wrm} \)

Water saturation at position \( y \), time \( t \) \( S_w(y,t) \)

Time \( t \)

Temperature \( T \)

Temperature of rock matrix \( T_m \)

Displacement in x, y, and z direction \( u_x, u_y, u_z \)

Oil velocity in fractures \( v_{o,f} \)

Oil velocity in the matrix \( v_{o,m} \)

Oil velocity in pores \( v_{o,p} \)

Water velocity in the matrix \( v_{w,m} \)

Water velocity in fractures \( v_{w,f} \)

Water velocity in pores \( v_{w,p} \)

Pore volume \( V_P \)

Volume \( V \)

Rock volume \( V_R \)

Partial volume of solute \( V_s \)

Partial volume of water \( V_w \)

Mole fraction of component \( i \) \( x_i \)

Valence of the electrolyte \( z \)
Position of the interface \( z_c \)

Biot tensor and Biot coefficient \( \alpha, \alpha \)

Phenomenological coefficients that relate the \( i^{th} \) flow to the \( j^{th} \) force \( \alpha_{ij} \)

Thermal expansion coefficient of rock matrix \( \beta \)

Interfacial tension \( \gamma \)

Oil specific gravity \( \gamma_o \)

Water specific gravity \( \gamma_w \)

Incremental \( \delta \)

Binary interaction coefficient between component \( m \) and \( n \) \( \delta_{mn} \)

Grid block dimension \( \Delta x, \Delta y, \Delta z \)

Time step for reservoir scale \( \Delta t \)

Time step for mass transport and geomechanics equations in matrix \( \Delta t_m \)

Density difference \( \Delta \rho \)

Dielectric constant \( \varepsilon \)

Elastic strain tensor \( \varepsilon_e \)

Swelling strain tensor \( \varepsilon_s \)

Thermal strain tensor \( \varepsilon_T \)

Horizontal swelling strain \( \varepsilon_{sh} \)

Vertical swelling strain \( \varepsilon_{sv} \)

Volumetric strain of fractures \( \varepsilon_{v,f} \)

Volumetric strain of matrix \( \varepsilon_{v,m} \)

Zeta potential \( \zeta \)

Contact angle \( \theta_c \)
Inverse Debye-Huckel length parameter \( \kappa \)

Lame coefficient \( \lambda \)

Mobility of oil in fractures \( \lambda_{o,f} \)

Mobility of water in fractures \( \lambda_{w,f} \)

Chemical potential of component \( i \) \( \mu_i \)

Viscosity of oil \( \mu_o \)

Viscosity of water \( \mu_w \)

Poisson’s Ratio of rock \( \nu \)

Disjoining pressure \( \Pi \)

Osmotic pressure \( \Pi_s \)

Oil density \( \rho_o \)

Solute density \( \rho_s \)

Water density \( \rho_w \)

Stress tensor \( \sigma \)

Effective stress tensor \( \sigma_{eff} \)

Shape factor \( \sigma_s, \sigma_z \)

Atomic collision diameter \( \sigma_c \)

Interfacial tension \( \sigma_i^{\gamma \gamma}, \sigma_i \)

Matrix tortuosity \( \tau \)

Shear stress \( \tau_{ij} \)

Fracture tortuosity \( \tau_f \)

Oil volumetric transfer function \( \tau_o \)

Total volumetric transfer between fractures and matrix \( \tau_t \)
Water volumetric transfer function \( \tau_w \)

Initial porosity \( \phi_o \)

Fracture porosity \( \phi_f \)

Matrix porosity \( \phi_m \)

Pore inclination angle \( \psi \)

Osmotic efficient coefficient or membrane efficiency \( \omega \)
<table>
<thead>
<tr>
<th>Abbreviation</th>
<th>Full Form</th>
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<tr>
<td>Annual Energy Outlook 2014</td>
<td>AEO2014</td>
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<tr>
<td>Cation Exchange Capacity</td>
<td>CEC</td>
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<tr>
<td>U.S. Energy Information Administration</td>
<td>EIA</td>
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<tr>
<td>Enhanced Oil Recovery</td>
<td>EOR</td>
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<tr>
<td>Improved Oil Recovery</td>
<td>IOR</td>
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<tr>
<td>Hydraulic Fracture</td>
<td>HF</td>
</tr>
<tr>
<td>High Salinity</td>
<td>HS</td>
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<tr>
<td>Inside Diameter</td>
<td>ID</td>
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<tr>
<td>Low Salinity</td>
<td>LS</td>
</tr>
<tr>
<td>Million barrels per day</td>
<td>MMbbl/d</td>
</tr>
<tr>
<td>Outside Diameter</td>
<td>OD</td>
</tr>
<tr>
<td>Pore Pressure Transmission</td>
<td>PPT</td>
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<tr>
<td>Society of Petroleum Engineers</td>
<td>SPE</td>
</tr>
<tr>
<td>Stimulated Reservoir Volume</td>
<td>SRV</td>
</tr>
<tr>
<td>Total Organic Carbon</td>
<td>TOC</td>
</tr>
<tr>
<td>Unconventional Natural Gas and Oil Institute</td>
<td>UNGI</td>
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<tr>
<td>Unstimulated Reservoir Volume</td>
<td>URV</td>
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<td>Water Activity</td>
<td>WA</td>
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CHAPTER 1
INTRODUCTION

In this chapter, the importance of multi-scale and multi-physics modeling in unconventional reservoir simulation for improvement of oil recovery and better production forecasting is presented. The objectives, scope, and methodology of this research study are also outlined.

1.1 Unconventional Resources

Unconventional reservoirs have quickly become a main contributor to the oil and gas production in the United States, replacing the depletion of conventional resources. The rapid development of unconventional resources is supported by the new technologies, particularly horizontal drilling and hydraulic fracturing. The growth of crude oil production from tight oil and shale formations has supported a nearly fourfold increase in tight oil production from 2008 to 2012 (EIA 2014). Tight oil and shale oil contribute more than one third of the total U.S. production. The Annual Energy Outlook 2014 (AEO2014) predicts that the total projected U.S. crude oil production can reach 9.6 MMbbl/d in 2019, that is 2.1 MMbbl/d more than in 2014. It is anticipated that the tight oil production growth of 2.5 MMbbl/d in 2012 will continue to reach 4.8 MMbbl/d in 2019. The estimated shale oil in the United States and in 137 shale formations in 41 other countries represent 10% of the world’s crude oil technically recoverable resources according to an EIA-sponsored study (EIA 2013). Shale gas reserves and production also grow rapidly and is becoming the dominant source of natural gas in the U.S. (Figure 1.1). The shale gas share of total U.S. natural gas production is projected to increase from 40% in 2012 to 53% in 2040 (EIA 2014). However, the current recovery factor from unconventional reservoirs is very low, especially for shale oil. EIA (2013) reports that the recovery factor for shale gas is typically around 20 to 30% while this recovery is significantly lower for shale oil, 3 to 7%. The production rate also declines
rapidly after the first year of production. Hence, understanding the transport mechanism and improving the hydrocarbon recovery from these formations are essential.

Figure 1.1: The U.S. historical and projected production of oil and natural gas by source, 1990 - 2040 (EIA, 2014).

Recent research studies suggest the use of waterflooding, low salinity waterflooding, chemical flooding, CO₂ injection, and gas injection for improving the recovery in shale oil reservoirs (Morsy et al. 2013a,b; Chen 2013; Nguyen et al. 2014; He et al. 2015; Sheng 2015). However, most of these studies are still in their experimental stages. We are currently using conventional models implemented in conventional simulators to evaluate the potential of each method. Which methods should be used is still an open question for further research since we currently lack of the understanding of the transport mechanisms in unconventional reservoirs. We are reporting the laboratory and field observation of the factors controlling the effect of low salinity water injection such as the change of the contact angle with water salinity rather than calculating amount of water imbibed into rock matrix. Further research on the mass transport mechanisms and modeling at various scales should be conducted to make any quantitative recommendations. Hence, modeling the mass transport in shale oil reservoirs and evaluating the overall effect of different factors on water injection enhanced oil recovery (EOR) are the main motivation of this study.
1.2 Unconventional Reservoir Modeling

Organic-rich shale reservoirs often contain the natural fractures and induced fractures by hydraulic fracturing. Therefore, unconventional reservoirs are often modeled using a dual-continuum model. In reservoir modeling, the dual-porosity or dual-permeability model is often used to model the fractured reservoirs. This concept was first introduced by Barenblatt et al. (1960). In 1963, Warren and Root reintroduced this concept to the petroleum engineering literature. Kazemi (1969) proposed a slab model using a similar solution method to Warren and Root’s model and introduced transient flow conditions between matrix and fracture systems. de Swaan (1976) presented a transient model that explicitly accounts for the matrix and fracture dimensions and flow properties. Kazemi et al. (1976) introduced the numerical modeling for reservoirs containing two phases, water and oil.

In a dual-porosity model, the reservoir consists of two systems, the fractures and the rock matrix. The fracture continuum has higher hydraulic conductivity and the flow in the fractures is the main flow in the reservoir. The matrix continuum has lower hydraulic conductivity and the flow in matrix is at a relatively lower velocity. Initially, fluids in the reservoir is at the thermodynamic equilibrium. When the flow in fractures occurs, this flow changes the equilibrium in the reservoir. To reach a new thermodynamic equilibrium, fluids move between fractures and rock matrix causing mass exchange between the fractures and the rock matrix. This mass exchange is very important from an enhanced oil recovery perspective because a high percent of oil in the reservoir is stored within the rock matrix. For shale formations, the amount of oil stored in the matrix is significantly higher than the amount of oil in fractures as shown in Figure 1.2. Therefore, to improve or enhance oil recovery from shale formations, it is critical to focus on the oil recovery from shale matrix. In other words, transfer functions should be accurately modeled.

The mass transfer between rock matrix and fractures is often modeled using mass transfer functions accounting for pressure gradient, gravity, and capillary pressure. For thick matrix blocks, gravity drainage often plays a more important role in production if it can overcome
the capillary pressure in oil-wetted matrix blocks. For water-wetted rock matrix, capillary force imbibes water into rock matrix and releases oil. In the early work of fractured reservoir modeling, only the pressure gradient was considered as the driving force for the mass exchange between the rock matrix and fractures (Warren and Root 1963). Later, some additional force such as capillarity and osmosis are added to transfer functions (Fakcharoenphol 2013; Kurtoglu 2014). Although accurate mass transfer modeling is important as emphasized by Al-Kobaisi et al. 2009; Ozkan et al. 2010; Ramirez et al. 2009, analytical models are currently used. Since shale matrix has very low permeability, the flow in the shale matrix is often transient over a long period of time. The contribution of osmotic pressure and wettability alteration become more important. The use of the steady-state transfer functions for very low permeability matrix may overestimate the contribution of the matrix on the oil recovery. This may lead to an over evaluation of the economic potential. Hence, research studies on enhanced oil recovery in shale formations should focus on this mass transfer.

1.3 Mass Transport between Fractures and Rock Matrix

The transport process between fluid in the fractures and the rock matrix includes advection, molecular, thermal and electrochemical diffusions, and thermal convection. In con-
ventional fractured reservoir modeling, analytical transfer functions are used to describe the mass transfer between the rock matrix and the fractures. The computation is average for matrix blocks meaning that each matrix has single value of phase pressure, saturation, and concentration. The variation of these parameters at different positions inside the matrix block is not considered. This transfer function typically accounts for convective transport described by Darcy’s law. However, in shale formations, very low matrix permeability decreases the effect of convection. Instead, molecular and electrochemical diffusions and mechanical dispersion play a more important role (Ozkan et al. 2010; Farrokhrouz and Asef 2013). Since diffusion and thermal convection are very slow processes compared to the convective, mass transport in shale matrix is time dependent and analytical mass transfer functions may often overestimate this mass exchange. Hence, more comprehensive models for fracture-matrix mass transport are needed for low permeability reservoir modeling.

1.4 Multi-scale and Multi-physics Reservoir Modeling

In fractured reservoir simulation the concept of multi-scale and multi-physics modeling is related to modeling of the flow at different scales, from pore scale to reservoir scale (Figure 1.3). The main objective is often to better model the mass exchange between the rock matrix and the fractures. In a multi-scale reservoir modeling study, three scales including pore scale, matrix block scale, and reservoir scale are often considered.

Figure 1.3: Step-wise procedural upscaling of recovery processes in naturally fractured reservoirs. Colors represent different phases (red=gas, green=oil, blue=water) (Elfell et al. 2013).
The imbibition of water into rock matrix is a complicated process required the understanding of mass transport at pore scale. The complexity of pore structure, electrochemical properties of rock, multi-componets of fluids, and fluid-rock interaction are the main obstacles for understanding this transport process. All of these complex factors make the upscaling from pore scale to larger scale more challenging. Hence, pore scale modeling used in this research study is for understanding the physics of transport at pore size. Elfeel et al. (2013) suggest that pore scale models can be used to predict multiphase displacement process and generate relative permeability and capillary pressure curves. Matrix block scale simulation is used to compute the mass exchange between the matrix block and its surrounding fractures. Hence, the effect of relative permeability, capillarity, wettability, and gravity can be investigated. For low salinity water injection, the contribution of osmotic transport and wettability alteration on oil recovery can also be evaluated. Reservoir scale provides the global contribution of various factors on the pressure, phase, and saturation change in the reservoir. It combines the effect of multi-physics at various scale on recovery and long term response in reservoirs.

One of the limitations of the multi-scale simulation is the computation time is much higher than normal simulation. Hence, multi-scale modeling was found to be not practical in the past and it is often used for research purposes only. However, the advancements of multi-core computing machines help to make this approach more feasible. In the near future, multi-scale approach will be used widely in the oil industry with cloud computing.

1.5 Shale Swelling

Shale swelling may have a significant effect on the economics of water injection enhanced oil recovery in shale reservoirs. To demonstrate the significant role of the swelling, we consider an unconventional reservoir with average porosity of 8%, initial oil saturation of 80%, and 5% recovery factor. The volume of oil that we can produce from this reservoir is estimated to be 0.32% of the reservoir volume. The volumetric change of the rock due to shale swelling may be higher than this volume depletion and pore pressure may be maintained by
pressure induced through swelling. In other words, swelling may enhance recovery from shale formations. The invasion of fluid into shale matrix also causes the pore pressure and effective stress alteration. Swelling may change the aperture of the fractures; therefore, it changes fracture permeability and porosity (Liu and Rutqvist 2009). This change creates a variation in the fracture and matrix permeability and porosity, especially for the matrix blocks near the hydraulic fracture face. Fracture permeability reduction blocks the transport of phases in fractures reducing oil production and injection rate. Ji and Geehan (2013) showed that the invasion of the water into shale matrix causes the deviatoric stress inside the sample to be higher than the yield strength of the sample creating the failure inside the shale matrix. Hence, this improves the permeability of shale matrix and facilitates the penetration of fluid along the existing “secondary” fractures deeper into shale matrix. In other words, shale swelling may have both a positive and negative effects on oil recovery. However, the effect of swelling on oil recovery is still not investigated and is one of the objectives of this study.

There are experimental evidences of the swelling behavior of shale when it contacts water. The displacement in different directions of an Eagle Ford shale sample when contacted with water, presented in Figure 1.4, indicates that shale does swell (Emadi et al. 2013). The experimental results for the Eagle Ford samples by Emadi et al. (2013) also show that the maximum volumetric swelling strain is about 0.69% when submerged into distilled water and about 0.15% when submerged into 7% KCl water for seven days. For their drilling calculations, this value is considered to be small. However, for reservoir engineering calculations, this is more than the volumetric percentage of oil produced from the reservoir depending on the volume of shale matrix in contact with injection water. Therefore, accounting for the effect of shale swelling is important for water injection. The effect of shale swelling on hydrocarbon recovery has been reported in literature (Lager et al. 2007; Morsy et al. 2013a,b; Kurtoglu 2014). However, the mechanism and the theoretical model to simulate the effect of shale swelling in reservoir is not well presented in the reservoir engineering literature.
In summary, developing a model for computing the mass exchange between fractures and the rock matrix is essential to capture the multi-physics at different scales. The multi-scale modeling approach has many applications for enhanced and improved oil recovery in fractured reservoirs, particularly in unconventional reservoirs. The effect of salinity and ion concentration on hydrocarbon recovery can be better modeled. This is also useful for selecting proper fracturing fluids in hydraulic fracturing operations for Stimulated Reservoir Volume (SRV) optimization. Multi-scale simulation provides a better understanding of the effect of salinity, electrochemical potential and surface energy on the oil recovery. With the advancement of cloud computing and multiple core computing machines, this approach is becoming feasible.

1.6 Objectives and Scope

The main motivation of this research study is how to model the multi-physics at different scales in liquid-rich unconventional reservoirs. The overall objective of this research study is to investigate the mass transport mechanism at various scales in the reservoir to develop a
multi-scale and multi-physics model with a better evaluation of the mass exchange between the fractures and the rock matrix. The developed model is used to investigate the effect of low salinity water injection on oil recovery from the reservoir. The detailed objectives include:

1. To investigate the contribution of interfacial tension-induced transport on the imbibition of water into oil-wetted pores in pore scale.

2. To model the mass transport between the fractures and the rock matrix and to better understand the mass transport within the reservoir at different scales.

3. To formulate a geomechanics model for evaluating the effect of shale swelling on oil recovery.

4. To investigate the effect of injected fluid properties (solute concentration), fluid type, and well and fracture spacing on the oil recovery during water injection operations.

The scope of this study is limited to three phases (water, oil and solute). The phase transfer and other phase behavior are not considered in this study.

1.7 Contributions of This Research

This research study emphasize the importance of interface tension-induced transport on the transport of water into rock matrix, particularly oil-wetted shale matrix as shown in pore-scale model as presented in Chapter 3. Our aim is to make contribute to our understanding and modeling of the mass transport in the reservoir at various scales. One of the main contributions of this study is the formulation of a mass transport model for computing mass exchange between fractures and the rock matrix accounting for the osmotic transport. The next contribution is the shale swelling model for evaluating the variation of porosity and permeability of fractures and the rock matrix during water injections. The developed model provides reservoir engineers a better methodology to simulate the fluid transport in unconventional reservoirs during water injection operations. Moreover, this study findings
also allow us to evaluate the potential of water injection on the oil recovery in liquid-rich unconventional reservoirs.

1.8 Dissertation Organization

This dissertation is presented in six chapters.

• An introduction to the research study is provided in Chapter 1. The motivation, objectives, scope, and the contribution of this research are presented. The importance of multi-scale and multi-physics modeling in unconventional reservoir simulation to improve/enhance oil recovery is outlined. The objectives, scope, and methodology of the study are summarized at the end of this chapter.

• Chapter 2 outlines the literature related to multi-scale and multi-physics modeling. Pore scale modeling, pore size physics and transport phenomena are briefly discussed first. Then, a review of the flow mechanisms in unconventional reservoirs and modeling approaches are introduced followed by the transport mechanisms between the fractures and the rock matrix with related physical phenomena. Finally, shale swelling mechanisms and modeling approaches are discussed.

• Chapter 3 introduces the interfacial tension-induced transport concept. A simplified pore scale model is presented to model the imbibition of the water into the pores by interfacial tension-induced transport helping to explain the transport of the water into oil-wetted shale matrix at pore scale. The mathematical model for a simplified pore-scale model is derived in this chapter along with numerical solution and results and discussion. This chapter concludes with a discussion on the model limitations and the future studies.

• Chapter 4 presents the mathematical model for fluid flow in two scales, reservoir scale and matrix block scale in a dual-porosity reservoir. A phenomenological mass transport model is derived and validated against experimental data. The chapter is concluded
with the clay-swelling model. The numerical solution of the mathematical model in this chapter is presented in Appendix B.

- The results from the numerical study for matrix block, and reservoir scales along with the discussion of the underlying physics are summarized in Chapter 5.

- The summary and recommendations are presented in Chapter 6. The research study presented in this dissertation along with the conclusions and the recommendation for the future research studies and field operations are summarized.
CHAPTER 2
LITERATURE REVIEW

This literature review briefly outlines research related to pore scale modeling, pore size physics, unconventional reservoir modeling, the mass transport between fractures and rock matrix, and shale swelling modeling. The flow mechanisms in unconventional reservoirs and the current approaches used in the modeling studies are discussed. The transport mechanisms between the fractures and rock matrix are reviewed. Finally, shale swelling mechanisms and modeling are discussed focusing on the effects of shale swelling on hydrocarbon recovery and porosity and permeability variation of rock matrix and fractures.

2.1 Pore Scale Modeling

The pore structure in rocks is very complicated partially due to the heterogeneous distribution of the minerals, varying lithology and facies. The porous media are often modeled as a sphere pack (Hazen 1892; Slichter 1899; Kozeny 1927; Carman 1937) and a bundle of tubes (Childs and Collis-George 1948; Purcell 1949; Gates and Lietz 1950). The pore network modeled as a network of tubes (Figure 2.1) is first introduced to the petroleum literature by Fatt (1956a,b,c). The pore network model have been used extensively in modeling of multiphase transport in porous media and various physical phenomena (Bryant et al. 1993; Bakke and Øren 1997; Patzek 2001; Varloteaux et al. 2013). With the advances in the imaging techniques, pore-network model has become more useful in reservoir engineering applications and porous media modeling (Al-Dhahli et al. 2012; Blunt et al. 2013; Thibodeaux et al. 2014). Blunt (2001) provided an extensive literature review on the use of pore network models. To better model the distribution of phase and the trapping mechanism in the pore, the variation of tube diameter to represent the main pore and pore throat is often used (Wardlaw 1982; Arriola et al. 1983; Bui et al. 2016).
Figure 2.1: Pore networks extracted from pore-space images of three quarry carbonates: (a) Estaillades; (b) Ketton; (c) Mount Gambier. The pore space is represented as a lattice of wide pores (shown as spheres) connected by narrower throats (shown as cylinders). The size of the pore or throat indicates the inscribed radius. The pores and throats have angular cross-sections—normally a scalene triangle—with a ratio of area to perimeter squared derived from the pore-space image (Blunt et al. 2013).

Even though pore scale models highly idealize the complexity of the porous media, they are useful for studying relationships between fundamental processes and phenomena at nanoscale and providing useful implications for large scale. The phenomena such as Knudsen diffusion, adsorption, capillary condensation, capillarity, and wettability alteration can be accurately modeled if we have sufficient understanding of the fundamental processes at pore scale. Without deeper fundamental research studies on the mass transport at pore scale, the current understanding will be limited to phenomenological description of the field and experimental evidence. In this study, a simplified pore model is introduced to investigate the importance of interfacial tension-induced transport on mass transport along a oil-wetted pore.
2.2 Interfacial Tension-Induced Transport in Pores

The distribution of pore sizes in porous rock is modeled using a distribution of capillaries with various radii. For oil-wetted rock, solid surfaces are in contact with oil. The water is surrounded by the oil phase and the water film at the contact may not be stable. Where the film is not stable, the surface wetting preference can change. This may lead to a situation of mixed wettability, where some parts of the pore surface are water-wetted and other parts are oil-wetted. Generally, the large pore spaces are more likely to be occupied by non-wetting phase, and the small pore spaces and interstices within pores are more likely to be occupied by the wetting phase (Abdallah et al. 2007).

The interfacial tension \( \sigma_i \) between phase 1 and phase 2 depends on temperature \( T \), pressure \( p \), curvature of the interface \( \kappa_c \) or interface radius \( r_c \), and the composition of the both phases \( (x_i, y_i) \). In general, the interfacial tension can be written as,

\[
\sigma_i = \sigma_i(p, T, r_c, x_1 \ldots x_{n_{c1}}, y_1 \ldots y_{n_{c2}}) \quad (2.1)
\]

where \( n_{c1} \) and \( n_{c2} \) are the number of components of phase 1 and phase 2.

The change of interfacial tension can be caused by temperature, pressure, interface curvature, and composition as,

\[
d\sigma_i = \left( \frac{\partial \sigma_i}{\partial p} \right)_{x,y,T,r_c} dp + \left( \frac{\partial \sigma_i}{\partial T} \right)_{x,y,p,r_c} dT + \left( \frac{\partial \sigma_i}{\partial r_c} \right)_{x,y,p,T} dr_c + \sum_{i=1}^{n_{c1}} \left( \frac{\partial \sigma_i}{\partial x_i} \right)_{x_k \neq i, y \neq i, p, T, r_c} dx_i + \sum_{i=1}^{n_{c2}} \left( \frac{\partial \sigma_i}{\partial y_i} \right)_{y_k \neq i, x \neq i, p, T, r_c} dy_i \quad (2.2)
\]

Equation 2.2 indicates that interfacial tension can be altered by changing the temperature, pressure, contact radius, and fluid composition. It is often reported that the interfacial tension decreases with temperature. However, both increase and decrease of interfacial tension are observed when pressure is increased. The variation of the water-oil interfacial tension depends on the composition of both water and oil phases. At the reservoir conditions, it is not often practical to change the composition of oil phase. However, the composition of the
water can be altered by changing the composition of injected water. Injecting low salinity water reduces the salinity of the water in the rock due to concentration-gradient diffusion. The variation of the water salinity changes the interfacial tension between oil and water depending on water and oil compositions and reservoir conditions. The contact angle also changes with the variation of salinity (Alotaibi 2011; Gupta and Mohanty 2011; Alameri et al. 2015).

In the reservoir, the variation of the interfacial tension between oil and water can be one important driving force for pushing oil out of its original place, particularly in the pore throat. The mass transfer along an interface between two fluids driven by the variation of the interfacial tension is often referred to as Marangoni flow, or the Gibbs–Marangoni flow. To illustrate how this phenomenon occur in the reservoir during low salinity water injection, we consider a cross section of a pore filled by oil as shown in Figure 2.2. The rock surface is oil-wetted. Initially, both sides of the pore is in contact with the same formation water (high salinity) as shown in Figure 2.2(a). Since the radius of the oil drop depends on the interfacial tension between water and oil and determined by Young-Laplace equation

\[ \left( p_i = p_o - p_w = \sigma_i \left( \frac{1}{r_1} + \frac{1}{r_2} \right) \right), \]

the interface radii on both sides are the same. The salinity of water in the right compartment is then decreased to duplicate the process during low salinity water injection. This salinity reduction decreases the oil-water interfacial tension of the right interface driving the transport of oil phase from the left to the right as shown in Figure 2.2(b). During this process both phase pressure and contact radius change until a new equilibrium is reached. This suggests that by reducing the interfacial tension, oil can be transported out of the oil-wetted rock matrix as observed in laboratory experiment by Kurtoglu (2014).

### 2.3 Determination of Oil Film Thickness on Pore Wall

The distribution of the fluid in the pore space is more complicated due to the complex structure of the pores and the thermodynamic balance of the fluid inside the pores. At pore scale, the surface forces and surface energy determine the distribution of water and oil
in the pores. For the oil-wetted pore wall, the water is not in direct contact with the wall but via a thin film of oil as shown in Figure 2.3. The wetted fluid sticks to the rock surface creating a thin film of fluid on the rock surface. The thickness of this film depends on the electrochemical potential and the interaction between the fluid and the rock. The electrochemical interaction between the fluid and the rock is determined by the disjoining pressure ($\Pi$) calculated from augmented Young-Laplace equation (Hirasaki 1991; Tutuncu 1992; Tutuncu and Sharma 1992; Kovscek et al. 1993) as,

$$ p^\alpha - p^\gamma = \Pi + 2H^\alpha\gamma \sigma_i^{\alpha\gamma} $$  \hspace{1cm} (2.3)

where $p^\alpha$ and $p^\gamma$ are pressure of phase $\alpha$ and $\gamma$; $H^\alpha\gamma$ is mean curvature; and $\sigma_i^{\alpha\gamma}$ is interfacial tension.

The contact angle ($\theta_c$) is calculated from surface energy as,

$$ 1 - \cos \theta_c = -\frac{1}{\sigma_i} \left[ \int_{h_o}^{\infty} \Pi dh - h_o \Pi (h_o) \right] $$

The disjoining pressure is the sum of all surface forces including van der Waals attraction, electrostatic repulsion and structural forces and Born repulsion (Israelachvili 1985). The disjoining pressure is a function of the separation distance between two interfaces (Hirasaki 1991; Israelachvili 1985; Tutuncu 1992; Bui and Tutuncu 2015):

$$ \Pi (h) = -\frac{A}{6\pi h^3} + \frac{64n_s kT}{\kappa} \beta^2 e^{-\kappa h} + K_l e^{-l} + \frac{1}{45} \frac{A\sigma_e^6}{h^9} $$  \hspace{1cm} (2.4)
Figure 2.3: The interfacial intension-induced transport of oil and water phases in simplified pores. When contacting with low salinity water, solute diffuse out of the pore toward low solute concentration to reach the new thermodynamic balance. The change of the salinity of the water inside the pore alters the interfacial and electrochemical properties of the fluid-rock system. This results in interfacial tension-induced transport inside the pore reducing the thickness of the oil layer stuck to the pore wall and forcing the oil trapping in the pore throat out of the pore. Oil is forced out and form small droplet. Then, nearby small oil drops merge to form bigger oil drops as observed in laboratory measurements. The core sample on the right (from Kurtoglu (2014)) is oil-wetted.

where $A$ is Hamaker constant; $\beta$ is coefficient calculated from zeta potential ($\zeta$); $K_l$ and $l$ are structural constants; $n_s$ is the ion concentration; $\sigma_s$ is atomic collision diameter; $k$ is the Boltzmann constant; $T$ is the absolute temperature; $\kappa$ is the inverse Debye-Huckel length. $\kappa$, $\beta$ are calculated as,

$$
\begin{align*}
\kappa &= \sqrt{\frac{8\pi n_s e^2 z^2}{e^2 k T}} \\
\beta &= \frac{\frac{z^2}{e^2} - 1}{e^2 + 1}
\end{align*}
$$

where $y = \frac{\zeta e}{k T}$, $e$ is electronic charge; $z$ is the valence of the electrolyte; $\epsilon$ is the dielectric constant of the fluid in between two interfaces.

The Hamaker constant that appears in Equation (2.4) is a chemical coefficient controlling the attractive van der Waals forces between bodies (Israelachvili 1985). It is calculated using
Lifshitz theory in terms of dielectric constants and refractive indices of materials involved (Israelachvili 1985; Hirasaki 1991; Tutuncu 1992):

\[
A = \frac{4}{3} kT \left( \frac{\epsilon_1 - \epsilon_3}{\epsilon_1 + \epsilon_3} \right) \left( \frac{\epsilon_2 - \epsilon_3}{\epsilon_2 + \epsilon_3} \right) + \frac{3\hbar \nu_e}{8\sqrt{2}} \frac{(n_1^2 - n_3^2)(n_2^2 - n_3^2)}{(n_1^2 + n_3^2)^{\frac{3}{2}}(n_2^2 + n_3^2)^{\frac{3}{2}} \left[ (n_1^2 + n_3^2)^{\frac{1}{2}} + (n_2^2 + n_3^2)^{\frac{1}{2}} \right]} \tag{2.6}
\]

where \(\epsilon_1\), \(\epsilon_3\), and \(\epsilon_2\) are the dielectric constant of the water, oil and the rock surface, respectively. \(\hbar\) is Plank’s constant, \(\nu_e\) is the absorption frequency of the fluid, \(n_1\), \(n_3\), and \(n_2\) are the refraction index for water, oil and the rock surface, respectively.

Having all properties of the pore surface and the fluid we can calculate the thickness of the oil film and the contact angle. At equilibrium, the thickness of the film is the value calculated for the separation distance. Therefore, the disjoining pressure is equal to the external force (Figure 2.4). The stable equilibrium position is the intercept at which the total surface force curve has a negative slope. In our case, the first intercept between the total surface force curve and the external force line is the separation distance (Figure 2.4).

This model can be helpful to evaluate the effect of fluid type and salinity on the hydrocarbon recovery at pore scale. The model can be used for evaluating the thickness of oil film variation with the salinity of water. The determination of the oil film thickness is not presented in this study since input data is not available. More experimental studies to determine the surface properties of rock are necessary to use the model confidently. Instead, the pore model, focusing on interfacial tension-induced transport along the pore, is introduced in this study in Chapter 3.

2.4 Flow Mechanisms and Unconventional Reservoir Modeling

The comparison of the permeability obtained from core experiment and that from field measurements often suggests that micro-fractures are present in shale formations as shown for Bakken Formation by Kurtoglu (2014). Hence, the dual-porosity or dual-permeability model is often used to model these kinds of reservoirs (Cipolla 2009; Ozkan et al. 2010;
Figure 2.4: Determination of thin film thickness

Abdulal et al. 2011; Apaydin 2012; Fakcharoenphol 2013; Morsy et al. 2013b; Kurtoglu 2014; Fuentes-Cruz and Valko 2015; Sun et al. 2015). It is also suggested by Sun et al. (2015) that dual-porosity or dual-permeability model with Knudsen diffusion is adequate to model the unconventional gas reservoir production. More detailed modifications are also proposed to model the complex flow in shale reservoirs.

Fuentes-Cruz and Valko (2015) presented a new approach to account for the effect of matrix-block size variation on the well performance of unconventional shale reservoirs. The characteristic length of the blocks depends on the distance from the main hydraulic-fracture plane. They assume that the density of micro-fractures (natural and induced) is high near the hydraulic-fracture face, but gradually decreases away from hydraulic-fracture face. In other words, the matrix-block size increases with the distance from the fracture face.

Due to the complexity of the fractures and the flow in rock matrix, triple-porosity and even multi-porosity models are used in some research studies for shale reservoirs (Schepers et al. 2009; Dehghanpour and Shirdel 2011; Hudson et al. 2012; Tivayanonda et al. 2012; Haghshenas et al. 2013; Li et al. 2013; Torcuk et al. 2013; Yan et al. 2013). Other modifications have also been proposed to capture the complexity of the pressure transient in shale reservoirs. Torcuk et al. (2013) presented a model accounting for multiple matrix size and the corresponding properties. Multi-porosity and multi-matrix block size model may offer a
better production forecast. However, as the model becomes more complex, the determination of the corresponding input parameters is more difficult for practical measurements in the field or in the laboratory.

The other modification of a dual-porosity model for shale reservoirs is the consideration of multi-components within the rock matrix. Shales often contain organic and inorganic materials. As the result of the hydrocarbon generation process, the organic matter is often hydrocarbon-wetted. The absorbed gas and free gas are proportional to the total organic carbon (TOC) content. In modeling, separation between inorganic and organic materials is used (Yan et al. 2013).

Coupling fluid flow model with geomechanics model also has received significant attention in unconventional reservoir modeling. One of the primary objectives of the coupled fluid flow and geomechanics modeling is to account for the effect of rock deformation on the flow and associated recovery factor of the reservoir. The fluid flow equation is related to geomechanics equation by the volumetric strain representing the volumetric variation of rock due to pressure, stress, and temperature. The flow properties of the reservoir, particularly permeability, is often related to the volumetric variation of rock due to fluid pressure, in situ stress, and temperature. Fakcharoenphol et al. (2013) used a coupled model to investigate the effect of water-induced stress on the existing fractures and the creation of new fractures. They suggested that water-induced stress is one of the mechanisms for enhancing permeability and hence improving gas recovery.

The recent development in coupled modeling includes the advancements in coupling techniques, dual-grid size technique, and more comprehensive physical coupling of fluid and rock interactions. Kim and Moridis (2012) presented a coupled geomechanics and fluid flow model using multiple porosity model for shale reservoirs. The multi-scale and multi-physics modeling studies are also conducted (Lerdahl et al. 2005; Ramirez 2010; Apaydin 2012; Elfeel et al. 2013). One of the common objectives of these modeling studies is to accurately model the mass exchange between the fractures and the rock matrix and simulate multi-physics at
matrix block scale. However, analytical mass transfer functions were used in these studies. The effectiveness of different fluid salinity has not been investigated in these studies.

With the development of new tools for fracture characterization using seismic data, seismic-driven reservoir simulation and monitoring are becoming the standard improving reservoir description (Ouenes et al. 2004; Li et al. 2014; Ramanathan et al. 2014). The new commercial software packages have provided a tool for modeling the fracture geometry and integration of the seismic and stimulation data in the reservoir modeling and production forecasting.

2.5 Mass Transport between Fractures and Rock Matrix

The success of the water injection in fractured reservoirs depends strongly on the knowledge of mass transport mechanisms in reservoir, particularly between fractures and rock matrix. This transport is governed by various natural forces including gravity, pressure, chemical, and thermal potential gradient. The transport of the solute phase between the fractures and the rock matrix also determines the salinity of the flow-back water and production rate improvement after a shut-in period.

Because the shale matrix permeability is very low, the Darcy flow is less significant and other flow mechanisms are more dominant. For gas reservoirs, Ozkan et al. (2010) incorporated the Darcy flow, diffusive flow in the shale matrix, and stress dependent permeability of fractures into a dual-porosity model and derived a new transfer function for fractured shale-gas reservoirs. They showed that the Darcy flow is dominated near the surface of the shale matrix and the diffusive flow is dominated near the core of the matrix. Diffusive flow is considered to make a significant contribution to production and becomes more important as the matrix permeability decreases. Apaydin (2012) suggested that the effect of stress dependent permeability and a better calculation of the mass transfer is critically important for low permeability formations.

Settari et al. (2002); Cheng (2012); Agrawal and Sharma (2013); Fakcharoenphol (2013); Ghanbari et al. (2013) also suggested that the imbibition of the injected water into the shale
matrix is considered to be the main reason for the improved early production rate after shut-in period. Imbibition experimental observation by Lan et al. (2014) suggested that the amount of water that imbibes into matrix depends on the clay content and TOC content of the matrix. They observed that the amount of imbibed water is inversely proportional to the TOC and matrix block size. Oil-wetting property of the organic material could be the main reason for this observation. Tensile induced micro-fractures are also observed in their experiment. However, the experiments were conducted at room conditions and no confining stress was applied. Hence, the recovery from matrix is higher than in the in situ reservoir conditions.

2.6 Flow-back Water Analysis

During hydraulic fracturing operations, fracturing fluid is pumped at high pressure into the formation to generate hydraulic fractures. This fluid invades the shale reservoir and then is returned to the surface through the wellbore after fracturing. In the early state of production, this fluid is called flow-back fluid or flow-back water. In the field operation, only a portion of the injected fluid is recovered during the clean-up phase followed by produced water.

The reasons behind the low water flow-back is still not well understood due to its significant dependence on the fluid and rock characteristics and their interactions. Hence, it varies from formation to formation. In several research studies (Fan et al. 2009; Ghanbari et al. 2013; Lan et al. 2014), it was suggested that this water may be trapped in secondary fractures or was imbibed into the rock matrix. The exchange of the solute concentration between the water in shale matrix and water in the fractures is considered as the main reason for the increase of salinity of the flow-back water. The field data and experiments conducted by Ghanbari et al. (2013) showed that the increasing salinity of flow-back water may be the result of solute exchange between the fractures and the shale matrix. Haluszczak et al. (2013) also showed that the mixing of injected fluid with the formation brine is the reason for salinity variation of the flow-back water. While Blauch et al. (2009) suggested
that the dissolution of the rock constituents is the main reason for the chemical alteration of the flow-back water salinity. This hypothesis may be questionable for formations with initial water saturation since the formation water salinity is typically less than the solubility of the solute. The concentration of the solute in formation water is often less than maximum concentration of solute that can be dissolved; hence, the salt may not be present in the solid form. Gale et al. (2014) observed that the mineral filled natural fractures and local precipitated salts may react with water and impact the composition of flow-back water.

Flow-back water analysis provides useful information for evaluating and optimizing hydraulic fracturing operations, estimating formation properties, and forecasting reservoir performance. Crafton and Gunderson (2007) showed that high frequency data collection of the flow-back fluid can be used to obtain hydraulic fracture properties such as fracture conductivity and length. Clarkson and Williams-Kovacs (2013) used the flow-back of shale-gas wells to obtain hydraulic-fracture properties. They suggested that the early fluid production and flowing pressure data gathered immediately after the hydraulic fracture stimulation can be used for long-term production forecasts. Fluid compositions and chemical tracers added during stage treatments may be monitored to determine the fluid recovery and to evaluate inflow from each stage. They also emphasized that the flow-back data should be tested for a greater data set and should not be used for reserve forecasting. In addition, the flow-back water chemical analysis can also be used for tracking the origin of ions and for evaluating environmental impact as shown by Warner et al. (2012).

2.7 Low Salinity Waterflooding

Low salinity water has been first reported to be effective by George (1967). In early 1990s, low salinity waterflooding has received further attention in the enhanced recovery research studies (Jadhunandan 1990). Low salinity water injection has been reported to improve the oil recovery by the field observations in conventional reservoirs (Webb et al. 2004). There are also field data suggesting that the recovery improvement potential of low salinity waterflooding in low permeability formations (Skrettingland et al. 2011). The first
pilot waterflooding project in a shale formation was conducted in the Bakken Formation in 2006 (Wood and Milne 2011). Although the effect of low salinity water injection was not investigated, the improvement of oil recovery from this project indicated the potential of water injection for enhancing the oil recovery. The results from a numerical simulation study conducted by Iwere et al. (2012) showed that using water injection can improve the oil recovery in Bakken Formation up to 6.7%.

There are many hypotheses explaining the effectiveness of low salinity water injection on oil recovery including the wettability alteration, osmotic pressure, and the expansion of electrical-double-layer. Wettability alteration from non-water-wetted towards more water-wetted formation is often considered as the first mechanism for improving hydrocarbon recovery (Austad et al. 2010; Masalmeh et al. 2014). Low salinity water changes the relative permeability curve, reducing the water relative permeability, increasing the oil relative permeability at a given water saturation, and reducing the residual oil saturation. At the same water saturation, the capillary pressure of the low salinity water is higher than that of the high salinity water. Looking further into the mechanism of wettability alteration, Nasralla and Nasr-El-Din (2014) suggested that the expansion of the electrical-double-layer can also be a dominant mechanism for oil recovery improvement by the low salinity waterflooding. However, most of this works were conducted for conventional reservoirs.

Austad et al. (2010) summarized the research studies by Lager et al. (2006), Lager et al. (2007), and Tang and Morrow (2010) to list the conditions for effective low salinity water flood in sandstone reservoirs. These conditions include: the formation must contain clay; oil contains polar components; initial formation water is required and it must contain divalent components. Morrow and Buckley (2011) reviewed the effect of low salinity water flooding on the hydrocarbon recovery from conventional reservoirs. They showed that the necessary conditions for successful low salinity waterflooding in Berea-sandstone core are the presence of clay fraction, connate water, and mixed-wettability conditions. The effectiveness of the low salinity waterflooding depends strongly on the initial water saturation, the ionic type
and the composition suggesting that low salinity waterflooding can also be effectively used for unconventional formations.

He et al. (2015) stated that the wettability alteration is the primary reason for recovery improvement from shale reservoirs. Their experimental data show that low salinity waterflooding and interfacial tension alteration increases the recovery in shale reservoirs. Experimental data on Mancos Shale by Morsy et al. (2014) suggested that reducing pH of the injected water can increase the recovery from samples up to 53%. The change of contact the angle and the wettability alteration are considered to be the reasons for recovery improvement in their experiments. Nguyen et al. (2014) emphasized the importance of wettability alteration from oil-wet to water-wet on the increase of the oil recovery from fractured oil-wetted reservoirs. The experimental results by Kathel and Mohanty (2013) also showed that wettability alteration has a positive effect on EOR in tight oil reservoirs.

To model the effect of low salinity water flooding on wettability alteration, different relative permeability and capillary pressure curves for low and high salinity were used (Jerauld et al. 2008; Al-Shalabi et al. 2014; Masalmeh et al. 2014). The difference in relative permeability curves for low and high salinity experiments (Figure 2.5) is considered to be the result of wettability alteration. For unconventional reservoirs, there are ongoing research studies that the effect of salinity on the contact angle and wettability alteration are being investigated. However, the evaluation overall effects of these factors on hydrocarbon recovery from unconventional reservoirs is still not available.

Osmotic pressure is recently added as one of the mechanisms for improving hydrocarbon recovery using low salinity water injection (Fakcharoenphol 2013; Kurtoglu 2014). The difference in salinity between the injected fluid and formation brine creates a concentration gradient and an osmotic pressure. This osmotic pressure induces the flow of water in fractures into the matrix with pore containing high-solute concentration. This process continues until the solute concentrations reach an equilibrium. To account for this additional driven force on gas recovery in low permeability formations, Fakcharoenphol (2013) suggested adding the
Figure 2.5: The effect of salinity on relative permeability. Low salinity (LS) water reduces the water relative permeability ($K_{rw}$) and increases oil relative permeability ($K_{ro}$) at a given water saturation as compared to high salinity (HS) water. Low salinity water also reduces the residual oil saturation (Jerauld et al. 2008).

Osmotic pressure into the transfer function. One of the factors we also need to consider is the very slow process of osmotic pressure driven flow in very tight rock matrix. Conventional approach using transfer functions, developed for Darcy’s flow, may overestimate the contribution of osmotic pressure due to time dependent characteristics and low permeability of the shale formations. In a recent study, Kristian et al. (2016) showed that the contribution of osmosis on oil recovery is overestimated. They emphasized paying more attention toward wettability alteration. Their conclusion is based on their experiment with relatively large pore sizes. For larger pore size, the membrane efficiency is almost zero as shown later in this modeling study, hence the contribution of osmosis is negligible as their data showed.

2.8 Shale Swelling Mechanisms and Modeling

In the reservoir engineering literature, the effect of shale swelling on geomechanical properties and hydrocarbon recovery has not been investigated comprehensively. In this section,
the swelling mechanism with governing factors and the effect of shale swelling on fractures and rock matrix porosity and permeability variation are reviewed. The effect of swelling on the hydrocarbon recovery is also discussed.

### 2.8.1 Shale Swelling Mechanism and Governing Factors

Not all shales swell when contacted with water. The swelling properties depend on the mineralogy and the transport properties of the shales. The amount of clay in the reservoir and the type of clays are the most important parameters determining the swelling properties of the rock. Shale with high smectite content tends to swell more while shale with high kaolinite tends to disintegrate and disperse, shale with high illite content also tends to disperse. A summary of mineral composition and clay contents of several shale formations that have been investigated at UNGI geomechanics research group are shown in Figure 2.6. For Eagle Ford Formation, Murphy et al. (2013) also showed that clay content is about 5-35% of the shale volume with high illite, smectite and kaolinite contents which suggests that the percentage of clay is considerable and accounting for the effect of shale swelling is essential.

Two types of shale swelling are crystalline swelling and osmotic swelling. Crystalline swelling is the result of cation exchange between clay minerals and the fluid due to negative charges on the clay layers. The exchange of cation increases the distance between clay platelets and results in the expansion of clay. Osmotic swelling is the result of the salinity difference between the original fluid in shale and the new fluid in contact with shale. Low salinity injected water diffuses into the shale matrix with higher salinity and hydrates the clay particle creating the double layer with repulsive potential and resulting in the expansion of the shale matrix. Zhang et al. (2004) showed that the shale swelling significantly change the volume of the shale sample depending on the amount of time shale sample is in contact with water as shown Figure 2.7. The cation exchange capacity (CEC) and surface area of four common clays as shown in Table 2.1 indicate that smectites have highest swelling tendency since it has the highest cation exchange capacity.
The swelling of shale depends also on the solute concentration and ion types (Mese 1988, 1995; Zhang et al. 2004; Ewy and Morton 2009). Low salt concentration solution often promotes shale swelling. The experimental results for Eagle Ford samples by Emadi et al. (2013) showed that the maximum volumetric swelling strain after 7 days is about 0.69% when submerged into distilled water and about 0.15% when submerged into 7% KCl water. The effect of salt concentration on the swelling of Eagle Ford shale also was confirmed from an experimental study by Morsy et al. (2013b) when they compared the difference between distilled water and 2% KCl solution. Injected fluid with higher water activity, or low salinity, tends to move into shale matrix and increases the pore pressure causing the shale to swell. While injected fluid with high salinity, water will move out of shale matrix reducing the pore pressure resulting dehydration induced cracks and fissures within the shale matrix. The invasion of the water often changes the cohesive force that keeps the clay particles sticking...
Figure 2.7: Effect of ion type and ion concentration (water activity, aw) on the swelling behavior of the Arco Shale. The swelling percentage is the elongational strain along the core sample (Zhang et al. 2014). It is showed that the higher the water activity, the higher the swelling strain of the shale sample. The swelling behaviors of the Arco Shale with two types of ions are considerably different.

to each other and may cause failure. This changes the permeability of shale matrix (Al-Arfaj et al. 2014).

Mese (1988) built a new apparatus to measure preloads necessary to prevent expansion. The sample volume was kept constant after it is introduced to the injection fluid and the load that is created by the sample was recorded as a function of time. Pressure recorded at the equilibrium time was assumed to be the swelling pressure of the sample for the particular fluid used during the measurements. An increase in montmorillonite concentration considerably decreased the equilibrium time for all clays tested. An experimental and theoretical investigation of the effects of saturation, stress and pore fluid type on the mechanical, acoustic and swelling characteristics for various pure clays and core shale samples was also conducted (Mese 1988, 1995). Mese 1995 also developed a model to include the fluid/clay interactions into calculation for estimation of percent swelling in each shale formation. A comparison of the measured expansion (swelling) data using kaolinite and Pierre shale sam-
Table 2.1: Cation exchange capacity and surface area of four common clays

<table>
<thead>
<tr>
<th>Clay type</th>
<th>CEC (meq./100 g)</th>
<th>Internal surface area (m²/g)</th>
<th>External surface area (m²/g)</th>
<th>Total surface area (m²/g)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Chlorite</td>
<td>1-30</td>
<td>0</td>
<td>15</td>
<td>15</td>
</tr>
<tr>
<td>Illite</td>
<td>10-40</td>
<td>0</td>
<td>30</td>
<td>30</td>
</tr>
<tr>
<td>Kaolinite</td>
<td>3-10</td>
<td>0</td>
<td>15</td>
<td>15</td>
</tr>
<tr>
<td>Smectite</td>
<td>80-150</td>
<td>750</td>
<td>50</td>
<td>800</td>
</tr>
</tbody>
</table>

Samples indicated a good agreement between his swelling predictions in these formations. Under 1 psig load with lateral restraint, Pierre Shale and kaolinite expanded 35% and 30%, respectively. Increasing the KCl concentration from zero (distilled water) to 10% decreased the expansion around 10% in kaolinite and 8% in Pierre Shale. However, increasing the load even from 1 to 50 psig decreased the expansion 13% in both samples tested. Mese (1988) reported similar conclusions for other pure clays (montmorillonite, API bentonite, attapulgite) and shale core samples (Mancos, Ekofisk, Andrews County and Mississippi shales).

Shale swelling also depends on the experimental conditions implemented such as temperature, pore pressure, and stress. Chenevert and Osisanya (1992) investigated swelling behavior of the Wellington Shale contacted with water under elevated temperatures and pressures. They showed that the increasing of the confining stress acting on the shale sample reduces the swelling rate. An increase in pore pressure and temperature results in higher swelling rates.

In addition, the swelling behavior of the shale sample strongly depends on the direction of the bedding. Emadi et al. (2014) showed that the maximum swelling occurs on the samples cored in the direction parallel to the bedding and minimum shale swelling occurs in the sample cored in the direction perpendicular to the bedding. This is the result of layering structure, fabric, texture, and directional dependence of permeability and other anisotropic geomechanical properties of shales.
2.8.2 Effect of Shale Swelling on Matrix and Fracture Porosity and Permeability

Matrix permeability and porosity can be changed as a result of shale swelling, especially for the shale matrix near the fracture face. Ji and Geehan (2013) used an analytical model for calculating the water content along the clay sample as a function of time. Then, a correlation was used to compute the vertical strain, horizontal strain, yield strength, Young’s modulus, and Biot coefficient. They solved the equation of motion to determine the stress along the core sample and determined if the swelling caused the failure of the shale sample. Since the deviatoric stress is high inside the sample, not at the surface, this creates the failure inside the shale sample. This failure improves the permeability of shale matrix and facilitated the penetration of fluid along the existing secondary fractures deeper in shale matrix. New “secondary” fractures will be created and they will continue to propagate deeper inside the shale matrix. Because the tensile strength is lowest in the direction perpendicular to the bedding, the secondary micro-fractures are often formed along the bedding plane. The formation of these induced fractures depends on the confining stress and boundary condition. The free movement near the wellbore and hydraulic fractures promotes the formation of these osmotic induced fractures. Away from the wellbore or hydraulic fractures, the confining pressure and in situ stress in the reservoir reduce the formation of these micro-fractures instead of the expansion of clay reducing the porosity and permeability of shale matrix. A correlation between matrix failure and permeability improvement should be developed experimentally to evaluate the effect of clay swelling on the matrix permeability in this case.

The fracture permeability and porosity can be altered by two key mechanisms. The first mechanism relates to the changes in the pressure of fluid phases in the fractures. High internal fracture pressure tends to mechanically open the fractures and enhance the fracture permeability. The second mechanism is related to the swelling of the matrix (volumetric strain) and thus reduces the fracture permeability by narrowing and even closing fracture apertures. These two mechanisms have been investigated and modeled by Liu and Rutqvist (2009) and other researchers for coal.
2.8.3 Effect of Shale Swelling on Hydrocarbon Recovery

The effect of shale swelling on hydrocarbon recovery can also be found in literature in core scale experiments (Lager et al. 2007; Lan et al. 2014; Morsy et al. 2013b; Kurtoglu 2014). However, shale swelling modeling in reservoir scale is still not available. Lager et al. (2007) showed that there is a linear correlation between clay content and oil recovery for the low-salinity water injection enhanced oil recovery. Clay minerals with high cation exchange capacity tend to be more favorable to low salinity effects (Austad et al. 2010). The experimental data from Morsy et al. (2013b) on the Eagle Ford core sample illustrated that the higher recovery oil recovery by spontaneous imbibition is due to shale swelling. They showed that the oil recovery during waterflooding with distilled water is higher than the recovery when 2% KCl solution was used. This could be due to the fact that water with lower salinity imbibes more into the core and cause more swelling. In other words, low salinity water injection results in more shale swelling. However, no confining stress was applied in their experiments. Hence their results may lead to a conclusion that swelling may increase the oil recovery. This may occur near the hydraulic fracture face but may not occur for the rock matrices away from the hydraulic fractures.
It has been observed in the laboratory measurements that water imbibes into the oil-wetted rock matrix. The amount of water imbibed into rock matrix increases when the salinity of the injected water decreases. Wettability alteration is often considered as the main reason for this phenomena. The main phenomenon behind wettability alteration is the variation of the interfacial tension and the contact angle. In this chapter, the mass transport mechanism of the water and oil at the pore scale caused by interfacial tension variation, or interfacial tension-induced transport, is investigated. First, a simplified pore scale model is presented to simulate the imbibition of water into an oil-wetted pore. Next, a numerical solution and procedure are outlined followed by the results and discussions. Finally, the limitations of the pore scale model and future works are discussed.

3.1 Simplified Pore Scale Model

We use a relatively simple conceptual capillarity model in porous media often referred to as “bundle of capillaries” model (Kayser et al. 2006). The distribution of pore sizes is modeled by a distribution of capillaries with various radii. Depending on the pore and pore-throat geometries, a part of the pore space are oil-filled and the other parts are water-filled. We focus on the mass flux into a single pore modeled as a series of tubes and cones to represent the pore and pore throat. The pore is oil-wetted. Oil fills in the pore throat and the rest of the pore on the right (Figure 3.1). The system is first at equilibrium and the pressures at two ends are equal to \( p_{o1} \) and \( p_{w1} \). The salt concentration of water in the pore is \( c_{si} \). Then, the concentration of water at the outlet is reduced to \( c_{sn} \) while keeping the pressure at the two ends constant. This initiates the diffusion of the salt from the pore to its inlet reducing the solute concentration of the water and changing the water-oil interfacial
tension. Because of the interfacial tension variation, the interface moves to reach a new equilibrium driving the flow of water and oil along the pore.

3.2 Mathematical Model for Mass Transport in Pores

To formulate the mathematical model describing the mass transport in the pore geometry, we consider a horizontal pore and ignore the effect of gravity. The geometry of the pore and the distribution of water and oil phase are shown in Figure 3.1. Since the pore geometry is symmetrical, only one half of the pore is presented in Figure 3.1. The reduction of the interfacial tension causes not only interface movement but also the change of phase pressure. This makes the modeling task more challenging. In order to investigate the contribution of only interfacial tension-induced transport on mass transport along the pore, we assume that pressures at two ends of the pore are constant. Fluids, water and oil, are modeled as Newtonian fluids with constant viscosity. To simplify the solution, we also assumed that system is isothermal. The deformation of the pore space due to the pressure reduction has not been considered in this research study.

Figure 3.1: Dimension and distribution of phase in simplified pore model.

3.2.1 Governing Equations

Assuming that the solute is only dissolvable in water, the continuity equation for water and oil phase in pores can be written as,
\[
\n\nabla \cdot \left[ (\rho_w \vec{v}_{w,p}) - \rho_w \frac{k_w}{\mu_w} \frac{\omega RT}{V_w} \nabla c_{s,p} \right] + \rho_w \dot{q}_{wp} = \frac{\partial}{\partial t} (\rho_w S_{wp}) \tag{3.1}
\]

\[
\nabla \cdot (\rho_o \vec{v}_{o,p}) + \rho_o \dot{q}_{op} = \frac{\partial}{\partial t} (\rho_o S_{op}) \tag{3.2}
\]

where the subscripts \( p, o, s, w \) are referred to pore, oil, solute, and water; \( c_{s,p} \) is solute concentration in pore; \( p_i, \rho_i, S_{i,p}, \vec{v}_{i,p} \) are pressure, density, saturation, and velocity of phase \( i \) \( (i = o, w) \); The sink/source term \( \dot{q}_{w,p} \) is the specific rate of phase \( i \) \( (i = o, w) \) entering or leaving the pore; \( R \) is the universal gas constant; \( T \) is the temperature; \( t \) is time; \( \omega \) is the membrane coefficient. When a single pore with sufficiently large pore throat diameter is considered, the membrane coefficient of the pore is zero.

The derivation of the transport equation for water phase is presented in Appendix A.

Using the Darcy’s Law and ignoring the gravity, these continuity equations can be written in 1-D as,

\[
\frac{\partial}{\partial x} \left[ \rho_w \frac{k_{wp}}{\mu_w} \left( \frac{\partial p_{wp}}{\partial x} \right) - \rho_w \frac{k_w}{\mu_w} \frac{\omega RT}{V_w} \frac{\partial c_{s,p}}{\partial x} \right] + \rho_w \dot{q}_{wp} = \frac{\partial}{\partial t} (\rho_w S_{wp}) \tag{3.3}
\]

\[
\frac{\partial}{\partial x} \left[ \rho_o \frac{k_{op}}{\mu_o} \left( \frac{\partial p_{op}}{\partial x} \right) \right] + \rho_o \dot{q}_{op} = \frac{\partial}{\partial t} (\rho_o S_{op}) \tag{3.4}
\]

where \( k_{ip}, \mu_i \) are permeability and viscosity of phase \( i \) \( (i = o, w) \) in the pore.

The right hand side of the equation for water phase can be expanded as,

\[
\frac{\partial}{\partial t} (\rho_w S_{wp}) = \rho_w \frac{\partial S_{wp}}{\partial t} + S_{wp} \frac{\partial \rho_w}{\partial t} = \rho_w \frac{\partial S_{wp}}{\partial t} + S_{wp} \frac{\partial p_{wp}}{\partial t} \frac{\partial \rho_w}{\partial p_{wp}} = \rho_w \frac{\partial S_{wp}}{\partial t} + S_{wp} c_w \rho_w \frac{\partial p_{wp}}{\partial t} \tag{3.5}
\]

Hence, the continuity equation for water and oil phases are simplified as,

\[
\frac{\partial}{\partial x} \left[ \rho_w \frac{k_{wp}}{\mu_w} \left( \frac{\partial p_{wp}}{\partial x} \right) - \rho_w \frac{k_w}{\mu_w} \frac{\omega RT}{V_w} \frac{\partial c_{s,p}}{\partial x} \right] + \dot{q}_{wp} = \frac{\partial S_{wp}}{\partial t} + S_{wp} c_w \frac{\partial p_{wp}}{\partial t} \tag{3.6}
\]

\[
\frac{\partial}{\partial x} \left[ \frac{k_{op}}{\mu_o} \frac{\partial}{\partial x} (p_{wp} - p_{cwop}) \right] + \dot{q}_{op} = \frac{\partial S_{op}}{\partial t} + S_{op} c_o \frac{\partial (p_{wp} + p_{cwop})}{\partial t} \tag{3.7}
\]

In the equation above, \( c_w \) and \( c_o \) are compressibilities of water and oil defined as,

\[
\begin{align*}
    c_w & = \frac{1}{\rho_w} \frac{\partial \rho_w}{\partial p_{wp}} \\
    c_o & = \frac{1}{\rho_o} \frac{\partial \rho_o}{\partial p_{op}}
\end{align*} \tag{3.8}
\]
The pressure of water phase is higher than that of the oil phase. At a certain interfacial radius, the capillary pressure in the pore, \( p_{cwop} \), is calculated from Young-Laplace equation as,

\[
p_{cwop} = p_{wp} - p_{op} = \sigma_i \left( \frac{1}{r_1} + \frac{1}{r_2} \right) = \sigma_i \left( \frac{1}{r_c} + \frac{1}{r_c} \right) \cos \theta_c = \frac{2\sigma_i \cos \theta_c}{r_c} \tag{3.9}
\]

where and \( r_1 \) and \( r_2 \) are the principal radii of curvature; \( \sigma_i \) is the water-oil interfacial tension; and \( r_c \) is contact radius; \( \theta_c \) is contact angle.

The summation of two equation gives

\[
\frac{\partial}{\partial x} \left[ \frac{k_{op}}{\mu_o} \frac{\partial}{\partial x} (p_{wp} + p_{cwop}) \right] + \frac{\partial}{\partial x} \left[ \frac{\rho_w k_{wp}}{\mu_w} \frac{\partial p_{wp}}{\partial x} \right] - \frac{\rho_w k_{wp}}{\mu_w} \frac{\omega RT}{V_w} \frac{\partial c_{s,p}}{\partial x} + \dot{q}_{wp} + \dot{q}_{op} = c_{tp} \frac{\partial p_{wp}}{\partial t}
\]

\[
\frac{\partial}{\partial x} \left[ \frac{k_{op}}{\mu_o} \frac{\partial}{\partial x} (p_{wp} + p_{cwop}) \right] + \frac{\partial}{\partial x} \left[ \frac{\rho_w k_{wp}}{\mu_w} \frac{\partial p_{wp}}{\partial x} \right] - \frac{\rho_w k_{wp}}{\mu_w} \frac{\omega RT}{V_w} \frac{\partial c_{s,p}}{\partial x} + \dot{q}_{wp} + \dot{q}_{op} = c_{tp} \frac{\partial p_{wp}}{\partial t} \tag{3.10}
\]

where \( c_{tp} = (S_{op}c_o + S_{wp}c_w) \) is the total compressibility. The last term is relatively small and is can be neglected.

\[
\frac{\partial}{\partial x} \left[ \frac{k_{op}}{\mu_o} \frac{\partial}{\partial x} (p_{wp} + p_{cwop}) \right] + \frac{\partial}{\partial x} \left[ \frac{\rho_w k_{wp}}{\mu_w} \frac{\partial p_{wp}}{\partial x} \right] - \frac{\rho_w k_{wp}}{\mu_w} \frac{\omega RT}{V_w} \frac{\partial c_{s,p}}{\partial x} + \dot{q}_{wp} + \dot{q}_{op} = c_{tp} \frac{\partial p_{wp}}{\partial t} \tag{3.11}
\]

The permeabilities of the phase \( i (i = w, o) \) is calculated from pore radius \( (R_p) \) as,

\[
k_{ip} = \frac{R_p^2}{8} \tag{3.12}
\]

Mass transport equation for solute is:

\[
\nabla \cdot (D_{eff,p} \nabla c_{s,p}) - \nabla \cdot (c_{s,p} v_{w,p}) + \dot{q}_{s,p} = \frac{\partial c_{s,p}}{\partial t} \tag{3.13}
\]

where \( D_{eff,p} \) is the effective diffusion coefficient in the pore, \( \dot{q}_{s,p} \) is solute specific rate entering or leaving the pore.

In 1-D, equation above can be simplified into Equation 3.14 as,

\[
\frac{\partial}{\partial x} \left( D_{eff,p} \frac{\partial c_{s,p}}{\partial x} \right) - \frac{\partial}{\partial x} (c_{s,p} v_{w,p}) + \dot{q}_{s,p} = \frac{\partial c_{s,p}}{\partial t} \tag{3.14}
\]
Velocity of water is defined as,

\[ v_{w,p} = -\frac{k_{w,p}}{\mu_w} \nabla (p_{wp}) \]  

(3.15)

### 3.2.2 Interface Position

The position of the interface satisfies the following constrain derived from Newton’s second law as,

\[
\frac{\partial}{\partial t} \left( \rho_w z_c \frac{\partial z_c}{\partial t} \right) = \frac{2\gamma \cos \theta_c}{r} - \frac{2\gamma_o \cos \theta_{c_o}}{r_o} + \frac{\mu_w}{k_{w,p}} z_c \frac{\partial z_c}{\partial t} - \Delta \rho g z_c \sin \psi \]  

(3.16)

or

\[
\rho_w z_c \frac{\partial^2 z_c}{\partial t^2} + \rho_w \left( \frac{\partial z_c}{\partial t} \right)^2 = \frac{2\gamma \cos \theta_c}{r} - \frac{2\gamma_o \cos \theta_{c_o}}{r_o} + \frac{\mu_w}{k_{w,p}} z_c \frac{\partial z_c}{\partial t} - \Delta \rho g z_c \sin \psi \]  

(3.17)

where \( z_c \) is the position of the interface; \( r_o \) is the initial contact radius; \( \psi \) is the inclination angle of the pore, for horizontal pore, \( \psi = 0 \); \( \Delta \rho \) is the density difference \( \Delta \rho = \rho_w - \rho_o \).

For nano pores, the derivative terms in the left hand side are relatively smaller than other terms. Ignoring these terms, Equation 3.17 is reduced to:

\[ 0 = \frac{2\gamma \cos \theta_c}{r} - \frac{2\gamma_o \cos \theta_{c_o}}{r_o} + \frac{\mu_w}{k_{w,p}} z_c \frac{\partial z_c}{\partial t} - \Delta \rho g z_c \sin \psi \]  

(3.18)

### 3.3 Numerical Solution of the Pore Scale Model

The meshing scheme for the pore is illustrated in Figure 3.2. The solution of the total pressure equation gives us the pressure of each phase in the pore. The saturation, contact radius, capillary pressure, and flow rates can be calculated when water pressure is obtained.

![Meshing scheme for pore scale model](image.png)

Figure 3.2: Meshing scheme for pore scale model
3.3.1 Phase Pressure in Pores

The finite difference equation to solve for water pressure (Equation 3.11) is written as,

$$M_{xpb}p_{wp_{i,j,k}}^{n+1} + M_{xpm}p_{wp_{i,j,k}}^{n+1} + M_{xf}p_{wp_{i+1,j,k}}^{n+1} = M_{xpR}$$ (3.19)

where

$$M_{xpb} = \frac{1}{\Delta x_{i,j,k}} \left( \frac{k_{op}}{\mu_o \Delta x} + \frac{k_{wp}}{\mu_w \Delta x} \right)_{i-\frac{1}{2},j,k}$$ (3.20)

$$M_{xpf} = \frac{1}{\Delta x_{i,j,k}} \left( \frac{k_{op}}{\mu_o \Delta x} + \frac{k_{wp}}{\mu_w \Delta x} \right)_{i+\frac{1}{2},j,k}$$ (3.21)

$$M_{xpm} = - \left\{ M_{xb} + M_{xf} + \frac{-c_{tp_{i,j,k}}^n}{\Delta t} \right\}$$ (3.22)

$$M_{xpR} = \frac{-1}{\Delta x_{i,j,k}} \left\{ \left( \frac{k_{op}}{\mu_o \Delta x} \right)_{i+\frac{1}{2},j,k} \left[ (p_{cwop}^n)_{i+1,j,k} - (p_{cwop}^n)_{i,j,k} \right] - \left( \frac{k_{wp}}{\mu_w \Delta x} \right)_{i-\frac{1}{2},j,k} \left[ (p_{cwop}^n)_{i,j,k} - (p_{cwop}^n)_{i-1,j,k} \right] \right\}$$

$$- \frac{(q_{wp} + q_{op})_{i,j,k}}{V_{i,j,k}} - c_{tp_{i,j,k}}^n \frac{p_{wp}^n}{p_{wp}^n} + \frac{1}{\Delta x_{i,j,k}} \left[ \frac{k_{wp}}{\mu_w \Delta x} (c_{s,p_{i+1,j,k}}^n - c_{s,p_{i,j,k}}^n) - \frac{k_{wp}}{\mu_w \Delta x} (c_{s,p_{i,j,k}}^n - c_{s,p_{i-1,j,k}}^n) \right)$$ (3.23)

3.3.2 Solute Concentration Equation

Solute concentration in the pore is calculated from the continuity equation for the solute in the pore (Equation 3.14) as,

$$c_{s,p_{i,j,k}}^{n+1} = \frac{\Delta t}{\Delta x_{i,j,k}} \left[ \left( \frac{D_{eff,p}}{\Delta x} \right)_{i+\frac{1}{2},j,k} \left( c_{s,p_{i+1,j,k}}^n - c_{s,p_{i,j,k}}^n \right) - \left( \frac{D_{eff,p}}{\Delta x} \right)_{i-\frac{1}{2},j,k} \left( c_{s,p_{i,j,k}}^n - c_{s,p_{i-1,j,k}}^n \right) \right]$$

$$- \Delta t \frac{c_{s,p_{i+1,j,k}}^{n+1} - c_{s,p_{i,j,k}}^n}{\Delta x_{i,j,k}} + \frac{\Delta t q_{sp}}{V_{i,j,k}} + c_{s,p_{i,j,k}}^n$$ (3.24)

where the water velocity is defined as,
\[
\begin{align*}
\frac{v_{w,p}^{n+1}}{\mu_w} &= \left( k_{w,p} \right) \frac{p_{w,p}^{n+1} - p_{w,p_i+1,j,k}^{n+1}}{\Delta x_{i+\frac{1}{2},j,k}} \\
\frac{v_{w,p}^{n+1}}{\mu_w} &= \left( k_{w,p} \right) \frac{p_{w,p_i,j,k}^{n+1} - p_{w,p_i-1,j,k}^{n+1}}{\Delta x_{i-\frac{1}{2},j,k}}
\end{align*}
\]  

(3.25)

### 3.3.3 Flow Rate Equation

Flow rate of oil phase and water phase is calculated from Darcy’s law as,

\[
\begin{align*}
q_{wp}^{n+1} &= \pi r_c^2 \left( k_{wp} \right) \frac{p_{wp_1,j,k}^{n+1} - p_{wp_{in}}^{n+1}}{\Delta x_{1/2,j,k}} \\
q_{op}^{n+1} &= \pi \left( r^2_p - r_c^2 \right) \frac{p_{op_1,j,k}^{n+1} - p_{op_{in}}}{\Delta x_{1/2,j,k}}
\end{align*}
\]  

(3.26)

### 3.3.4 Solution Procedure

The solution involves determining the contact radius, solving the governing equation for pressure distribution, and calculating the phase saturation and flow rate of the inlet node. The step-by-step solution procedure is presented as follows.

1. Determine the initial contact radius and the phase pressure from the initial saturation.
2. Solve the total pressure equation for pressure of water phase.
3. Find the water and oil saturations of each grid cell.
4. Determine the contact radius, capillary pressure, and oil phase pressure from saturation geometric relation and constrain.
5. Calculate the flow rate at the inlet and the outlet.
6. Obtain the solute concentration from the continuity equation of the solute.
7. Repeat step 2 through step 6 until reaching the simulation time \( t_{max} \).
3.4 Pore Scale Result

Reservoir fluids often compose of multiple components and the water-oil interfacial tension is a function of many variables. This complicates our problem yet does not change the underlying physics. For simplicity, we select a single oil component n-Heptane ($C_7H_{16}$) for numerical calculation. The data from Kumar (2012) for n-Heptane is used to obtain the n-Heptane - water interfacial tension as shown in Figure 3.3. For simplicity, diffusion coefficient is assumed to be constant.

Figure 3.3: Effect of salt concentration on the interfacial tension between water and n-heptane at 23°C and atmospheric pressure (modified after Kumar (2012)).

The dimension of the pore and other input data for the numerical calculation are provided in Table 3.1. The absolute permeability of the pore throat is 112.5 nm$^2$ ($k_{abs} = \frac{r_p^2}{8}$). If we consider this pore size as the average pore size of a rock matrix with porosity 8 % and tortuosity of $\tau = 45$, then the estimated matrix permeability is about 200 nD. Initially, the contact radius is 45 nm and the interface is contained in the cone part of the pore. The pressure at the inlet and the outlet of the pore is kept constant. The pressure at the outlet is equal to the initial pressure of oil phase ($p_{o,p}^{initial} = 10.1 \times 10^5$) Pa and the pressure at the inlet is equal to the initial pressure of the water phase. The pressure difference between the inlet and the outlet is equal to the initial capillary pressure $p_{cwo,p}^{initial} = \frac{2\gamma^{initial}\cos(\theta^{initial})}{r_{c}^{initial}}$. The initial interfacial tension and the diffusion coefficient for three different solutions, NaCl,
Na₂SO₄, CaCl₂ are presented in Table 3.1. The initial salinity of the water phase inside the pore is 60,000 ppm the the inlet salinity is reduced to 1000 ppm. These salinity values are selected based on the salinity of the native formation water (60,000 ppm) and slick water (1000 ppm) typically used in Eagle Ford Shale hydraulic fracturing operations.

Table 3.1: Input parameters for pore scale simulation

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
<th>Unit</th>
<th>Parameter</th>
<th>Value</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>(p_{\text{w,p}}^{\text{initial}})</td>
<td>(p_{\text{w,p}}^{\text{initial}} + p_{\text{cwo,p}}^{\text{initial}})</td>
<td>Pa</td>
<td>(c_{s,p}^{\text{initial}})</td>
<td>60,000</td>
<td>ppm</td>
</tr>
<tr>
<td>(p_{\text{o,p}}^{\text{initial}})</td>
<td>1.01*10⁵</td>
<td>Pa</td>
<td>(c_{\text{s,inlet}})</td>
<td>1,000</td>
<td>ppm</td>
</tr>
<tr>
<td>(\gamma_{\text{NaCl}}^{\text{initial}})</td>
<td>50.93</td>
<td>mN/m</td>
<td>(\mu_{w})</td>
<td>1</td>
<td>cp</td>
</tr>
<tr>
<td>(\gamma_{\text{Na}_2\text{SO}_4}^{\text{initial}})</td>
<td>49.99</td>
<td>mN/m</td>
<td>(\mu_{\text{n-Heptane}})</td>
<td>0.386</td>
<td>cp</td>
</tr>
<tr>
<td>(\gamma_{\text{CaCl}_2}^{\text{initial}})</td>
<td>50.51</td>
<td>mN/m</td>
<td>(D_{\text{pore}})</td>
<td>100</td>
<td>nm</td>
</tr>
<tr>
<td>(c_{\text{n-Heptane}})</td>
<td>5*10⁻⁷</td>
<td>Pa⁻¹</td>
<td>(D_{\text{throat}})</td>
<td>60</td>
<td>nm</td>
</tr>
<tr>
<td>(c_{w})</td>
<td>5*10⁻⁷</td>
<td>Pa⁻¹</td>
<td>(L_{\text{pore}})</td>
<td>100</td>
<td>nm</td>
</tr>
<tr>
<td>(D_{\text{NaCl}}^{\text{eff}})</td>
<td>1.99*10⁻⁹</td>
<td>m²/sec</td>
<td>(L_{\text{cone}})</td>
<td>100</td>
<td>nm</td>
</tr>
<tr>
<td>(D_{\text{CaCl}_2}^{\text{eff}})</td>
<td>1.49*10⁻⁹</td>
<td>m²/sec</td>
<td>(L_{\text{throat}})</td>
<td>50</td>
<td>nm</td>
</tr>
<tr>
<td>(D_{\text{Na}_2\text{SO}_4}^{\text{eff}})</td>
<td>1.04*10⁻⁹</td>
<td>m²/sec</td>
<td>(\omega)</td>
<td>0</td>
<td>%</td>
</tr>
<tr>
<td>(\rho_{w})</td>
<td>1000</td>
<td>kg/m³</td>
<td>(V_w)</td>
<td>1.8*10⁻⁶</td>
<td>m³/mole</td>
</tr>
<tr>
<td>(\rho_{\text{n-Heptane}})</td>
<td>679.5</td>
<td>kg/m³</td>
<td>(g)</td>
<td>0</td>
<td>m/s²</td>
</tr>
<tr>
<td>(\theta_{\text{c(oil-rock)}})</td>
<td>20</td>
<td>deg.</td>
<td>Time step, (dt)</td>
<td>10⁻⁹</td>
<td>sec</td>
</tr>
</tbody>
</table>

The interfacial tension of a curved surface differs from that of a flat surface (Tolman 1949). In our case, the interfacial tension of the interface is lower than that of the flat surface at the same thermodynamic conditions. For the vapor and liquid interface, the curvature dependence of the interfacial tension is important in determining the position of the interface and the phase behavior of the liquid inside the pore throat. For the interfacial radius higher than 30 nm, the variation of the interfacial tension with curvature is small (Erik and Firoozabadi 2006). To simplify the solution, the variation of the interfacial tension with its curvature is neglected in this work. It is also assumed that the change of interfacial tension with the change of pressure is small.
3.4.1 Pressure Transient and Interface Movement

When the solute concentration is reduced at the inlet of the pore, the solute inside the pore diffuses out of the pore. Water moves into the pore to achieve the mass balance. Since the mass fraction of the solute is very small, the amount of water moves into the pore to achieve this balance is insignificant meaning that the transport of the water into the pore by the diffusion of the solute in the pore is also small. However, when the solute concentration decreases, it changes the interfacial tension between oil and water. In our case, the interfacial tension decreases as solute concentration decreases. Since the pressure at the inlet and the outlet of the pore is keep constant, the reduction of the interfacial tension drives the movement of the interface toward the outlet of the pore. This process increases the pressure of the oil nearby the interface, the pressure increase propagates to the outlet forcing the oil out of the pore and the water pressure near the interface decreases as interface move toward the outlet. This pressure reduction propagates to the inlet promoting the flux of water into the pore.

To track the movement of the interface, interface position as a function of simulation time and the variation of contact radius is shown in Figure 3.4(a) and Figure 3.4(b), respectively. The interface position is the distance from the interface to the inlet of the pore as shown in Figure 3.1. We can observe that the interface only moves when the concentration of the grid block contains the interface changes. Diffusion coefficient determines how fast the solute diffuses out of the pore. Since the diffusion coefficient of NaCl is the highest among the three fluids investigated in this study, the interface of NaCl case moves faster than the other cases. The interfacial tension decreases as more solute is transported out of the pore as shown in Figure 3.5 for NaCl concentration in the water phase at different times. When solute concentration inside and outside the pore is balanced, the interface reaches a stable position.

The movement of the interface is small, yet quite significant since a very high pressure gradient is needed to move the interface the same distance. The incremental pressure needed
to be imposed at the inlet of the pore to change the interface from its original radius $r_o = 45$ nm to a radius $r_n = 43.5$ nm is presented in Figure 3.6. The corresponding pressure gradient needed to create the differential pressure is also included in the same figure. To reduce the contact radius from 45 nm to 43.5 nm, we need to increase the pressure at the inlet about 10.5 psi. Upscaling the pore scale to the reservoir scale, we need to create a pressure gradient of about 7200 kpsi/ft to achieve this interface movement. It is nearly “impossible” to create this pressure gradient in the reservoir. This calculation indicates that the interfacial tension-induced transport is a very important mechanism for water imbibition into pores.
Figure 3.6: Pressure required at the inlet to reduce the contact radius for three solutes used.

3.4.2 Mass Transport in Pore

Along with the movement of the interface, there is the transport of the water into the pore and associated oil forced out of the pore at the outlet. Initial mass flow rate into the pore is zero. When solute concentration at the grid cell containing the interface reduces, the interface moves driving water flux into the pore and oil flux out of the pore. The mass transport rate for the three solutions studied here is shown in Figure 3.7(a). It is observed that the mass flow rate reaches a peak value and gradually decreases. How fast the flow rate reaches to the peak value depends on the diffusion coefficient of the solute. The maximum value of flow rate at the peak depends on the slope of the concentration - interfacial tension curve in Figure 3.3. The corresponding cumulative mass flux is also shown in Figure 3.7(b). The stable value of cumulative mass flux indicates that no more water flux into the pore and the pore reaches the equilibrium.

3.4.3 Effects of Solute Type and Salinity

Different solute types have different diffusion coefficients and have varying effect on the interfacial tension. This results in different cumulative recovery from the pore as illustrated in Figure 3.8. Hence, how fast the oil is forced out of the pore depends on the type of solute used. The change of salinity initiates the change of interfacial tension driving the
(a) Mass flow rate.  
(b) Cumulative mass flux.

Figure 3.7: Mass flow rate and cumulative mass flux as functions of time for the three solutes used in this study.

movement of the interface. When inlet salinity is lower more solute diffuses out of the pore resulting in higher cumulative recovery from the pore. Since a linear correlation between solute concentration and interfacial tension is used, a linear correlation between the solute concentration and cumulative recovery is observed as shown in Figure 3.8. For the oil and brine system with the interfacial tension varies with salinity in a complex manner, we can find the optimum value of salinity for the injected water to obtain higher oil recovery from the same reservoir. That value of salinity is considered as optimum brine salinity as suggested by (Alotaibi 2011).

Figure 3.8: Effect of salinity on cumulative mass recovery from the pore for three solutes used.
3.4.4 Effects of Contact Angle Variation

Contact angle is often reported in the literature to be changed with the variation of water salinity (Alameri et al. 2015; Alotaibi 2011). However, a correlation between contact angle and the salinity of the water has not been available. The change of the contact angle also has strong effect on the interface movement as shown in Figure 3.9(a) and the cumulative recovery from the pore (Figure 3.9(b)). Higher contact angle change with respect to the variation of salinity results in higher interface movement and higher cumulative recovery.

![Figure 3.9: Interface movement and cumulative recovery dependence on the rate of change of contact angle for three solutes used](image)

3.5 Limitations and Future Work

Since the objective of this pore scale model is to quantify the interfacial-induced transport at pore scale, assumptions have been made to simplify the problem. The physical phenomena taking place at pore scale are much more complicated and deserves further effort. The main limitation of this pore scale model is it may over simplifies the pore structure, hence does not account for pore complexity. In addition, upscaling from pore scale to larger scale is still a challenging task. Further effort on pore characterization and modeling is necessary for more realistic modeling of the mass transport phenomena along the pores. Advanced imaging techniques should be used for more realistic modeling of the mass transport at pore scale.
The diffusion of the solute inside the pore in this research accounts only for the concentration gradient. The surface forces at the pore wall should also be considered to accurately evaluate the rate of solute transport in future research studies as a continuation of the pore modeling effort presented in this chapter. Reducing the interfacial tension between oil and water forces oil out of the pores and may have many applications in improved/enhanced oil recovery. Further research on the mechanism to reduce the interfacial tension is essential for effective implementation of EOR projects. A comprehensive investigation of surface forces, surface charge and surface energy should also be conducted before any recommendation of low salinity water injection for EOR field applications.
CHAPTER 4
RESERVOIR AND MATRIX BLOCK SCALE MATHEMATICAL MODELING

In this chapter, the mathematical models for fluid transport in the fractured reservoirs at different scales are presented. First, the equation for fluid flow in a dual-porosity reservoir is summarized. Then, the mass transport models, including the general model and a new phenomenological model, are derived followed by the geomechanical model formulation for shale swelling along with the models to account for the effect of shale swelling on fracture, matrix permeability and porosity. The validation of the newly developed mass transport model using the experimental data is also presented in this chapter. The numerical solution of the governing equations in this chapter is summarized in Appendix B. The numerical solution validation is presented in Appendix C.

4.1 Fluid Flow Modeling

The governing equations for fluid flow and solute transport in the fractures are presented. First, the governing equation for each phase is outlined in this section. Then, the total pressure equation is derived to obtain the equation for calculating the phase pressure. Finally, the equation for solute transport in fractures is presented.

4.1.1 Governing Equations

For fractured reservoirs, the flow in the fractures is dominant and the matrix functions as fluid storage. The contribution of the concentration diffusion on the phase transport in fractures is small compared to the hydraulic diffusion. Hence, the continuity equations for water and oil phases in fracture are written as,

\[
- \nabla \cdot (\rho_w \mathbf{v}_{w,f}) - \rho_w \tau_w + \rho_w \dot{q}_w = \frac{\partial}{\partial t} [(1 - \epsilon_{v,f}) \rho_w \phi_f S_{w,f}] 
\]  

\[
- \nabla \cdot (\rho_o \mathbf{v}_{o,f}) - \rho_o \tau_o + \rho_o \dot{q}_o = \frac{\partial}{\partial t} [(1 - \epsilon_{v,f}) \rho_o \phi_f S_{o,f}] 
\]
where $S_{i,f}$, $v_{i,f}$ are saturation and velocity of phase $i$ ($i = o, w$) in the fracture; $\tau_i$ is volumetric transfer of phase $i$ between fractures and rock matrix; $\hat{q}_i$ are specific rate of phase $i$ ($i = o, w$) entering or leaving the reservoir; $\phi_f$ is the fracture porosity; $\epsilon_{v,f}$ is the volumetric strain of the fracture.

The right hand side of Equations 4.1 and 4.2 can be simplified as,

$$\frac{\partial}{\partial t}[(1 - \epsilon_{v,f}) \rho_w \phi_f S_{w,f}] = -\rho_w \phi_f S_{w,f} \frac{\partial \epsilon_{v,f}}{\partial t}$$
$$+ \phi_f \rho_w \left[ \frac{\partial S_{w,f}}{\partial t} + S_{w,f} (c_w + c_\phi) \frac{\partial p_{o,f}}{\partial t} + S_{w,f} \beta_w \frac{\partial T_f}{\partial t} \right] \quad (4.3)$$

$$\frac{\partial}{\partial t}[(1 - \epsilon_{v,f}) \rho_o \phi_f S_{o,f}] = -\rho_o \phi_f S_{o,f} \frac{\partial \epsilon_{v,f}}{\partial t}$$
$$+ (1 - \epsilon_{v,f}) \phi_f \rho_o \left[ \frac{\partial S_{o,f}}{\partial t} + S_{o,f} (c_o + c_\phi) \frac{\partial p_{o,f}}{\partial t} + S_{o,f} \beta_o \frac{\partial T_f}{\partial t} \right] \quad (4.4)$$

where $T_f$ is the temperature in the fracture; $\beta_i$ is the thermal conductivity of phase $i$ ($i = o, w$)

The continuity equation for water and oil phases in fractures can be rewritten as,

$$- \nabla \cdot (\rho_w v_{w,f}) - \rho_w \tau_w + \rho_w \hat{q}_w = -\rho_w \phi_f S_{w,f} \frac{\partial \epsilon_{v,f}}{\partial t}$$
$$+ \phi_f (1 - \epsilon_{v,f}) \rho_w \left[ \frac{\partial S_{w,f}}{\partial t} + S_{w,f} (c_w + c_\phi) \frac{\partial p_{o,f}}{\partial t} + S_{w,f} \beta_w \frac{\partial T_f}{\partial t} \right] \quad (4.5)$$

$$- \nabla \cdot (\rho_o v_{o,f}) - \rho_o \tau_o + \rho_o \hat{q}_o = -\rho_o \phi_f S_{o,f} \frac{\partial \epsilon_{v,f}}{\partial t}$$
$$+ \phi_f (1 - \epsilon_{v,f}) \rho_o \left[ \frac{\partial S_{o,f}}{\partial t} + S_{o,f} (c_o + c_\phi) \frac{\partial p_{o,f}}{\partial t} + S_{o,f} \beta_o \frac{\partial T_f}{\partial t} \right] \quad (4.6)$$

where $\tau_w$ and $\tau_o$ are the rate of volumetric water and oil transferring between fractures and rock matrix; $\epsilon_{v,f}$ is the volumetric strain of the fracture accounting for the variation of fracture volume. The compressibilities of the water ($c_{w,f}$), oil ($c_{o,f}$), and formation ($c_{\phi,f}$) are defined as,
\[
\begin{align*}
   c_{w,f} &= \frac{1}{\rho_w} \frac{\partial \rho_w}{\partial p_{o,f}} \\
   c_{o,f} &= \frac{1}{\rho_o} \frac{\partial \rho_o}{\partial p_{o,f}} \\
   c_{\phi,f} &= \frac{1}{\phi_f} \frac{\partial \phi_f}{\partial p_{o,f}}
\end{align*}
\]  

(4.7)

Since

\[
\begin{align*}
   \nabla \cdot (\rho_w \mathbf{v}_{w,f}) &= \rho_w \nabla \cdot (\mathbf{v}_{w,f}) + \mathbf{v}_{w,f} \cdot \nabla (\rho_w) \approx \rho_w \nabla \cdot (\mathbf{v}_{w,f}) \\
   \nabla \cdot (\rho_o \mathbf{v}_{o,f}) &= \rho_o \nabla \cdot (\mathbf{v}_{o,f}) + \mathbf{v}_{o,f} \cdot \nabla (\rho_o) \approx \rho_o \nabla \cdot (\mathbf{v}_{w,f})
\end{align*}
\]  

(4.8)

the continuity equation can be written using Darcy’s Law as,

\[
- \nabla \cdot \left\{ k_{f,\text{eff}} \left[ (\lambda_{w,f} \nabla p_{w,f} - (\lambda_{w,f} \gamma_{w,f}) \nabla D) \right] \right\} - \tau_w + \dot{q}_w = \phi_f (1 - \epsilon_{v,f}) \left[ \frac{\partial S_{w,f}}{\partial t} + S_{w,f} (c_w + c_\phi) \frac{\partial p_{o,f}}{\partial t} + S_{w,f} \beta_w \frac{\partial T_f}{\partial t} \right] - \phi_f S_{w,f} \frac{\partial \epsilon_{v,f}}{\partial t}
\]  

(4.9)

\[
- \nabla \cdot \left\{ k_{f,\text{eff}} \left[ (\lambda_{o,f} \nabla p_{o,f} - (\lambda_{o,f} \gamma_{o,f}) \nabla D) \right] \right\} - \tau_o + \dot{q}_o = \phi_f (1 - \epsilon_{v,f}) \left[ \frac{\partial S_{o,f}}{\partial t} + S_{o,f} (c_o + c_\phi) \frac{\partial p_{o,f}}{\partial t} + S_{o,f} \beta_o \frac{\partial T_f}{\partial t} \right] - \phi_f S_{o,f} \frac{\partial \epsilon_{v,f}}{\partial t}
\]  

(4.10)

where \( D \) is the elevation; \( k_{f,\text{eff}} \) is the effective permeability of fracture; \( \lambda_i \gamma_i,f \) are the mobility and specific gravity of phase \( i \) (\( i = o, w \)).

The sum of Equations (4.9) and (4.10) gives us the total pressure equation in fractures:

\[
- \nabla \cdot \left\{ k_{f,\text{eff}} \left[ (\lambda_{w,f} + \lambda_{o,f}) \nabla p_{o,f} - (\lambda_{w,f} \gamma_{w,f} + \lambda_{o,f} \gamma_{o,f}) \nabla D) \right] \right\} - (\tau_w + \tau_o) \]

\[
+ (\dot{q}_w + \dot{q}_o) = \phi_f (1 - \epsilon_{v,f}) \left[ (S_{w,f} c_w + c_\phi + S_{o,f} c_o) \frac{\partial p_{o,f}}{\partial t} - \beta_o \frac{\partial T_f}{\partial t} \right] - \phi_f \frac{\partial \epsilon_{v,f}}{\partial t}
\]  

(4.11)

For isothermal case, ignoring the volumetric strain of fracture, Equation 4.11 can be simplified as,

\[
- \nabla \cdot \left\{ k_{f,\text{eff}} \left[ (\lambda_{w,f} + \lambda_{o,f}) \nabla p_{o,f} - (\lambda_{w,f} \gamma_{w,f} + \lambda_{o,f} \gamma_{o,f}) \nabla D) \right] \right\} - (\tau_w + \tau_o) \]

\[
+ (\dot{q}_w + \dot{q}_o) = \phi_f \left[ (S_{w,f} c_w + c_\phi + S_{o,f} c_o) \frac{\partial p_{o,f}}{\partial t} \right]
\]  

(4.12)
The continuity Equation 4.12 can be written in term of total transfer function \((\tau_t = \tau_w + \tau_o)\) and total fracture compressibility \((c_{t,f} = S_{w,f}c_w + c_\phi + S_{o,f}c_o)\) as,

\[
- \nabla \cdot \{ k_{f,eff} \left[ (\lambda_{w,f} + \lambda_{o,f}) \nabla p_{o,f} - \lambda_{w,f}p_{cw0,f} - (\lambda_{w,f} \gamma_{w,f} + \lambda_{o,f} \gamma_{o,f}) \nabla D \right] \} - \tau_t + (\hat{q}_w + \hat{q}_o) = \phi_f c_{t,f} \frac{\partial p_{o,f}}{\partial t} \tag{4.13}
\]

The oil and water transfer functions are conventionally defined as,

\[
\tau_o = \frac{\lambda_{of/m}}{\lambda_t} \phi_m c_{t,m} \frac{\partial p_{om}}{\partial t} - \sigma_s k_m \lambda_{wf/m} \left\{ (p_{o,f} - p_{o,m}) + \frac{\sigma_z}{\sigma_s} \gamma_o (h_{w,f} - h_{w,m}) \right\} \tag{4.14}
\]

\[
\tau_w = \frac{\lambda_{wf/m}}{\lambda_t} \phi_m c_{t,m} \frac{\partial p_{om}}{\partial t} + \sigma_s k_m \lambda_{wf/m} \left\{ (p_{o,f} - p_{cw0,f}) - (p_{o,m} - p_{cw0,m}) \right\} + \frac{\sigma_z}{\sigma_s} \gamma_w (h_{w,f} - h_{w,m}) \tag{4.15}
\]

where \(\sigma_s\) and \(\sigma_z\) are shape factors; \(p_{cw0,f}\) is the fracture capillary pressure (see Appendix D.3). A review of these shape factor models are summarized by Heel and Boerrigter (2006).

The fluid level heights in the equations above are defined as,

\[
\begin{align*}
    h_{w,f} &= \left( \frac{S_{w,f} - S_{wr,f}}{1 - S_{rw,f} - S_{or,f}} \right) L_z = S_{w,f}D L_z \\
    h_{w,m} &= \left( \frac{S_{w,m} - S_{wr,m}}{1 - S_{rw,m} - S_{or,m}} \right) L_z = S_{w,m}D L_z
\end{align*} \tag{4.16}
\]

In this research, these conventional mass transfer functions were not used. A new approach was introduced to compute the mass exchange between the fractures and rock matrix as presented in detail in Section 4.2.

### 4.1.2 Solute Transport in Fractures

Assuming the solute is only dissolved in water phase, the continuity equation for solute can be expressed as,

\[
- \nabla \cdot J_{sf} + \rho_s \dot{q}_{swm/f} + \rho_s \dot{q}_{sw} + \rho_s \dot{q}_{som/f} + \rho_s \dot{q}_{so} =
\]

\[
\frac{\partial}{\partial t} \left[ \phi_f \left( S_{w,f} \rho_w \frac{c_{sw,f}}{1 - c_{sw,f}} + S_{of} \rho_o \frac{c_{so,f}}{1 - c_{so,f}} \right) + (1 - \phi_f) \rho_s a_{sf} \right] \tag{4.17}
\]
where $J_{sf}$ is the mass flux of solute in fracture; $\rho_s$ is solute density; $c_{swf}$ and $c_{sof}$ are solute fractional mass concentration in water and oil phase; the sink/source terms $\dot{q}_{sw}$ and $\dot{q}_{so}$ are the specific rate of solute entering or leaving the fractures from the well in water and oil phase; $\dot{q}_{swm/f}$ and $\dot{q}_{som/f}$ are specific volumetric rate of solute entering or leaving fracture from the rock matrix representing the solute mass exchange between matrix and fracture; $a_{sf}$ is the solute adsorption on the fracture walls determined using Langmuir Equation,

$$a_{sf} = \frac{b c_{sf}}{1 + b c_{sf}} a_{max}$$  \hspace{1cm} (4.18)

where $a_{max}$ is the ; $b$ is the coefficient.

For simplicity, $a_{sf}$ is neglected in the transport equation for solute.

The specific rates of solute entering the fracture from rock matrix ($\dot{q}_{swm/f}$ and $\dot{q}_{som/f}$) are obtained from the solution of mass exchange between fracture and matrix (see section 4.2). Since only water is injected into the reservoir, $\dot{q}_{so} = 0$. The specific rate of solute from injected water is calculated as,

$$\dot{q}_{sw} = \frac{c_{swj}}{1 - c_{swj}} \frac{\rho_w}{\rho_s} \dot{q}_w$$  \hspace{1cm} (4.19)

where $c_{swj}$ is salt fractional mass concentration of injected water.

The mass flux of solute in fracture is the summation of the flux of solute in water and oil phase.

$$J_{sf} = J_{swf} + J_{sof} = \left[J_{swf}^d + \frac{c_{swf}}{(1 - c_{swf})} J_{wf}^d \right] + \left[J_{sof}^d + \frac{c_{sof}}{(1 - c_{sof})} J_{of}^d \right]$$  \hspace{1cm} (4.20)

where $J_{swf}$ and $J_{sof}$ are the mass flux of solute in water and oil phase; $J_{wf}$ and $J_{of}$ are the flux of water and oil in fracture; $J_{swf}^d$ and $J_{sof}^d$ are the diffusion of solute in water and oil phase obtained from the diffusion equation.

$$\begin{align*}
\begin{cases}
J_{swf}^d &= \left(\rho_s \frac{D_{sw}}{\tau_f \phi_{Sw}} \right)_f \nabla c_{swf} \\
J_{sof}^d &= \left(\rho_s \frac{D_{so}}{\tau_f \phi_{So}} \right)_f \nabla c_{sof}
\end{cases}
\end{align*}$$  \hspace{1cm} (4.21)

where $D_{sw}$ and $D_{so}$ are the diffusion coefficients of the solute in water and oil; $\tau_f$ is the tortuosity of the fractures.
Ignoring the solute diffusion in fracture and assuming that the solute does not dissolve in oil, we obtain the simplified equation for the solute transport in the fractures:

\[
- \nabla \cdot \left\{ \frac{\rho_w c_{swf}}{1 - c_{swf}} \mathbf{v}_{wf} \right\} + \rho_s \hat{q}_{sm/f} + \frac{c_{swj}}{1 - c_{swj}} \rho_w \hat{q}_w = \frac{\partial}{\partial t} \left[ S_{wf} \rho_w \phi_f \frac{c_{swf}}{1 - c_{swf}} \right]
\] (4.22)

For incompressible water, equation above can be reduced as,

\[
- \nabla \cdot \left\{ \frac{c_{swf}}{1 - c_{swf}} \mathbf{v}_{wf} \right\} + \rho_s \hat{q}_{sm/f} + \frac{c_{swj}}{1 - c_{swj}} \rho_w \hat{q}_w = \frac{\partial}{\partial t} \left[ S_{wf} \phi_f \frac{c_{swf}}{1 - c_{swf}} \right]
\] (4.23)

The solute flux due to diffusion in the fracture is small and was ignored in this research study. For low solute fractional mass concentration of initial water and injected water, following equations can be obtained.

\[
\begin{align*}
\frac{c_{swf}}{1 - c_{swf}} & \approx c_{swf} \\
\frac{c_{swj}}{1 - c_{swj}} & \approx c_{swj}
\end{align*}
\] (4.24)

Solute transport equation is simplified as,

\[
- \nabla \cdot \left\{ c_{swf} \mathbf{v}_{wf} \right\} + \frac{\rho_s}{\rho_w} \hat{q}_{sm/f} + c_{swj} \hat{q}_w = \frac{\partial}{\partial t} \left[ S_{wf} \phi_f c_{swf} \right]
\] (4.25)

The flow velocities of oil and water phases in fractures are defined as,

\[
\begin{align*}
\mathbf{v}_{wf} &= -k_{f,eff} \lambda_{wf} \nabla (p_{wf} - \gamma_w D) \\
\mathbf{v}_{of} &= -k_{f,eff} \lambda_{of} \nabla (p_{of} - \gamma_o D)
\end{align*}
\] (4.26)

### 4.2 Mass Transport between Fractures and Rock Matrix

In this section, the governing equation for mass transport between fractures and rock matrix is formulated. A general model from the literature for transport of the component \(i\) based on the thermodynamics laws and conservation of mass is summarized. A simplified phenomenological model is derived to replace the general model for computing the mass exchange. The geomechanical model for shale swelling is also outlined at the end of this section.
4.2.1 Osmosis and Osmotic Pressure

Osmotic pressure is the pressure applied by a solution to prevent the inward flow of water across a semipermeable membrane. Osmosis is the process in which a liquid passes through a membrane which allows the passage of the solvent molecules but is too small for the larger solute molecules to pass through as shown in Figure 4.1. Because the molecules are in random motion, there will be more molecules moving from the high concentration region to the low concentration region than in the opposite direction. The motion of a substance from a high concentration region to a low concentration region is known as diffusion. In the absence of the perfect membrane, diffusion would continue until the concentrations of all substances are uniform throughout the liquid phase. With the perfect membrane in place, if one compartment contains the pure solvent, the equilibrium can never happen no matter how much liquid flows through the membrane, the solvent in the right side will always be more concentrated than that in the left side. Osmosis will continue indefinitely until we run out of solvent, or something else stops the process (Lower 2014).

Figure 4.1: Osmosis and osmotic flow: Water molecules (blue) moving freely in both directions through the semipermeable membrane, while the larger solute molecules remain trapped in the left compartment. This results in a net osmotic flow of water from the right side to the left side (Lower 2014).

In the absence of the hydraulic pressure gradient and capillarity, the movement of fluid filtrate into shale is mainly governed by the chemical potential difference between the pore fluid and the injected fluid, and this results in the osmotic transport of water (Ewy and
However, the osmotic potential generated between shale matrix and fluid in fractures is greatly influenced by the flow of ions into or out of shale caused by the ionic concentration imbalances. Therefore, the actual osmotic effect is often less than the osmotic potential. The determination of the impact of ionic flow on the osmotic potential initiates the concept of shale membrane efficiency (Osuji et al. 2008).

### 4.2.2 Shale Membrane

The transport of the solute in shale depends strongly on the membrane properties of the shale matrix. The membrane efficiency or modified diffusion potential is used to describe the ability of the membrane to prevent solute transport. Understanding the mechanism of membrane efficiency of the shale is often important for selecting the fluid for injection operations. Membrane efficiency is the measure of how well a membrane can prevent ion movement. Membrane efficiency has the value from zero for non-selective membrane to one for perfect membrane. Shales are often classified as leaky semi-permeable membrane. The membrane efficiency of shale depends on its petrophysical properties such as permeability and porosity (Figure 4.2), clay surface area, cation exchange capacity, the ion size (Figure 4.3) and concentration or water activity (Mese 1988, 1995; van Oort et al. 1995; Osuji et al. 2008; Zhang et al. 2008).

![Figure 4.2: Measured membrane efficiency of Atoka Shale as a function of matrix permeability and porosity (Osuji et al. 2008).](image-url)
Figure 4.3: Membrane efficiency versus calculated salt radius and CEC/surface area for Pierre type I shale exposed to chloride salt solutions at a water activity of 0.76 (van Oort et al. 1995).

The ratio of the ion size to shale pore throat determines the ability of shale to restrict solutes from entering the pore space in the shale matrix. The pore throat diameter of the shale is often larger than the diameter of most molecular and ion sizes (Figure 4.4). Hence, the membrane efficiency is often very low. Zhang et al. (2008) showed that when exposed to salt solutions membrane efficiency of shale is low ranging from 0.18% to 1.78% for Pierre Shale as presented in Table 4.1. They point out that the membrane efficiency of shales is directly proportional to the ratio of the cation exchange capacity of the shale. When permeability and porosity decrease, the shale membrane efficiency increases. Several researchers including van Oort et al. (1996), Ewy and Stankovich (2000), Mody et al. (2002), Zhang et al. (2008), and Osuji et al. (2008) focused on quantitatively estimating the membrane efficiency of the shale. They all showed that the membrane efficiency of shale is often less than 10% and particularly very small if permeability of the shale matrix is greater than 1 nD.

4.2.3 General Mass Transport Model in Rock Matrix

The mass flux of component \( i \) across the boundary of a control volume is calculated from electro-chemical potential, pressure, and gravitational gradient as (Hoteit and Firoozabadi 2009),
Figure 4.4: Sizes of molecules and pore throats in siliciclastic rocks on a logarithmic scale covering seven orders of magnitude. Measurement methods are shown at the top of the graph, and scales used for solid particles are shown at the lower right (Nelson 2009).

\[
J_i = \rho_i \sum_{j=1}^{n_c} L_{ij} \nabla \mu_i + L_{ip} \nabla (p_{im} - \rho_i g) \tag{4.27}
\]

where \(J_i\), \(\rho_i\), \(p_{im}\), \(i\) are the solute flux, density, pressure, and chemical potential of component \(i\) \((i = 1 - n_c)\); \(n_c\) is number of component; \(g\) is gravitational acceleration vector; \(L_{ij}\) and \(L_{ip}\) are the phenomenological coefficients.

The phenomenological coefficients associated with the pressure and gravity \(\nabla (p_{im} - \rho_i g)\) in Equation 4.27 must satisfy the Darcy’s flow as following:

\[
\frac{k_m}{\mu_o} = \sum_{i=1}^{n_c} \rho_i L_{ip} \tag{4.28}
\]
Table 4.1: The membrane efficiency of Pierre Shale for different solutions (Zhang et al. 2008)

<table>
<thead>
<tr>
<th>Salt Solution</th>
<th>Water Activity</th>
<th>Measured Osmotic Pressure [psi]</th>
<th>Membrane Efficiency [%]</th>
</tr>
</thead>
<tbody>
<tr>
<td>NaCl</td>
<td>0.93</td>
<td>12.4</td>
<td>1.21</td>
</tr>
<tr>
<td></td>
<td>0.85</td>
<td>25.6</td>
<td>0.92</td>
</tr>
<tr>
<td>KCl</td>
<td>0.93</td>
<td>2.9</td>
<td>0.28</td>
</tr>
<tr>
<td></td>
<td>0.85</td>
<td>5</td>
<td>0.18</td>
</tr>
<tr>
<td>CaCl₂</td>
<td>0.93</td>
<td>11.9</td>
<td>1.16</td>
</tr>
<tr>
<td></td>
<td>0.85</td>
<td>49.8</td>
<td>1.78</td>
</tr>
<tr>
<td>KCOOH</td>
<td>0.93</td>
<td>4</td>
<td>0.39</td>
</tr>
<tr>
<td></td>
<td>0.85</td>
<td>6.2</td>
<td>0.22</td>
</tr>
</tbody>
</table>

The chemical potential ($\mu_i$) is a function of the mole fraction, temperature and pressure. Hence the gradient of the chemical potential can be calculated using Equation 4.29,

$$\nabla \mu_i = \sum_{i=1}^{n_c} \left( \frac{\partial \mu_i}{\partial x_k} \right)_{p_m, T, x_{j \neq i}} \nabla x_k + \left( \frac{\partial \mu_i}{\partial p_m} \right)_{T, x} \nabla p_m + \left( \frac{\partial \mu_i}{\partial T_m} \right)_{p_m, x} \nabla T_m
$$

where $S_i$, $x_i$ are the entropy and mole fraction of component $i$ ($i = 1 - n_c$).

In Equation 4.29, the partial derivative of the chemical potential with respect to the component and pressure can be written in term of fugacity ($f_i$) as,

$$\begin{align*}
\left( \frac{\partial \mu_i}{\partial x_k} \right)_{p_m, T, x_{j \neq i}} & = \frac{RT_m}{MW_i} \left( \frac{\delta_i}{x_k} + \frac{1}{f_i} \frac{\partial f_i}{\partial p_m} \right) \\
\left( \frac{\partial \mu_i}{\partial p_m} \right)_{T, x} & = \frac{RT_m}{MW_i} \left( \frac{1}{p_m} + \frac{\partial f_i}{\partial p_m} \right)
\end{align*}$$

where the fugacity and its derivatives can be calculated from equation of state as long as the composition of fluids are given. If the pore size is larger than the mean free path of the molecules, the mobility of each component is equal to that of the bulk flow. Substituting Equations 4.30 and 4.29 into Equation 4.27, we obtain the equation for mass flux of component $i$ across the boundary of a control volume as,
\[ \mathbf{J}_i = \rho_i \sum_{j=1}^{n_c} \left\{ L_{ij} \sum_{i=1}^{n_c} \frac{RT_m}{MW_i} \left( \frac{\delta_{ik}}{\mu_k} + 1 \frac{\partial f_i}{\partial p_m} \right) \nabla x_k + \left( \frac{\partial \mu_k}{\partial T} \right) \nabla T_m + \frac{RT_m}{MW_i} \left( \frac{\partial f_i}{\partial p_m} \right) \nabla p_m + L_{ip} \nabla \left( p_{im} - \rho_i g \right) \right\} \] (4.31)

where \( MW_i \) is the molecular weight of component \( i \) (\( i = 1 \sim n_c \)).

Equation 4.31 can be written as the combination of four components (Montel et al. 2003):

\[ \mathbf{J}_i = \mathbf{J}_i^{\text{thermal}} + \mathbf{J}_i^{\text{chemical}} + \mathbf{J}_i^{\text{gravity}} + \mathbf{J}_i^{\text{pressure}} \] (4.32)

where thermal flux (\( \mathbf{J}_i^{\text{thermal}} \)), chemical flux (\( \mathbf{J}_i^{\text{chemical}} \)), gravity flux (\( \mathbf{J}_i^{\text{gravity}} \)), and pressure (\( \mathbf{J}_i^{\text{pressure}} \)) flux are calculated as,

\[
\begin{align*}
\mathbf{J}_i^{\text{thermal}} &= \rho_i L_{iq} \nabla T_m \\
\mathbf{J}_i^{\text{chemical}} &= \rho_i D_{i}^{\text{eff}} \sum_{k=1}^{n_c} \left( \frac{\delta_{ik}}{\mu_k} + 1 \frac{\partial f_i}{\partial x_k} \right) \nabla x_k \\
\mathbf{J}_i^{\text{gravity}} &= \rho_i \left( \rho_m \frac{k_m}{\mu_m} - D_{i}^{\text{eff}} \frac{MW_i}{RT} \right) g \\
\mathbf{J}_i^{\text{pressure}} &= \rho_i \left( \rho_m \frac{k_m}{\mu_m} - D_{i}^{\text{eff}} \right) \left( \frac{1}{p_m} + \frac{\partial f_i}{\partial p_m} \right) \nabla p_m
\end{align*}
\] (4.33)

Using the flux term in the continuity equation for fluid flow in the matrix, we obtain:

\[ -\nabla \cdot \mathbf{J}_i + \rho_i \dot{\mathbf{q}}_i = \frac{\partial}{\partial t} \left( \rho_i S_i \phi_m \right) \] (4.34)

where \( c_{t,m}, \phi_m \) are total compressibility and porosity of rock matrix.

The solution of Equation 4.34 for refined grid size on each matrix block will provides us the mass transfer between fractures and rock matrix for every component at every time step. The general formulation of the mass transport equation above is theoretically complete and accurate for each component and has been used in conventional reservoir modeling by Hoteit and Firoozabadi (2009). However, the solution of this equation requires a sufficient computing power to obtain the solution for each component. It took Hoteit and Firoozabadi (2009) one day to obtain the numerical solution for gas injection in 10-m spacing of factor network using a 2.5 GHz, Pentium 4 computing machine. Hence using this approach for large scale reservoirs is computationally impractical as it increases the simulation time and
complicates the numerical solution. Moreover, the model presented above does not account for the interactions taking place between the injected fluid and the rock. Hence, fluid and rock interaction may reduce the accuracy of this model. To overcome this challenges, the phenomenological model is used for practical applications (Yu 2002; Farrokhrouz and Asef 2013). The main advantage of using the phenomenological model is to incorporate the effect of all parameters including the fluid and rock interaction.

4.2.4 Simplified Phenomenological Mass Transport Model in the Matrix

We assume that solute does not dissolve in the oil phase but water phase. The osmotic pressure creates the flow of water phase only. This causes the change of water and oil saturations. The continuity equations for water, oil, and solute are written as,

- For water:

\[-\nabla \cdot \mathbf{J}_{{wm}} + \rho_w \hat{q}_{{wm}} = \nabla \cdot \rho_w \mathbf{v}_{w,m} + \rho_w \hat{q}_w = \frac{\partial}{\partial t} \left( (1 - \epsilon_{vm}) S_{wm} \rho_w \phi_m \right) \] (4.35)

- For oil:

\[-\nabla \cdot \mathbf{J}_{{om}} + \rho_o \hat{q}_{{om}} = \nabla \cdot \rho_o \mathbf{v}_{o,m} + \rho_o \hat{q}_o = \frac{\partial}{\partial t} \left( (1 - \epsilon_{vm}) S_{om} \rho_o \phi_m \right) \] (4.36)

- For solute

\[-\nabla \cdot \mathbf{J}_{{sm}} + \rho_s \hat{q}_{{sm}} = \frac{\partial}{\partial t} \left( (1 - \epsilon_{vm}) S_{wm} \rho_w \phi_m \frac{c_{sm}}{1 - c_{sm}} \right) \] (4.37)

where subscript \( m \) is used to represent matrix; \( \mathbf{J}_{im}, \mathbf{v}_{im}, \rho_i \) are the mass flux, velocity, and density of phase \( i \) \( (i = o, s, w) \), respectively; \( c_{sm} \) is the solute fractional mass concentration, \( 1 - c_{sm} = c_{wm} \) is the fractional mass concentration of water; The sink/source term \( \hat{q}_{im} \) represents the specific rate of the phase \( i \) \( (i = o, s, w) \) entering or leaving the matrix.

The mass fluxes of water and solute are calculated using the following phenomenological equation (Manassero and Dominijanni 2003):
The second term represent the mass transport of solute by the flow of the water phase. The solute flux due to diffusion is calculated as,

\[ J_{sm}^d = \alpha_{21} \rho_s V_w \nabla (p_{wm} - \gamma_w D_m) + \alpha_{22} \rho_s \frac{RT_m}{c_{sm}} \nabla c_{sm} \]  

(4.40)

where \( p_{im} \) and \( \gamma_i \) are the pressure and specific gravity of phase \( i \); \( D_m \) is the elevation; \( V_m \) is the partial volume of water; \( \alpha_{ij} = \alpha_{ji} \) are phenomenological coefficients. Experiments need to be conducted to determine these coefficients. Following simplification can be used to determine the coefficients and the correlation among these coefficients and other parameters.

First, we observe that when there is no concentration gradient, \( \nabla c_{sm} = 0 \), the mass flux of water is obtain from the Darcy’s law as,

\[ J_{wm} = \alpha_{11} \rho_w V_w \nabla (p_{wm} - \gamma_w D_m) = -\rho_w k_{wm} \frac{RT_m}{\mu_w} \nabla (p_{wm} - \gamma_w D_m) \]  

(4.41)

Hence, we obtain:

\[ \alpha_{11} V_w = \frac{k_{wm}}{\mu_w} \Rightarrow \alpha_{11} = -\frac{1}{V_w} \frac{k_{wm}}{\mu_w} \]  

(4.42)

Second, we can assume that we can impose a pressure or potential gradient that balances with the osmotic pressure gradient to prevent any water flux due to osmotic pressure. Since the osmotic pressure drives the flow, we can impose a pressure, or potential, that acts in the opposing direction to prevent the flow. This pressure or potential gradient is referred to as the balance gradient, \( \nabla (p_{wm} - \gamma_w D_m) \). At this gradient, \( J_{wm} = 0 \), the coefficient \( \alpha_{12} \) can be determined using equation 4.38 as,

\[ \alpha_{12} = -\frac{c_s \alpha_{11} V_w [\nabla (p_{wm} - \gamma_w D_m)]_b}{RT_m} = \frac{k_{wm}}{\mu_w c_{sm}} \frac{[\nabla (p_{wm} - \gamma_w D_m)]_b}{RT_m \nabla c_{sm}} \]  

(4.43)

Manassero and Dominijanni (2003) used the van’t Hoff equation, \( \nabla \Pi_s = \frac{RT_m}{V_w} \nabla c_{sm} \), to obtain the equation for \( \alpha_{12} \) as,
$$\alpha_{12} = \alpha_{21} = c_{sm} \frac{k_{wm}}{V_w \mu_w} \omega$$  \hspace{1cm} (4.44)$$

where \( \omega \) is the osmotic or reflection coefficient. The membrane efficiency or membrane selectivity is pressure dependence as suggested by Geren et al. (2014). For simplicity, we assume that membrane is constant and given by:

$$\omega = \frac{\nabla (p_{wm} - \gamma_w D_m)}{\nabla \Pi_s} = \frac{V_w [\nabla (p_{wm} - \gamma_w D_m)]_b}{RT_m \nabla c_{sm}}$$  \hspace{1cm} (4.45)$$

when no water flux occurs, transport of the solute is purely due to the diffusion. Hence, substituting Fick’s Law equation, \( J^d_{sm} = -\rho_s \phi_m D^{eff} \nabla c_{sm} \), into equation for the solute flux (Equation 4.40), Manassero and Dominijanni (2003) obtained Equation 4.46,

$$J^d_{sm} = -\rho_s \phi_m D^{eff} \nabla c_{sm} = \alpha_{21} \rho_s V_w [\nabla (p_{wm} - \gamma_w D_m)]_b + \alpha_{22} \rho_s \frac{RT_m}{c_{sm}} \nabla c_{sm}$$  \hspace{1cm} (4.46)$$

or

$$\alpha_{22} = -\frac{\phi_m D^{eff}}{RT_m} c_{sm} - \alpha_{21} c_{sm} \omega = -\frac{\phi_m D^{eff}}{RT_m} c_{sm} - \frac{k_{wm}}{V_w \mu_w} c_{sm}^2 \omega^2$$  \hspace{1cm} (4.47)$$

The effective bulk diffusion of the porous medium is defined as,

$$D^{eff} = \theta \tau D_o$$  \hspace{1cm} (4.48)$$

where \( \tau \) is the tortuosity; \( D_o \) is the diffusivity in free solution; and \( \theta \) is the effective solute porosity ratio; defined as the ratio of the connected porosity by total porosity. Manassero and Dominijanni (2003) used a model from the literature to relate \( \theta \) to osmotic efficiency as, \( \theta = 1 - \omega \).

The continuity equation for water reduces to

$$\nabla \cdot \left[ \rho_w \frac{k_{wm}}{\mu_w} \nabla (p_{wm} - \gamma_w D_m) - c_{sm} \rho_w \frac{k_{wm}}{V_w \mu_w} \omega \frac{RT_m}{c_{sm}} \nabla c_{sm} \right] + \rho_w \dot{q}_{wm} = \frac{\partial}{\partial t} \left[ (1 - \epsilon_{wm}) S_{wm} \rho_w \phi_m \right]$$  \hspace{1cm} (4.49)$$

In terms of water mobility in matrix \( \left( \lambda_{wm} = \frac{k_{wm}}{\mu_w} \right) \), Equation 4.49 is re-written as,
\[ \nabla \cdot \left[ \rho_w k_m \lambda_{wm} \nabla (p_{wm} - \gamma_w D_m) - c_{sm} \rho_w \frac{k_{wm}}{V_w \mu_w} \frac{RT_m}{c_{sm}} \nabla c_{sm} \right] \]
\[ + \rho_w q_{wm} = \frac{\partial}{\partial t} [(1 - \epsilon_{vm}) S_{wm} \rho_w \phi_m] \] (4.50)

where \( k_m \) is the matrix absolute permeability.

For incompressible water phase, the continuity equation for water reduces to:

\[ \nabla \cdot \left[ \frac{k_{wm}}{\mu_w} \nabla (p_{wm} - \gamma_w D_m) \right] - \nabla \cdot \left( \frac{k_{wm}}{V_w \mu_w} \omega RT_m \nabla c_{sm} \right) \]
\[ + \hat{q}_{wm} = \frac{\partial}{\partial t} [(1 - \epsilon_{vm}) S_{wm} \phi_m] \] (4.51)

The continuity equation for oil in matrix is:

\[ \nabla \cdot \left[ \rho_o k_{om} \lambda_{om} \nabla (p_{om} - \gamma_o D_m) \right] + \rho_o \hat{q}_{om} = \frac{\partial}{\partial t} [(1 - \epsilon_{vm}) S_{om} \rho_o \phi_m] \] (4.52)

In term of oil mobility in the matrix \( \left( \lambda_{om} = \frac{k_{om}}{\mu_o} \right) \), Equation 4.52 is re-written as,

\[ \nabla \cdot \left[ \rho_o k_{om} \lambda_{om} \nabla (p_{om} - \gamma_o D_m) \right] + \rho_o \hat{q}_{om} = \frac{\partial}{\partial t} [(1 - \epsilon_{vm}) S_{om} \rho_o \phi_m] \] (4.53)

where \( k_{om} \) is the relative permeability of oil in the matrix.

For incompressible oil:

\[ \nabla \cdot \left[ \frac{k_{om}}{\mu_o} \nabla (p_{om} - \gamma_o D_m) \right] + \hat{q}_{om} = \frac{\partial}{\partial t} [(1 - \epsilon_{vm}) S_{om} \phi_m] \] (4.54)

Expanding the right hand side of the equation for water and oil and canceling the density from both sides of the equation (as shown in Section 4.1.1), we obtain:

\[ \nabla \cdot \left[ k_m \lambda_{wm} \nabla (p_{wm} - \gamma_w D_m) - c_{sm} k_{wm} \omega \frac{RT_m}{c_{sm}} \nabla c_{sm} \right] + \hat{q}_{wm} \]
\[ = (1 - \epsilon_{vm}) \phi_m S_{wm} (c_\phi + c_w) \frac{\partial p_{wm}}{\partial t} + (1 - \epsilon_{vm}) \phi_m \frac{\partial}{\partial t} (S_{wm}) - \phi S_w \frac{\partial}{\partial t} (\epsilon_{vm}) \] (4.55)
\[ \nabla \cdot [k_m \lambda_{om} \nabla (p_{om} - \gamma_o D_m)] + \dot{q}_{om} = (1 - \epsilon_{vm}) \phi_m S_{om} (c_\phi + c_o) m \frac{\partial p_{om}}{\partial t} \]
\[ + (1 - \epsilon_{vm}) \phi_m \frac{\partial}{\partial t} (S_{om}) - \phi S_o \frac{\partial}{\partial t} (\epsilon_{vm}) \]  
(4.56)

The summation of Equation 4.55 and Equation 4.56 gives,
\[ \nabla \cdot [k_m \lambda_{wm} \nabla (p_{wm} - \gamma_w D_m) - k_m \lambda_{wm} \omega \frac{RT_m}{V_w} \nabla c_{sm}] + \nabla \cdot [k_m \lambda_{om} \nabla (p_{om} - \gamma_o D_m)] \]
\[ + \dot{q}_{wm} + \dot{q}_{om} = (1 - \epsilon_{vm}) \phi_m c_{tm} \frac{\partial p_{wm}}{\partial t} - \phi_m \frac{\partial}{\partial t} (\epsilon_{vm}) \]  
(4.57)

where the total compressibility of matrix \((c_{t,m})\) is calculated as,
\[ c_{t,m} = S_{o,m} (c_\phi + c_o) m + S_{w,m} (c_\phi + c_w) m = c_\phi + S_{o,m} c_o + S_{w,m} c_{wm} \]  
(4.58)

The total pressure Equation 4.57 can be solved for water pressure or oil pressure depending on the wettability of rock matrix. For water-wetted rock matrix, we solve for water phase pressure. For oil-wetted rock matrix, we solve for oil phase pressure.

Similarly, we obtain the equation for solute assuming solute is only dissolved in water.
\[ - \nabla \cdot \left\{ \alpha_{21} \rho_s V_w \nabla (p_{wm} - \gamma_w D_m) + \alpha_{22} \rho_s \frac{RT_m}{c_{sm}} \nabla c_{sm} + \frac{c_{sm}}{(1 - c_{sm})} J_{wm} \right\} \]
\[ + \rho_s \dot{q}_{sm} = \frac{\partial}{\partial t} \left[ (1 - \epsilon_w) S_{w,m} \rho_w \phi_m \frac{c_{sm}}{(1 - c_{sm})} \right] \]  
(4.59)

Substituting the phenomenological coefficients into the equation above, we obtain:
\[ - \nabla \cdot \left\{ c_{sm} \rho_s \frac{k_{wm}}{\mu_w} \omega \nabla (p_{wm} - \gamma_w D_m) - \rho_s \left[ \phi_m \frac{D^f}{RT_m} \frac{c_{sm}}{c_{sm}^2} \omega^2 \right] \frac{RT_m}{c_{sm}} \nabla c_{sm} \right\} \]
\[ + \frac{c_{sm}}{(1 - c_{sm})} \left[ -\rho_w \frac{k_{wm}}{\mu_w} \nabla (p_{wm} - \gamma_w D_m) + \frac{k_{wm}}{\mu_w \rho_w} \omega RT_m \nabla c_{sm} \right] \]
\[ + \rho_s \dot{q}_{sm} = \frac{\partial}{\partial t} \left[ (1 - \epsilon_w) S_{w,m} \rho_w \phi_m \frac{c_{sm}}{(1 - c_{sm})} \right] \]  
(4.60)

Reorganizing the equation above, we obtain:
\[ \nabla \cdot \left\{ c_{sm} \rho_s \frac{k_{wm}}{\mu_w} \left( \frac{\rho_w}{\rho_s} \frac{c_{sm}}{1 - c_{sm}} - \omega \right) \right\} \left[ \nabla \left( p_{wm} - \gamma_w D_m \right) - \frac{\omega RT_m}{V_w} \nabla c_{sm} \right] + \phi_m \rho_s D_{eff} \nabla c_{sm} \]
\[ + \rho_s \dot{c}_{sm} = \frac{\partial}{\partial t} \left[ (1 - \epsilon_v) S_{w,m} \rho_w \frac{c_{sm}}{1 - c_{sm}} \right] \quad (4.61) \]

\[ \nabla \cdot \left\{ c_{sm} \rho_s k_{lm} \lambda_{wm} \left( \frac{\rho_w}{\rho_s} \frac{c_{sm}}{1 - c_{sm}} - \omega \right) \right\} \left[ \nabla \left( p_{wm} - \gamma_w D_m \right) - \frac{\omega RT_m}{V_w} \nabla c_{sm} \right] + \phi_m D_{eff} \nabla c_{sm} \]
\[ + \rho_s \dot{c}_{sm} = \frac{\partial}{\partial t} \left[ (1 - \epsilon_v) S_{w,m} \rho_w \frac{c_{sm}}{1 - c_{sm}} \right] \quad (4.62) \]

For incompressible solute, equation above can be reduces as,

\[ \nabla \cdot \left\{ c_{sm} k_{lm} \lambda_{wm} \left( \omega + \frac{\rho_w}{\rho_s} c_{sm} \right) \right\} \left[ \nabla \left( p_{wm} - \gamma_w D_m \right) - \frac{\omega RT_m}{V_w} \nabla c_{sm} \right] + \phi_m D_{eff} \nabla c_{sm} \]
\[ + \dot{c}_{sm} = \frac{\partial}{\partial t} \left[ (1 - \epsilon_v) \frac{\rho_w}{\rho_s} S_{w,m} \phi_m \frac{c_{sm}}{1 - c_{sm}} \right] \quad (4.63) \]

For low solute fractional mass concentration, \( \frac{c_{sm}}{1 - c_{sm}} \approx c_{sm} \), equation above is simplified as,

\[ \nabla \cdot \left\{ c_{sm} k_{lm} \lambda_{wm} \left( \omega + \frac{\rho_w}{\rho_s} c_{sm} \right) \right\} \left[ \nabla \left( p_{wm} - \gamma_w D_m \right) - \frac{\omega RT_m}{V_w} \nabla c_{sm} \right] + \phi_m D_{eff} \nabla c_{sm} \]
\[ + \dot{c}_{sm} = \frac{\partial}{\partial t} \left[ (1 - \epsilon_v) \frac{\rho_w}{\rho_s} S_{w,m} \phi_m c_{sm} \right] \quad (4.64) \]

Velocity of water phase is defined as,

\[ \begin{cases} v_{wm} = \frac{k_w}{\mu_w} \nabla \left( p_{wm} - \gamma_w D_m \right) \\ v_{om} = \frac{k_o}{\mu_o} \nabla \left( p_{of} - \gamma_o D_m \right) \end{cases} \quad (4.65) \]

Equation 4.49, 4.52, and 4.62 are the most important equations developed in this study to simulate the mass transport of water, oil, and solute in matrix. These transport equations, along with the geomechanical equation formulated in Section 4.3, are solved numerically for every matrix block in the reservoir to compute the mass exchange between the matrix and the fractures. The validation of this mass transport model is presented in the next section.
4.2.5 Mass Transport Model Validation

This section summarizes the experimental validation on the core sample from the experimental data. The experimental set-up, experimental procedure, and sample descriptions are also presented.

4.2.5.1 Experimental facility

Several experimental assemblies have been designed for measurement of pore pressure alteration due to chemically induced flow (Mese 1988, 1995; Ewy and Stankovich 2000; Yu 2002). Tutuncu and her research team at Colorado School of Mines UNGI Geomechanics Group at Unconventional Natural Gas and Oil Institute has built a 4th generation laboratory to conduct coupled geomechanics, fluid flow, acoustics, resistivity and permeability measurements under elevated pore pressure using various salinity fluids, pore pressure penetration measurements were conducted for monitoring the rock-fluid interaction induced pore pressure alteration Padin 2016. Experimental data from Yu (2002) for model validation in this study. Yu (2002) conducted experiments similar to the experiments by Ewy and Stankovich (2000) to validate his model and obtained the parameters for wellbore stability analysis.

A generalized schematic of the sample assembly is shown in Figure 4.5. A preserved shale sample is placed between two steel end caps and surrounded by an impermeable jacket which is sealed to the end caps. The top end cap has ports to slowly circulated fluid at the top end of the sample. The pressure and concentration of the fluid circulated at this end are different from these of the original fluid in the sample and kept constant during the test. A porous metal disk is placed at the top of the sample to allow the test fluid to travel along the surface of the sample and also provide a medium to transfer axial stress to the sample. The bottom end cap has a pressure sensor to measure the pore pressure change at this end of the sample. The sample assembly is set on a load cell within a pressure vessel to provide confining pressure. Two high-pressure accumulators are arranged nearby the pressure vessel to provide fluid source and fluid collection, and these are instrumented
to provide measurements of the volume flow rate (Ewy and Stankovich 2000).

Figure 4.5: Schematic of shale sample assembly and loading (Ewy and Stankovic 2010).

4.2.5.2 Experimental description

A preserved shale sample, fully saturated with the native pore fluid, is first jacketed to the end caps. Then, the entire assembly is placed within the pressure vessel. The confining pressure, acting in all directions on the sample, is increased to a designated level. If no pore pressure buildup is observed, the confining pressure is increased, in order to ensure full saturation of the sample before the test. When the sample reaches full saturation, pore pressure is drained off through the top cap. This procedure helps to ensure zero uniformed pore pressure before the experiment (Ewy and Stankovich 2000).

At the beginning, the flow lines for the test fluid is remained empty. The test fluid is then circulated through the top end of the sample. The test fluid is flowed past the top end of the sample at a rate of 0.1 to 0.5 ccl/hour, in order to prevent stagnation and keep the chemical content of the fluid constant (Ewy and Stankovich 2000; Yu 2002). The pressure and concentration of the circulated fluid are kept constant. This inlet boundary is treated as constant pressure and concentration boundary. The bottom end is maintained as a no-flow boundary. The pore pressure at this end of sample is monitored as a function of time and used to validate the model. Because it is a no-flow boundary, the pore pressure rises and finally reaches an equilibrium value. The deformable jacket around the sample, which is
pressed against the sample by the confining fluid pressure, seals around the outside of the sample to prevent any channel for flow. The test fluid pressure, with slow flow, is held on top of the sample for a period of several days until the test is finished.

4.2.5.3 Sample description

In both experimental studies by (Ewy and Stankovich 2000; Yu 2002), three different preserved shale cores were tested. Shale A1 is Cretaceous in age, while shales, A2 and N1 are both Tertiary. Sample A1 has high permeability, the pressure transient is not observed and is not be considered to be used here. The mineralogy of the two shales, A2 and N1, is presented in Table 4.2. Mineralogy was determined through a combination of X-ray diffraction (XRD) and complete rock geochemical analysis. The N1 shale contains 65% - 70% clay, while the A2 shale is more variable, containing anywhere from 50% to 75% clay. Shale A2 and N1 were reported to have a permeability of 2 to 8 and 1 to 4 nano darcies, respectively. The CEC and surface area data can be obtained from Ewy and Stankovich (2000).

Table 4.2: Sample mineralogy (wt%) determined by XRD combined with rock chemistry (Ewy and Stankovich 2000)

<table>
<thead>
<tr>
<th>Composition</th>
<th>N1-1a</th>
<th>N1 - 1b</th>
<th>A2 - 1c</th>
<th>A2 - 1b</th>
</tr>
</thead>
<tbody>
<tr>
<td>Kaolinite</td>
<td>10</td>
<td>11</td>
<td>16</td>
<td>8</td>
</tr>
<tr>
<td>Illite+mica</td>
<td>52</td>
<td>52</td>
<td>56</td>
<td>39</td>
</tr>
<tr>
<td>Mixed-layer IIS (20% III.)</td>
<td>4</td>
<td>4</td>
<td>3</td>
<td>2</td>
</tr>
<tr>
<td>Mixed-layer IIS (80% Ill.)</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Chlorite</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Total Clay</td>
<td>66</td>
<td>67</td>
<td>75</td>
<td>49</td>
</tr>
<tr>
<td>Quartz</td>
<td>20</td>
<td>19</td>
<td>10</td>
<td>41</td>
</tr>
<tr>
<td>K-Feldspar</td>
<td>4</td>
<td>4</td>
<td>2</td>
<td>4</td>
</tr>
<tr>
<td>Albite</td>
<td>4</td>
<td>3</td>
<td>5</td>
<td>2</td>
</tr>
<tr>
<td>Siderite</td>
<td>4</td>
<td>5</td>
<td>5</td>
<td>2</td>
</tr>
<tr>
<td>Organic matter</td>
<td>2</td>
<td>2</td>
<td>2</td>
<td>2</td>
</tr>
</tbody>
</table>
4.2.5.4 Governing equation for core scale

The formulated mass transport model accounts for the transport of three phases, water, oil, and solute to simulate the transport in the reservoir condition. Yet, only experiments for two phases (water and solute) are available. Therefore, the following transport equations are solved for pressure and concentration.

For water phase:

$$\nabla \cdot \left[ \rho_w \frac{k_{wm}}{\mu_w} \nabla (p_{wm} - \gamma_w D_m) - \rho_w \frac{k_{wm}}{\mu_w} \frac{RT_m}{V_w} \nabla c_{sm} \right] + \rho_w \hat{q}_{wm} = \frac{\partial}{\partial t} (\rho_w \phi_m) \quad (4.66)$$

and for solute phase:

$$\nabla \cdot \left\{ c_{sm} \rho_s \frac{k_{wm}}{\mu_w} \left( \frac{\rho_w}{\rho_s} \frac{c_{sm}}{1 - c_{sm}} - \omega \right) \right\} \left[ \nabla (p_{wm} - \gamma_w D_m) - \frac{\omega RT_m}{V_w} \nabla c_{sm} \right] + \phi_m \rho_s D_{eff} \nabla c_{sm} \right\} + \rho_s \hat{q}_{sm} = \frac{\partial}{\partial t} (\rho_s \phi_m c_{sm}) \quad (4.67)$$

4.2.5.5 Numerical solution

The mesh scheme for core sample is showed in Figure 4.6.

![Figure 4.6: Meshing scheme for core sample.](image)

a. Pressure of Water Phase in the Matrix: From the matrix total pressure Equation 4.66 we obtain the algebraic equation to obtain the pressure along the core as,

$$M_{xb}p_{wm_{i-1,j,k}}^{n+1} + M_{xm}p_{wm_{i,j,k}}^{n+1} + M_{xf}p_{wm_{i+1,j,k}}^{n+1} = M_{xR} \quad (4.68)$$

where
\[ M_{xb} = \frac{1}{\Delta x_{i,j,k}} \left( \frac{k_{wm}}{\mu_w \Delta x} \right)^n \]  
\[ M_{xf} = \frac{1}{\Delta x_{i,j,k}} \left( \frac{k_{wm}}{\mu_w \Delta x} \right)^n \]  
\[ M_{xm} = - \left\{ M_{xb} + M_{xf} + \frac{1}{\Delta t_m} \left[ \phi_m c_{tm} \right]_{i,j,k}^n \right\} \]  
\[ M_{xR} = \frac{1}{\Delta x_{i,j,k}} \left\{ \left( \frac{k_{wm}}{\mu_w \Delta x} \right)^n \left[ \gamma_{wi,j,k} (D_{i+1,j,k} - D_{i,j,k}) \right] \right. \]  
\[ \frac{\omega R T_m}{\Delta x_{i,j,k}} \left[ \left( \frac{k_{wm}}{\mu_w \Delta x} \right)^n \left[ \gamma_{wi,j,k} (D_{i,j,k} - D_{i-1,j,k}) \right] \right] - \left[ \phi_m c_{tm} \right]_{i,j,k}^n \frac{p_{wm}}{\Delta t_m} \]  
\[ c_{sm}^{n+1} = \frac{\Delta t}{(1 - \epsilon_{wm})_k^{n+1} \phi_m V_k} q_{sm} + \left[ (1 - \epsilon_{wm})_k^{n+1} \phi_m V_k \right]_{c_{sm} \mu_w - c_{sm} \mu_w}^n \frac{\Delta t}{(1 - \epsilon_{wm})_k^{n+1} \phi_m \Delta z_k}^* \]  
\[ - \left[ \left( c_{sm} \mu_w \Delta z \right)^n \omega + \left( c_{sm} \mu_w \Delta z \right)^n \phi_m \Delta z_k \right]_{c_{sm} \mu_w - c_{sm} \mu_w}^n \left[ \left( p_{wmk+1} - p_{wmk} \right) \gamma_w (D_{k+1} - D_k) \right] \]  
\[ \left\{ - \left[ \frac{\omega R T_m}{V_k} \nabla c_{sm} \right]_{c_{sm} \mu_w - c_{sm} \mu_w}^n \left[ \frac{c_{smk} - c_{smk-1}}{\Delta z_{k+1/2}} \right] + \left[ \frac{\omega R T_m}{V_k} \nabla c_{sm} \right]_{c_{sm} \mu_w - c_{sm} \mu_w}^n \left[ \frac{c_{smk+1/2} - c_{smk}}{\Delta z_{k+1/2}} \right] \right\} \]  
\[ - \phi_m D_{eff} \left( \frac{c_{smk+1/2} - c_{smk}}{\Delta z_{k+1/2}} - \frac{c_{smk} - c_{smk-1}}{\Delta z_{k-1/2}} \right) \]  
\[ 4.2.5.6 \text{ Model validation} \]

The input parameters for the simulation are summarized in Table 4.3. The initial and boundary conditions in term of pressure and concentration for each sample are shown in Table 4.4.

By curve fitting the experimental result, the four parameters were determined by Yu (2002). In our model, only membrane coefficient is varied to fit the experimental data.
All parameters for the numerical simulation are obtained from Yu (2002). The membrane efficiency for the same sample and same fluid is considered to be constant. For example the membrane efficiency for sample N1 with NaCl is 3.5% regardless of concentration. Varying the membrane efficiency with concentration may provide a better fit. However, for simplicity, we keep it constant. The transport properties of the same sample are also considered to be the same when different concentrations are used.

Table 4.3: Input parameters used in numerical simulation to validate the mass transport model

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
<th>Unit</th>
<th>Parameter</th>
<th>Value</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>$c_w$</td>
<td>4.8*10^{-10}</td>
<td>Pa^{-1}</td>
<td>$c_{sm_{initial}}$(NaCl)</td>
<td>1.5</td>
<td>M</td>
</tr>
<tr>
<td>$c_{\phi}$</td>
<td>1.45*10^{-9}</td>
<td>Pa^{-1}</td>
<td>$c_{sm_{initial}}$(CaCl$_2$)</td>
<td>0.1</td>
<td>M</td>
</tr>
<tr>
<td>$g$</td>
<td>0</td>
<td>m/s$^2$</td>
<td>$\frac{k_m}{\mu_w}$ (sample N1)</td>
<td>1.134*10^{-18}</td>
<td>m$^2$sec/kg</td>
</tr>
<tr>
<td>$\omega_{N1}$(CaCl$_2$)</td>
<td>3.5</td>
<td>%</td>
<td>$\frac{k_m}{\mu_w}$ (sample A2)</td>
<td>2.344*10^{-18}</td>
<td>m$^2$sec/kg</td>
</tr>
<tr>
<td>$\omega_{N1}$(NaCl)</td>
<td>7</td>
<td>%</td>
<td>Temperature</td>
<td>295</td>
<td>deg. K</td>
</tr>
<tr>
<td>$\omega_{A2}$(CaCl$_2$)</td>
<td>4.5</td>
<td>%</td>
<td>$\phi_m$ (sample N1)</td>
<td>7</td>
<td>%</td>
</tr>
<tr>
<td>$\omega_{A2}$(NaCl)</td>
<td>7.5</td>
<td>%</td>
<td>$\phi_m$ (sample A2)</td>
<td>8</td>
<td>%</td>
</tr>
<tr>
<td>$D_{o}^{eff}$(NaCl)</td>
<td>8.94*10^{-11}</td>
<td>m$^2$/sec</td>
<td>Sample thickness</td>
<td>0.5</td>
<td>in</td>
</tr>
<tr>
<td>$D_{o}^{eff}$(CaCl$_2$)</td>
<td>8.94*10^{-11}</td>
<td>m$^2$/sec</td>
<td>Sample diameter</td>
<td>0.75</td>
<td>in</td>
</tr>
<tr>
<td>$V_w$</td>
<td>1.8*10^{-6}</td>
<td>m$^3$/mole</td>
<td>$R$</td>
<td>8.3145</td>
<td>$\frac{Pa.m^3}{deg.K.mol}$</td>
</tr>
<tr>
<td>$\rho_s$(CaCl$_2$)</td>
<td>2150</td>
<td>kg/m$^3$</td>
<td>Outer boundary</td>
<td>No-flow</td>
<td></td>
</tr>
<tr>
<td>$\rho_s$(NaCl)</td>
<td>2165</td>
<td>kg/m$^3$</td>
<td>Time step, $dt$</td>
<td>20</td>
<td>sec</td>
</tr>
<tr>
<td>$\rho_{water}$</td>
<td>1000</td>
<td>kg/m$^3$</td>
<td>Number of grid cells</td>
<td>40</td>
<td></td>
</tr>
</tbody>
</table>

The rate of propagation of pore pressure into the shale is controlled by both the hydraulic and concentration gradient diffusions. The pressure profiles show two regions of propagation, early time and late time. The first region in the early time of the pressure propagation is dominant by the hydraulic diffusion, Darcy flow. The second region in the late time of
Table 4.4: Experimental data for each sample used in the validation of the mass transport model in matrix (Yu 2002).

<table>
<thead>
<tr>
<th>Parameter</th>
<th>N1</th>
<th>N1</th>
<th>N1</th>
<th>N1</th>
<th>A2</th>
<th>A2</th>
<th>A2</th>
<th>A2</th>
</tr>
</thead>
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<tr>
<td>Circulation fluid</td>
<td>CaCl₂</td>
<td>CaCl₂</td>
<td>NaCl</td>
<td>NaCl</td>
<td>CaCl₂</td>
<td>CaCl₂</td>
<td>NaCl</td>
<td>NaCl</td>
</tr>
<tr>
<td>$c_{initial}$ (M)</td>
<td>0.1</td>
<td>0.1</td>
<td>1.5</td>
<td>1.5</td>
<td>0.1</td>
<td>0.1</td>
<td>1.5</td>
<td>1.5</td>
</tr>
<tr>
<td>$c_{circulation}$ (g/l)</td>
<td>267</td>
<td>413</td>
<td>272</td>
<td>156</td>
<td>267</td>
<td>413</td>
<td>272</td>
<td>156</td>
</tr>
<tr>
<td>$p_{initial}$ (psi)</td>
<td>15</td>
<td>60</td>
<td>10</td>
<td>120</td>
<td>5</td>
<td>50</td>
<td>0</td>
<td>15</td>
</tr>
<tr>
<td>$p_{circulation}$ (psi)</td>
<td>985</td>
<td>995</td>
<td>965</td>
<td>940</td>
<td>1020</td>
<td>955</td>
<td>1030</td>
<td>1035</td>
</tr>
<tr>
<td>Result in Figure</td>
<td>4.8(a)</td>
<td>4.8(b)</td>
<td>4.9(a)</td>
<td>4.9(b)</td>
<td>4.10(a)</td>
<td>4.10(b)</td>
<td>4.11(a)</td>
<td>4.11(b)</td>
</tr>
</tbody>
</table>

the pressure propagation is controlled by concentration diffusion. If the hydraulic diffusion coefficient, or hydraulic diffusivity, $k_{wm}/\phi_m \epsilon_m \mu_w$, is small, the pressure buildup is very slow. However, if it is large, the rate of pore pressure propagation is fast. Since the hydraulic diffusivity is function of permeability, viscosity, total compressibility, and porosity. For rocks with high permeability, the hydraulic diffusivity is dominant and the concentration-driven diffusion is often not observable from the Pore Pressure Transmission (PPT) experiments. Higher membrane efficiency results in a large contribution from the osmotic transport. The pressure plateau observed in the pore pressure curves is not a true equilibrium in that the solute flux is still finite and still results in small changes of the pore pressure over a long period of time. This explains the upward of the curve in the late time. The pressure and solute concentration after 8 hours is shown in Figure 4.7 for sample N1 contacting with 267 g/l CaCl₂ with $p_w = 985$ psi, $p_{initial} = 15$ psi. We can observe that the pressure propagates faster than the solute concentration and it almost reaches the equilibrium but the solute only invades a very small portion of the core sample near the inlet. Hence, after 8 hours, the transport by diffusion still continues and will continue for a long period of time.

The experimental result and model prediction for Shale N1 contacting with 267 g/l and 413 g/l CaCl₂ solution are shown in (Figure 4.8(a)) and (Figure 4.8(b)), respectively. Yu
(2002) used the experiment with 267 g/l CaCl$_2$ solution to obtain his model parameter by curve fitting then predicted the result for experiment with 413 g/l CaCl$_2$ solution. He obtained $K_I = 1.1344 \times 10^{-18}$ m$^2$/s/kg, $K_{II} = -7.494 \times 10^{-20}$ m$^3$/s/kg, $D^{eff}_o = 8.942 \times 10^{-11}$ m$^2$/s. His parameter $K_I$ is equivalent to water mobility $\left(\frac{k_{wm} \mu_w}{\rho_w}\right)$ in the model presented in this research. Hence, $K_I$ and $D^{eff}_o$ are reused. By curve fitting, the membrane coefficient of 3.5% shown a good fit to the experimental data as shown in Figure 4.8(a). Because the same shale and same type of solutions were used in the experiment, parameters $\frac{k_{wm}}{\rho_w}$, $\omega$, and $D^{eff}_o$ are kept the same. Keeping all parameters the same and changing the initial and boundary condition, the model prediction for Shale N1 contacting with 413 g/l CaCl$_2$ solution is presented in Figure 4.8(b). In this case, the model over-predicts the pore pressure.

When circulating fluid was changed from CaCl$_2$ to NaCl as shown in Figure 4.9(a) and Figure 4.9(b), membrane coefficient is different. However, mobility remains the same because the same sample is used in both experiments. A new membrane coefficient, $\omega = 7\%$, is obtained for the Shale N1 contacting with NaCl solution. A good match is obtained for Shale N1 contacting with 272 g/l NaCl solution. The model predictions also indicate a very good agreement with the experimental data for the Shale N1 contacting with 156 g/l NaCl solution as shown in Figure 4.8(b).
Figure 4.8: Comparison of the model predictions with experimental data for shale N1 contacting with: (a) 267 g/l CaCl$_2$, $p_w = 985$ psi, $p_{initial} = 15$ psi; (b) with 413 g/l CaCl$_2$, $p_w = 995$ psi, $p_{initial} = 60$ psi.

Figure 4.9: Comparison of the model predictions with experimental data for shale N1 contacting with: (a) 272 g/l NaCl, $p_w = 965$ psi, $p_{initial} = 10$ psi; (b) 156 g/l NaCl, $p_w = 940$ psi, $p_{initial} = 120$ psi.

The same procedure is used for sample A2. The membrane coefficient $\omega = 4.5\%$ is used for CaCl$_2$ solution and $\omega = 7.5\%$ is used for NaCl solution. Figure 4.10(a), Figure 4.10(b), Figure 4.11(a) and Figure 4.11(b) show the experiments and model predictions for shale A2 contacting CaCl$_2$ and NaCl solutions at different concentrations. A good agreement of model predictions with experimental data is obtained for all data sets.
Figure 4.10: Comparison of the model predictions with experimental data for shale A2 contacting with: (a) 267 g/l CaCl$_2$, $p_w = 1020$ psi, $p_{initial} = 5$ psi; (b) 413 g/l CaCl$_2$, $p_w = 955$ psi, $p_{initial} = 50$ psi.

Figure 4.11: Comparison of the model predictions with experimental data for shale A2 contacting with: (a) 272 g/l NaCl, $p_w = 1030$ psi, $p_{initial} = 0$ psi; (b) 156 g/l NaCl, $p_w = 1035$ psi, $p_{initial} = 15$ psi.

4.2.6 Limitations and Future Works

A phenomenological approach was used to derive the mass transport model. This approach is often used in biology and chemical engineering (Demirel 2002) rather than in reservoir engineering. Hence, validation against more experimental data set is recommended. One of the limitation of this approach is the use of a constant membrane efficiency as a key input parameter. The membrane efficiency used here is an average value determined from labo-
ratory experiments. Since the membrane efficiency depends on solute composition and ion size, a more comprehensive model for membrane efficiency should be developed to account for multiple component mixtures. As suggested by Geren et al. (2014), membrane efficiency is a strong function of pressure and components. To achieve better results, further study should be devoted to incorporating this into the model. Recently, Padin and Torcuk developed a novel model for mass transport of two phases, water and solute, under the supervision of Dr. Hossein Kazemi at Colorado School of Mines (Padin 2016). Their model does not require the use of membrane efficiency which they considered to be ambiguous and does not present any physical process. Their model was validated using one experimental data set and has shown many advantages. This can be a valuable approach to use in reservoir engineering applications and can be recommended for future work.

4.3 Geomechanical Modeling

To model swelling, we need to solve the mass transport equation and the geomechanical equations including conservation of momentum and conservation of energy equations, for the rock matrix. In the case of isothermal conditions, only the equation of motion is solved along with the transport equation.

The equation of motion is derived for the incremental effective stress \( \delta \sigma_{m,eff} = \sigma_{m,eff}^{n+1} - \sigma_{m,eff}^n \) and total strain \( \delta \epsilon = \epsilon^{n+1} - \epsilon^n \). The incremental effective stress is related to total strain as,

\[
\delta \sigma_{m,eff} = C_s : \delta \epsilon \quad (4.74)
\]

where \( C_s \) is the stiffness tensor, \( \sigma_{m,eff} \) and \( \epsilon \) are the effective stress and total strain tensor.

The total strain tensor \( \epsilon \) is the summation of elastic strain \( \epsilon_e \), thermal strain \( \epsilon_T \), and swelling strain \( \epsilon_s \), \( \epsilon = \epsilon_e + \epsilon_T + \epsilon_s \). The swelling strain tensor is a diagonal tensor. The elastic strain is expressed in terms of displacement \( u_i \) as,
\[ \epsilon_e = \begin{bmatrix} \frac{\partial u_x}{\partial x} & \frac{1}{2} \left( \frac{\partial u_x}{\partial y} + \frac{\partial u_y}{\partial x} \right) & \frac{1}{2} \left( \frac{\partial u_x}{\partial z} + \frac{\partial u_z}{\partial x} \right) \\ \frac{1}{2} \left( \frac{\partial u_x}{\partial y} + \frac{\partial u_y}{\partial x} \right) & \frac{\partial u_y}{\partial y} & \frac{1}{2} \left( \frac{\partial u_y}{\partial z} + \frac{\partial u_z}{\partial y} \right) \\ \frac{1}{2} \left( \frac{\partial u_x}{\partial z} + \frac{\partial u_z}{\partial x} \right) & \frac{1}{2} \left( \frac{\partial u_y}{\partial z} + \frac{\partial u_z}{\partial y} \right) & \frac{\partial u_z}{\partial z} \end{bmatrix} \] (4.75)

Thermal strain tensor is related to temperature as,
\[ \epsilon_T = \begin{bmatrix} \beta T_m & 0 & 0 \\ 0 & \beta T_m & 0 \\ 0 & 0 & \beta T_m \end{bmatrix} \] (4.76)

where \( \beta \) is thermal expansion of rock matrix.

Swelling strain tensor is a diagonal tensor in the following form:
\[ \epsilon_s = \begin{bmatrix} \epsilon_{sx} & 0 & 0 \\ 0 & \epsilon_{sy} & 0 \\ 0 & 0 & \epsilon_{sz} \end{bmatrix} \] (4.77)

Using Voigt notation, the constitutive equation can be written as,
\[ \begin{bmatrix} \sigma_{m,eff_{xx}} \\ \sigma_{m,eff_{yy}} \\ \sigma_{m,eff_{zz}} \\ \sigma_{m,eff_{xy}} \\ \sigma_{m,eff_{xz}} \\ \sigma_{m,eff_{yz}} \end{bmatrix} = \begin{bmatrix} C_{11} & C_{12} & C_{13} & C_{14} & C_{15} & C_{16} \\ C_{21} & C_{22} & C_{23} & C_{24} & C_{25} & C_{26} \\ C_{31} & C_{32} & C_{33} & C_{34} & C_{35} & C_{36} \\ C_{41} & C_{42} & C_{43} & C_{44} & C_{45} & C_{46} \\ C_{51} & C_{52} & C_{53} & C_{54} & C_{55} & C_{56} \\ C_{61} & C_{62} & C_{63} & C_{64} & C_{65} & C_{66} \end{bmatrix} \begin{bmatrix} \frac{\partial u_x}{\partial x} + \beta T_m + \epsilon_{sx} \\ \frac{\partial u_y}{\partial y} + \beta T_m + \epsilon_{sy} \\ \frac{\partial u_z}{\partial z} + \beta T_m + \epsilon_{sz} \\ \frac{1}{2} \left( \frac{\partial u_x}{\partial y} + \frac{\partial u_y}{\partial x} \right) \\ \frac{1}{2} \left( \frac{\partial u_x}{\partial z} + \frac{\partial u_z}{\partial x} \right) \\ \frac{1}{2} \left( \frac{\partial u_y}{\partial z} + \frac{\partial u_z}{\partial y} \right) \end{bmatrix} \] (4.78)

where \( C_{ij} \) are the elastic coefficient, \( \epsilon_{si} \) is swelling strain in \( i \) direction, \( \beta \) is thermal expansion coefficient.

For orthotropic material, material with three orthogonal planes of symmetry, the stiffness tensor is simplified as,
\[ C_s = \begin{bmatrix} C_{11} & C_{12} & C_{13} & 0 & 0 & 0 \\ C_{21} & C_{22} & C_{23} & 0 & 0 & 0 \\ C_{31} & C_{32} & C_{33} & 0 & 0 & 0 \\ 0 & 0 & 0 & C_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & C_{55} & 0 \\ 0 & 0 & 0 & 0 & 0 & C_{66} \end{bmatrix} \] (4.79)

For isotropic material:
The equation of motion for the rock matrix can be written as,

$$\nabla \cdot \sigma_m + F = \rho_m \frac{dv_m}{dt}$$  \hspace{1cm} (4.84)
where $\mathbf{F}$ is the external force vector; $\mathbf{v}_m$ is the velocity of matrix; $\rho_m$ is the density of matrix.

For slow deformation process, the acceleration term can be ignored, the equilibrium equation is written in terms of the incremental stress as,

$$\nabla \cdot \delta \mathbf{\sigma}_m = 0 \Leftrightarrow \begin{cases} \frac{\partial \delta \sigma_{mxx}}{\partial x} + \frac{\partial \delta \sigma_{mxy}}{\partial y} + \frac{\partial \delta \sigma_{mxz}}{\partial z} = 0 \\ \frac{\partial \delta \sigma_{myx}}{\partial x} + \frac{\partial \delta \sigma_{myy}}{\partial y} + \frac{\partial \delta \sigma_{mzy}}{\partial z} = 0 \\ \frac{\partial \delta \sigma_{mzx}}{\partial x} + \frac{\partial \delta \sigma_{mzy}}{\partial y} + \frac{\partial \delta \sigma_{mzz}}{\partial z} = 0 \end{cases}$$ (4.85)

In 3-D Cartesian coordinates, equation above can be expanded as follows,

In $x$-direction:

$$\frac{\partial}{\partial x} \left[ C_{11} \frac{\partial \delta u_x}{\partial x} + C_{12} \frac{\partial \delta u_y}{\partial y} + C_{13} \frac{\partial \delta u_z}{\partial z} \right] + \frac{\partial}{\partial y} \left[ C_{44} \left( \frac{\partial \delta u_x}{\partial y} + \frac{\partial \delta u_y}{\partial x} \right) \right] + \frac{\partial}{\partial z} \left[ \frac{C_{66}}{2} \left( \frac{\partial \delta u_z}{\partial x} + \frac{\partial \delta u_x}{\partial z} \right) \right] = -\beta (C_{11} + C_{12} + C_{13}) \frac{\partial \delta T_m}{\partial x} - \alpha_{xx} \frac{\partial}{\partial x} [\delta p_{w,m} + \delta (S_{o,m}p_{cwom})] - \alpha_{yx} \frac{\partial}{\partial y} [\delta p_{w,m} + \delta (S_{o,m}p_{cwom})] - \alpha_{zx} \frac{\partial}{\partial z} [\delta p_{w,m} + \delta (S_{o,m}p_{cwom})]$$ (4.86)

In $y$-direction:

$$\frac{\partial}{\partial x} \left[ \frac{C_{44}}{2} \left( \frac{\partial \delta u_x}{\partial y} + \frac{\partial \delta u_y}{\partial x} \right) \right] + \frac{\partial}{\partial y} \left[ C_{21} \frac{\partial \delta u_x}{\partial x} + C_{22} \frac{\partial \delta u_y}{\partial y} + C_{23} \frac{\partial \delta u_z}{\partial z} \right] + \frac{\partial}{\partial z} \left[ \frac{C_{55}}{2} \left( \frac{\partial \delta u_z}{\partial x} + \frac{\partial \delta u_x}{\partial z} \right) \right] = -\beta (C_{11} + C_{12} + C_{13}) \frac{\partial \delta T_m}{\partial x} - \alpha_{xx} \frac{\partial}{\partial x} [\delta p_{w,m} + \delta (S_{o,m}p_{cwom})] - \alpha_{yx} \frac{\partial}{\partial y} [\delta p_{w,m} + \delta (S_{o,m}p_{cwom})] - \alpha_{zy} \frac{\partial}{\partial z} [\delta p_{w,m} + \delta (S_{o,m}p_{cwom})]$$ (4.87)

In $z$-direction:
\[
\frac{\partial}{\partial x} \left[ \frac{C_{66}}{2} \left( \frac{\partial \delta u_z}{\partial x} + \frac{\partial \delta u_x}{\partial z} \right) \right] + \frac{\partial}{\partial y} \left[ \frac{C_{55}}{2} \left( \frac{\partial \delta u_y}{\partial z} + \frac{\partial \delta u_z}{\partial y} \right) \right] +
\frac{\partial}{\partial z} \left[ C_{31} \frac{\partial \delta u_x}{\partial x} + C_{32} \frac{\partial \delta u_y}{\partial y} + C_{33} \frac{\partial \delta u_z}{\partial z} \right] = -\beta (C_{11} + C_{12} + C_{13}) \frac{\partial \delta T_m}{\partial x} -
\frac{\partial}{\partial z} \left( C_{31} \delta \epsilon_{sx} + C_{32} \delta \epsilon_{sy} + C_{33} \delta \epsilon_{sz} \right) - \alpha_{xz} \frac{\partial}{\partial x} \left[ \delta p_{w,m} + \delta (S_{o,m} p_{cwom}) \right] -
\alpha_{yz} \frac{\partial}{\partial y} \left[ \delta p_{w,m} + \delta (S_{o,m} p_{cwom}) \right] - \alpha_{zz} \frac{\partial}{\partial z} \left[ \delta p_{w,m} + \delta (S_{o,m} p_{cwom}) \right]
\]
(4.88)

We still need the constitutive equations relating the swelling strain to the water content. The correlations used in this study are presented in section 4.4.

4.4 Shale Swelling Modeling

One of the common approaches to model the shale swelling is to use the swelling strain. The swelling strain can be measured in the laboratory and is often correlated to the water saturation of the shale.

4.4.1 Constitutive Equation for Shale Swelling

Shale swelling strain is often correlated to the water saturation or water content. The experimental study by Ewy and Stankovic (2010) showed that the swelling property of shale depends on shale type, fluid, and confining stress. Yew et al. (1990) used the following second order correlation:

\[
\epsilon_{sv} = K_1 \Delta S_w (y, t) + K_2 \Delta S^2_w (y, t)
\]
(4.89)

where constants \( K_1 \) and \( K_2 \) are expansion coefficients that can be determined from the moisture-adsorption experiment. For Mancos shale (Figure 4.12), they obtained the following correlation:

\[
\epsilon_{sv} = 0.0708 \Delta S_w (y, t) + 11.08 \Delta S^2_w (y, t)
\]
(4.90)

where \( \epsilon_{sv} \) is the vertical swelling strain, water saturation variation \( \Delta S_w (y, t) \), is a function of position, \( y \), and saturated time, \( t \). The horizontal swelling strain is often obtained from
the vertical strain as $\epsilon_{sv} = f\epsilon_{sh}$, where $f$ is a constant ($0 \leq f \leq 1$).

The yield strength and Young’s modulus of the shale change with water content. The experimental data often shows that yield strength and Young’s modulus are linearly related to the increase of the water content (Chenevert 1970; Yew et al. 1990). Due to the layering structure of the shale matrix, the variation of the shale tensile and compressive strength are direction dependent. For Mancos Shale, Yew et al. (1990) used the following correlation for Young’s modulus (Figure 4.12):

$$E(y,t) = E_o + K_3 \Delta S_w(y,t) = 10^6 (3.1 - 80 \Delta S_w(y,t))$$  \hspace{1cm} (4.91)

where $K_3$ is coefficient that can be determined from the experiments; $E_o$ is the intact Young’s modulus of the shale matrix.

The variation of the strength and Young’s modulus depends on the salinity of the water, confining pressure, and the type of the shale formation. The increase of these parameters when shale samples are exposed to a solution is also reported in literature (Zhang et al. 2006; Ewy et al. 2008). The Biot coefficient also varies with water saturation. Ji and Geehan (2013) used the following correlation for determining Biot coefficient from shale grain modulus, $K_G$, Poisson’s ratio, $\nu$, and Young’s modulus, $E(y,t)$.

$$\alpha = 1 - \frac{E(y,t)}{3K_G (1 - 2\nu)}$$  \hspace{1cm} (4.92)

### 4.4.2 Stress-Dependent Fracture Porosity and Permeability

Cho et al. (2013) evaluated different model for stress-dependent fracture porosity and permeability for shale samples and suggested that model proposed by Raghavan and Chin (2002) best matches to their experimental data for core sample from Bakken Formation. The following correlation from Raghavan and Chin (2002) have been used.

$$\begin{cases} k_f = k_{fi} e^{-c_{f_{\alpha}} \Delta \sigma_{\text{eff}}} \\ \phi_f = \phi_{fi} e^{-c_{f_{\phi}} \Delta \sigma_{\text{eff}}} \end{cases}$$  \hspace{1cm} (4.93)
Figure 4.12: Vertical strain and Young’s modulus versus distilled water adsorption for Man-
cos Shale tested under atmospheric conditions. The experimental data fitted well into the
model presented in Equation (4.90) for vertical strain and in Equation (4.91) for Young’s
modulus (Yew et al. 1990).

where $c_{fk}$ and $c_{fp}$ are fracture porosity and permeability proportionality coefficients; $k_{fi}$ and
$\phi_{fi}$ are the initial fracture permeability and porosity; $\sigma_{eff}$ is the effective stress.

### 4.4.3 Stress Dependence Matrix Porosity and Permeability

There are many theoretical and experimental models for stress dependent porosity and
permeability of rock. Reyes and Osisanya (2002) compared several available models for shale
and suggested that simple exponential models in the following form can be used for shale
matrix.

\[
\begin{align*}
\phi_m &= \phi_{mo} e^{-c_p \sigma_{eff}} \\
k_m &= k_{mo} e^{-c_k \sigma_{eff}}
\end{align*}
\]

where $c_p$ and $c_k$ are matrix porosity and permeability proportionality coefficients; $\phi_{mo}$ and
$k_{mo}$ are porosity and permeability at zero effective stress.
This chapter summarizes the results from the numerical study along with the discussion of the underlying physics for several case studies for matrix block scale and reservoir scale.

5.1 Matrix Block Scale

This section focuses on a single cubic matrix block representing a matrix block in a dual-porosity reservoir. The matrix block contains both oil and water at initial water saturation of 0.52. Both water and oil are considered to be movable in this research initially. Water in the reservoir is often at the residual water saturation. When pressure of fractures surrounding the matrix block decreases, oil flows out of matrix block reducing the oil saturation. Hence, water becomes movable and can be imbibed into shale matrix. The matrix block is submerged into NaCl solution to duplicate the invasion of the injected water into rock matrix in reservoirs during water injection (Figure 5.1). Initially, the block is at equilibrium with initial NaCl concentration equal to the concentration of the water surrounding the block ($c_{sm}^{initial} = 60,000$ ppm). While keeping all other parameters constant, the matrix block size, salinity and pressure of the surrounding water, and the membrane coefficient are varied. The oil recovery factor, ratio of oil flux out of the matrix block and total amount of oil originally in the matrix block, is used for comparison. To determine the contribution of only osmotic transport, gravity was ignored ($g = 0$ ft/s$^2$). We keep the pressure outside the matrix block constant and is equal to the initial pressure, in order to assure that the transport mechanisms are osmotic and capillarity transport only.

All the input parameters have been selected at the reservoir conditions. The input parameters for relative permeability and capillary pressure curves for the shale matrix is provided on (Table 5.1) and plotted in Figure 5.2. The input parameters for the simulation are summarized in Table 5.2. One of the difficulty of waterflooding in shale reservoir is
the very narrow saturation window of the relative permeability curve where both water and hydrocarbon are movable. In the case study here, it is from 0.5 to 0.8. Also, water must reach a relatively high saturation before it becomes movable as shown for Middle Bakken by Karimi et al. (2015). The narrow saturation window may be the result of low resolution of the measurement device and associated errors introduced during the laboratory measurements. This often results in the misinterpretation that at the early injection time with low initial water saturation, water is not imbibed into the rock matrix by advection. However, when rock matrix is contacted with water, water molecules diffuse into the rock matrix. The rate of this diffusion depends on the diffusion coefficient, thermal and chemical potential gradient. When water diffuses into shale matrix, it changes the surface electrochemical balance and water becomes movable at saturation even lower than residual water saturation. Because this diffusion and residual saturation alteration processes are very slow, we may not be able to capture this phenomena in permeability measurement.

<table>
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<th>Value</th>
<th>Parameter</th>
<th>Value</th>
<th>Parameter</th>
<th>Value</th>
</tr>
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<td>(S_{wmx})</td>
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<tr>
<td>(k^*_{rom})</td>
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<td>(S_{orm})</td>
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<td>(\alpha_{m1})</td>
<td>-85</td>
</tr>
<tr>
<td>(n_{wm})</td>
<td>2.0</td>
<td>(S_{wrm})</td>
<td>0.5</td>
<td>(\alpha_{m2})</td>
<td>127.5</td>
</tr>
</tbody>
</table>
When the salinity outside the matrix is reduced to 1000 ppm, water surrounding the matrix block with higher activity fluxes into the matrix block creating pressure variation in the matrix block forcing the oil to move out. The pressure, solute concentration, and saturation after 12 hours the matrix block is submerged into the lower salinity water is shown in Figure 5.3. The concentration gradient - driven diffusion process is a very slow process, particularly in very tight matrix. Hence, only a very small portion of the matrix block is invaded by water (Figure 5.3). Inside the matrix block, the solute concentration still remains the same as the initial concentration (60000 ppm).

5.1.1 Contribution of Osmotic Transport on Oil Recovery from Shale Matrix

The recovery factor from matrix block accounting for the effect of capillary and osmotic pressure is shown in Figure 5.4. The recovery is up to 25% after 1000 days. With the contribution of osmotic transport, the oil recovery is significantly higher depending on the membrane coefficient. Higher membrane coefficient results in higher oil recovery. The recovery factors for four membrane coefficients, 0.05, 0.1, 0.2, and 0.4 are compared in Figure 5.4. The recovery factor in 1000 days increases from 25% to 42% when membrane efficiency is
Table 5.2: Input parameters for matrix block simulation

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
<th>Unit</th>
<th>Parameter</th>
<th>Value</th>
<th>Unit</th>
</tr>
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<tbody>
<tr>
<td>$p_{\text{initial}}$</td>
<td>4351.1</td>
<td>psi</td>
<td>$c_0$</td>
<td>3.44*10^{-6}</td>
<td>psi^{-1}</td>
</tr>
<tr>
<td>$p_{\text{inlet}}$</td>
<td>4351.1</td>
<td>psi</td>
<td>$c_w$</td>
<td>2.41*10^{-6}</td>
<td>psi^{-1}</td>
</tr>
<tr>
<td>$T_m$</td>
<td>380</td>
<td>deg.K</td>
<td>$c_\phi$</td>
<td>3.44*10^{-6}</td>
<td>psi^{-1}</td>
</tr>
<tr>
<td>$c_{\text{initial}}$</td>
<td>60,000 ppm</td>
<td></td>
<td>$\phi_m$</td>
<td>8</td>
<td>%</td>
</tr>
<tr>
<td>$c_{\text{inj}}$</td>
<td>1,000 ppm</td>
<td></td>
<td>$D_{\text{eff}}$</td>
<td>3.88*10^{-9}</td>
<td>ft^{2}/sec</td>
</tr>
<tr>
<td>$k_m$</td>
<td>300</td>
<td>nD</td>
<td>$\omega$</td>
<td>0.1</td>
<td>-</td>
</tr>
<tr>
<td>$\rho_m$</td>
<td>62.43</td>
<td>lb/ft^{3}</td>
<td>$V_w$</td>
<td>63.56*10^{-6}</td>
<td>ft^{3}/mole</td>
</tr>
<tr>
<td>$\rho_o$</td>
<td>50.88</td>
<td>lb/ft^{3}</td>
<td>$g$</td>
<td>0</td>
<td>ft/s^{2}</td>
</tr>
<tr>
<td>$\rho_s$</td>
<td>135.16</td>
<td>lb/ft^{3}</td>
<td>Matrix block size</td>
<td>2<em>2</em>2 ft^{3}</td>
<td></td>
</tr>
<tr>
<td>$\mu_w$</td>
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<td>cp</td>
<td>$R$</td>
<td>8.314</td>
<td>J K^{-1}mol^{-1}</td>
</tr>
<tr>
<td>$\mu_o$</td>
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<td>cp</td>
<td>Number of grid</td>
<td>100<em>1</em>1</td>
<td></td>
</tr>
</tbody>
</table>

increased from 0.05 to 0.4. With high membrane efficiency, fewer solute molecules diffuse out of the matrix. Hence, the concentration imbalance remains longer resulting in more water fluxing into the matrix forcing the oil to move out of the matrix. With low membrane efficiency, the solute molecules move out of the matrix easier. The concentration imbalance quickly vanishes reducing the effect of osmosis on the oil recovery. For conventional reservoirs, the pore size is significantly larger than the diameter of the solute molecules, and the membrane coefficient is very small. Hence the contribution of osmosis on oil recovery from conventional reservoirs is small. However, for unconventional reservoirs, membrane coefficient is higher resulting in a higher contribution of osmosis on oil recovery from rock matrix.

To evaluate the contribution of only osmotic transport on oil recovery from matrix block, we set the capillary pressure to zero. Comparing the osmotic transport to the Darcy’s transport helps to quantify the contribution of the osmotic transport on oil recovery. The recovery factor from the matrix block as the result of salinity reduction is compared with solely pressure - driven flow, or Darcy transport as shown in (Figure 5.5). The results suggest
Figure 5.3: Water pressure, solute concentration, and water saturation after 12 [hours] submerged into water.

that injecting the water with salinity of 1000 ppm results in the same recovery as reducing the pressure surrounding the matrix block about 2650 psi (Figure 5.5). With membrane efficiency of 0.05, the osmotic transport can recover 0.55% total oil in the matrix block. Osmotic flow is much slower than pressure-driven flow. But in long term, the contribution of osmotic transport is considerable. At the beginning, pressure-driven flow is dominant. But in a longer time frame, osmotic transport becomes significant. In pressure-driven flow, pressure drop propagates faster into the matrix to reach the pressure balance. How fast the pressure propagate depends on the hydraulic conductivity of the fluid in the matrix. When the pressure balance is reached, no more fluid flow out of the matrix, the recovery curve starts to flatten out. Meanwhile the osmotic transport is a very slow process, water slowly flux into matrix block and solute molecules diffuse out of the matrix. This process continues until a concentration balance is reached. At that time, the osmotic transport process stops. This implies that incorporating osmotic pressure into transfer function may overestimate the contribution of osmosis.

The contribution of osmotic transport on oil recovery, however, is much smaller for lower membrane efficiency. The recovery curve is flattened when the contribution of osmotic
transport on oil recovery is cease. The osmotic transport stops earlier when membrane efficiency is smaller as shown in Figure 5.5. Since the membrane efficiency is much smaller when permeability is higher, the contribution of the osmotic transport on oil recovery of high permeability matrix is smaller. This implies that the effect of osmotic transport in unconventional reservoirs is more important than it is in conventional reservoirs. The main reason is that the unconventional reservoirs have very low permeability and very small pore sizes. Small pore size reduces the transport of the solute out of the matrix block resulting in higher membrane efficiency. Hence, the concentration imbalance remains longer and the osmotic transport last longer.

5.1.2 Effect of Salinity on Oil Recovery from Shale Matrix

To determine the effect of salinity on the oil recovery, the solute concentration of the fluid surrounding rock matrix is reduced to initiate the osmotic transport. Pressure outside the matrix block is the same as the initial pressure and kept constant. Different solute concentrations may result in different membrane efficiencies. But for the sake of simplicity, the membrane efficiency is kept constant ($\omega = 0.1$). The oil recovery factors for different value of salinities are shown in Figure 5.6. The results indicate that lower salinity increases the amount of oil flux out of the matrix block.
5.1.3 Effect of Matrix Block Size on Oil Recovery from Shale Matrix

Matrix blocks are fractured reducing their sizes during hydraulic fracturing. The matrix block size depends on the distance from the main hydraulic-fracture plane. The density of the micro-fractures (natural and induced) is high near the hydraulic-fracture face, but gradually decreases away from it as a result of the hydraulic-fracturing treatment. This affects the well performance of unconventional shale reservoirs (Fuentes-Cruz and Valko 2015). The contribution of the osmotic transport on oil recovery also depends on the matrix block size as shown in Figure 5.7. Six values of matrix block dimensions (1, 2, 3, 4, 5, 6, 7, and 8 ft)
are used for comparison. The contribution of osmotic transport on oil recovery is more for smaller matrix block sizes. Smaller matrix block results in a higher surface area and a higher recovery factor by osmotic transport. This is important for unconventional reservoirs since the surface area is significantly high after hydraulic fracturing. Since the osmotic transport is a very slow process, matrix block size is more important in very low permeability formations.

5.1.4 Effect of Fluid Type on Oil Recovery from Shale Matrix

The effect of the fluid type on the mass exchange between rock matrix and fractures can be explained by using membrane efficiency and the diffusivity concepts. Diffusion coefficient determines how fast the solute diffuses out of the sample determining the rate of recovery. Figure 5.8 suggests that higher diffusion coefficient lower the contribution of osmotic transport on the oil recovery. Higher diffusion coefficients result in a higher rate of solute diffused into the matrix block reducing the concentration gradient and reducing the effectiveness of the osmotic transport.

The overall oil recovery depends strongly on the membrane efficiency as shown in Figure 5.4. Since the membrane coefficient is the ability of the membrane to filter the solute molecules, solute diameter and the pore size determine the membrane efficiency of shale matrix. Different solutes have different diameters and different electrical charges, hence dif-

![Figure 5.7: Effect of matrix block size on oil recovery by osmotic transport.](image)

(a) with the contribution of osmosis only  
(b) with the contribution of osmosis and capillarity
different membrane coefficients. Larger hydrated ion diameter often results in higher membrane efficiency. The experimental data by Zhang et al. (2008) suggest that at the same concentration, the membrane efficiency of the calcium chloride ($\text{CaCl}_2$) is higher than that of sodium chloride ($\text{NaCl}$) and sodium chloride has higher membrane efficiency than potassium chloride ($\text{KCl}$). As shown in Table 5.3, the hydrated diameter of the calcium is higher than that of sodium and potassium. Even though, potassium has higher dehydrated diameter than sodium, it has a smaller hydrated diameter than potassium, hence, lower membrane efficiency. The concentration of the solute inside the rock matrix also determines the membrane efficiency of shale. The higher the solute concentration, the higher the driving force pushing the solute molecules out of the shale matrix. Hence, higher solute concentration in the matrix often results in lower membrane efficiency as reported by Zhang et al. (2008).

It is important to point out that at the in-situ reservoir conditions, the contribution of osmotic transport to the oil recovery is smaller than the results presented in this research. One of the main reasons is the salinity of the fluid surrounding the matrix increases as solute molecules diffuse from rock matrix with high concentration to fractures with lower concentration. This is one of the reasons why the salinity of the flow-back water is higher than injected water and increases with time.
Table 5.3: The dehydrated, hydrated and average hydrated diameters of some ions (Zhang et al. 2008)

<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Sodium</td>
<td>1.9</td>
<td>5.5-11.2</td>
<td>8.35</td>
</tr>
<tr>
<td>Potassium</td>
<td>2.66</td>
<td>4.64-7.6</td>
<td>6.12</td>
</tr>
<tr>
<td>Cesium</td>
<td>3.34</td>
<td>4.6-7.2</td>
<td>5.9</td>
</tr>
<tr>
<td>Calcium</td>
<td>1.3</td>
<td>21.6</td>
<td>21.6</td>
</tr>
<tr>
<td>Magnesium</td>
<td>1.9</td>
<td>19</td>
<td>19</td>
</tr>
</tbody>
</table>

In addition to the effect of different factors investigated above, other petrophysical properties of rock such as porosity, tortuosity, pore size structure also have important effects on the contribution of osmosis on oil recovery. Low porosity and small pore throat size and higher tortuosity likely promote the effect of osmotic transport. The tortuosity of unconventional reservoirs is high and strongly direction dependent. Anisotropic resistivity and tortuosity measurements by Revil et al. (2013) showed that vertical tortuosity in a Bakken core is around 100 in the vertical direction and 15 in the horizontal direction. It is also noted that the transport properties of shale formation is highly anisotropic, the tortuosity and permeability are strongly direction dependent that may also effect the result and is subject to further research.

5.1.5 Effect of Wettability on Oil Recovery from Shale Matrix

The wettability of shale matrix strongly determines the mass exchange between rock matrix and fractures. To investigate the role of wettability on the mass exchange, simulations are conducted for three matrix blocks with different wettability including water-wetted, oil-wetted, and mix-wetted as shown in (Figure 5.9) using the input data summarized in Table 5.4.

The recovery factors in Figure 5.10 show a considerable amount of water is imbibed into water-wetted and mixed-wetted matrix blocks. Figure 5.10 also suggests that water also
Figure 5.9: Relative permeability and capillary pressure for different wettability matrix blocks.

Table 5.4: Input parameters for obtaining the relative permeability and capillary pressure curves

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Water-wet</th>
<th>Oil-wet</th>
<th>Mixed-wet</th>
</tr>
</thead>
<tbody>
<tr>
<td>$k_{rwm}^*$</td>
<td>0.025</td>
<td>0.12</td>
<td>0.08</td>
</tr>
<tr>
<td>$k_{rom}^*$</td>
<td>0.12</td>
<td>0.025</td>
<td>0.06</td>
</tr>
<tr>
<td>$n_{wm}$</td>
<td>2.5</td>
<td>2.5</td>
<td>2.5</td>
</tr>
<tr>
<td>$n_{om}$</td>
<td>2.5</td>
<td>2.5</td>
<td>2.5</td>
</tr>
<tr>
<td>$S_{orm}$</td>
<td>0.2</td>
<td>0.2</td>
<td>0.2</td>
</tr>
<tr>
<td>$S_{wrm}$</td>
<td>0.8</td>
<td>0.8</td>
<td>0.5</td>
</tr>
<tr>
<td>$S_{wxm}$</td>
<td>0.799</td>
<td>0.5</td>
<td>0.6</td>
</tr>
<tr>
<td>$\alpha_m$</td>
<td>0.1</td>
<td>-30</td>
<td>65</td>
</tr>
</tbody>
</table>

imbibes into the oil-wetted matrix block due to osmotic transport, yet it is very small. Hence, there must be other mechanisms for the imbibition of water into oil-wetted matrix block. The nano-scale modeling results presented previously suggest that interfacial-induced transport could be one of the mechanisms for imbibing water into hydrocarbon-wetted rock matrix.
Surface property alterations, or wettability alterations, may provide a better explanation of this imbibition. In other words, pore scale studies looking at the fluid-rock interaction using the physics of interfacial phenomena are highly recommended for further research.

![Figure 5.10: Recovery factor for different wettability](image)

5.1.6 Matrix Geomechanical Property Alteration with Water Content

The simulation is set up for matrix block scale accounting for swelling and the simulation results are compared with the case without the swelling effect. In addition to input parameters provided in Table 5.2, Table 5.5 lists the input parameters for swelling modeling. The following constitutive equations, in field units, are used to model the swelling strain ($\epsilon_{sv}$) and Young’s modulus($E_o$) with the increase of water content.

\[
\begin{align*}
\epsilon_{sv} &= 0.000708\Delta S_w(y,t) + 0.1108\Delta S_w^2(y,t) \\
E(y,t) &= 3758859 - 2282000\Delta S_w(y,t)
\end{align*}
\]

The equation above is the dependence of Young’s modulus on water saturation for Barnett Shale by Lin and Lai (2013). The variation of the strains and Young’s modulus with the change of the water content is shown in Figure 5.11.

Swelling stress is calculated from the water content via swelling strain. The swelling stress is proportional to the water content, therefore, it is also dependent on the membrane efficiency and salinity. High membrane efficiency promotes the imbibition of the water into
Table 5.5: Geomechanical parameters for matrix block simulation

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
<th>Unit</th>
<th>Parameter</th>
<th>Value</th>
<th>Unit</th>
</tr>
</thead>
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<tr>
<td>$E_o$</td>
<td>3.76</td>
<td>Mpsi</td>
<td>$K_1$</td>
<td>0.00708</td>
<td>-</td>
</tr>
<tr>
<td>$\nu$</td>
<td>0.2</td>
<td></td>
<td>$K_2$</td>
<td>1.108</td>
<td>-</td>
</tr>
<tr>
<td>$f$</td>
<td>0.3</td>
<td></td>
<td>$K_3$</td>
<td>2.28</td>
<td>Mpsi</td>
</tr>
</tbody>
</table>

Figure 5.11: Variation of Young's modulus and strains with incremental water saturation.

The reduction of the Young’s modulus as the result of the invasion of the water into rock matrix depends on the amount of water imbibed into the rock matrix. The variation of Young’s modulus after 100, 500, and 1000 days submerged into water is shown in Figure 5.12. It is important to point out that the variation of Young’s modulus with the water content may have different effect on the pressure balance in the wellbore. If the Young’s modulus reduction is significant, the imbibition of the water into shale matrix reduces the shale compressive strength and may cause matrix shrinking enhancing fracture porosity and permeability.

Since there are two phases, oil and water, in the matrix block, there exist a counter current flow. Water is imbibed into rock matrix to reach the chemical potential balance. The transport of oil is pressure-driven transport as the result of pressure change in water phase. Hence, the rate of mass transport in reservoir condition is significantly lower than that at the lab condition. If the sample is not preserved well, water may evaporate and three phases, water, oil, and air may coexist. When submerged the sample into the water, air
easily get out of the sample allowing more water to imbibe into the sample. This increase in the swelling rate. In other words, the experimental results may overestimate the effect of swelling if it does not represent the reservoir conditions.

### 5.1.7 Effect of Swelling on Matrix Permeability and Porosity

For this matrix block simulation, the model by McKee et al. (1988) is used for evaluating the matrix porosity and permeability with the variation of the effective stress. Matrix porosity and permeability is determined from the change of effective stress as,

\[
\phi_m = \phi_{m_0} \frac{e^{-c\phi_m \Delta \sigma}}{1 - \phi_{m_0} (1 - e^{-c\phi_m \Delta \sigma})} \quad (5.2)
\]

\[
k_m = k_{m_0} \frac{e^{-3c\phi_m \Delta \sigma}}{1 - \phi_{m_0} (1 - e^{-c\phi_m \Delta \sigma})} \quad (5.3)
\]

The expansion of rock matrix as the result of the swelling stress reduces the matrix pore volume, porosity, and permeability of the rock matrix. As observed from Figure 5.13, the reduction of the porosity can be up 50% after 100 days and up to 84% after 1000 days. The reduction of the porosity of the outer layer is up to 44% after 1000 days as shown in Figure 5.14. Since the reduction of permeability is faster than that of porosity, swelling
reduces oil recovery from shale matrix as shown in Section 5.1.9.

![Figure 5.13: Matrix permeability after 100, 500, and 1000 days submerged into water. The imbibition is driven by osmosis only.](image)

![Figure 5.14: Matrix porosity after 100, 500, 1000 days submerged into water. The imbibition is driven by osmosis only.](image)

### 5.1.8 Effect of Swelling on Fracture Permeability and Porosity

The expansion of rock matrix due to swelling reduces the fracture aperture and volume reducing fracture porosity and permeability. The variation of fracture permeability and
porosity depends on the amount of water imbibed into rock matrix and the swelling characteristics of the matrix (Figure 5.15(a) and Figure 5.15(b)). This variation also depends on the fracture pressure since this fracture is the boundary condition for matrix block. Higher fracture pressure results in higher water imbibition into shale matrix, but also confines the matrix expansion. Fracture permeability and porosity reduce significantly for matrix that easily swells and easily imbibes water.

![Graph](image)

(a) Dimensionless fracture permeability.  
(b) Dimensionless fracture porosity.

Figure 5.15: Fracture permeability and porosity variation with time.

### 5.1.9 Effect of Swelling on Oil Recovery from Shale Matrix

The reduction of the pore space in shale matrix due to swelling of shale matrix forces fluid out of the shale matrix. This also reduces the matrix permeability, hence reducing the mass exchange between rock matrix and fractures. Since the diffusion of the water into rock matrix by osmosis is relatively slower than permeability reduction by swelling, swelling significantly reduces the rate of the mass exchange between the matrix and fractures (Figure 5.16). It should be emphasized that the matrix block in this numerical study is under confined stress. The reduction of oil recovery from shale matrix may be different from some imbibition experimental results obtained from experiments conducted at atmospheric condition without applying any confining stress. Shale swelling induces the formation of micro-fractures enhancing matrix permeability and recovery factor in such unconfined conditions. Therefore,
imbibitions should be conducted with confining stress of the reservoir conditions for realistic applications.

Figure 5.16: Effect of swelling on the oil recovery from rock matrix.

5.2 Reservoir Scale

The reservoir scale simulation is conducted to investigate the effectiveness of the low salinity water injection in a liquid-rich low permeability reservoir. The model is setup to simulate the water injection from a hydraulically fractured horizontal well and production from the other horizontal well as shown in Figure 5.17. Two fracture patterns, zipper fracture (Figure 5.17(a)) and modified zipper fracture (Figure 5.17(b)), are investigated. The input parameters for the reservoir scale simulation are summarized in Table 5.6.

As the result of hydraulic fracturing stimulation, the region nearby the fracture have higher permeability as shown in Figure 5.18. The effective permeability of hydraulic fracture (HF) is 4000 mD. The effective permeability of the stimulated reservoir volume (SRV) is 1 mD while that of the unstimulated reservoir volume (URV) is 0.1 mD. This effective fracture permeability is adapted from Xiong (2015). To prevent too early water breakthrough, a relatively small water injection rate of 1800 $ft^3/day$ is used.

The input parameters used for obtaining the relative permeability and capillary pressure curves are summarized in Table 5.7. The relative permeability and capillary pressure for
fractures are shown in Figure 5.20(a) and Figure 5.21(a). Both organic shale matrix and inorganic shale matrix are present in the reservoir. The percentage of organic matrix is about
<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
<th>Unit</th>
<th>Parameter</th>
<th>Value</th>
<th>Unit</th>
</tr>
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<tr>
<td>$p_i$</td>
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<td>psi</td>
<td>$c_{\phi_m}$</td>
<td>$3 \times 10^{-6}$</td>
<td>psi$^{-1}$</td>
</tr>
<tr>
<td>$c_i$</td>
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<td>ppm</td>
<td>$c_w$</td>
<td>$3 \times 10^{-6}$</td>
<td>psi$^{-1}$</td>
</tr>
<tr>
<td>$c_{inj}$</td>
<td>1000</td>
<td>ppm</td>
<td>$c_o$</td>
<td>$4 \times 10^{-6}$</td>
<td>psi$^{-1}$</td>
</tr>
<tr>
<td>$\phi_f$</td>
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<td>%</td>
<td>$T$</td>
<td>380</td>
<td>K</td>
</tr>
<tr>
<td>$k_{HF}$</td>
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<td>mD</td>
<td>$D_{eff}$</td>
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<td>ft$^2$/sec</td>
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<tr>
<td>$k_{SRV}$</td>
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<td>mD</td>
<td>$\omega$</td>
<td>5</td>
<td>%</td>
</tr>
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<td>$k_{URV}$</td>
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<td>mD</td>
<td>Reservoir width</td>
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<td>ft</td>
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<tr>
<td>$\phi_m^{organic}$</td>
<td>4</td>
<td>%</td>
<td>Reservoir length</td>
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<td>ft</td>
</tr>
<tr>
<td>$\phi_m^{inorganic}$</td>
<td>6</td>
<td>%</td>
<td>Reservoir thickness</td>
<td>100</td>
<td>ft</td>
</tr>
<tr>
<td>$k_m$</td>
<td>300</td>
<td>nD</td>
<td>Reservoir grid size</td>
<td>$10 \times 10 \times 10$</td>
<td>ft$^3$</td>
</tr>
<tr>
<td>$\rho_w$</td>
<td>62.8</td>
<td>lbm/ft$^3$</td>
<td>Number of grid on matrix</td>
<td>50<em>1</em>1</td>
<td></td>
</tr>
<tr>
<td>$\rho_o$</td>
<td>48</td>
<td>lbm/ft$^3$</td>
<td>Simulation time</td>
<td>1500</td>
<td>days</td>
</tr>
<tr>
<td>$\mu_w$</td>
<td>0.5</td>
<td>cp</td>
<td>$\Delta t$</td>
<td>0.1</td>
<td>days</td>
</tr>
<tr>
<td>$\mu_o$</td>
<td>0.38</td>
<td>cp</td>
<td>$p_{producer}$</td>
<td>2000</td>
<td>psi</td>
</tr>
<tr>
<td>$c_{\phi_m}$</td>
<td>$3 \times 10^{-6}$</td>
<td>psi$^{-1}$</td>
<td>Injection rate</td>
<td>1800</td>
<td>ft$^3$/day</td>
</tr>
<tr>
<td>$c_{tf}$</td>
<td>$3 \times 10^{-6}$</td>
<td>psi$^{-1}$</td>
<td>$\Delta t_m$</td>
<td>0.01</td>
<td>days</td>
</tr>
</tbody>
</table>

9% distributed randomly in the reservoir using normal distribution with standard deviation of 0.5% as shown in Figure 5.19. The organic shale matrix is oil-wetted, while the inorganic shale matrix is water-wetted. The relative permeability and capillary pressure for matrix is presented in Figure 5.20(b) and Figure 5.21(b), respectively. Since the percentage of the inorganic matrix is higher than that of the organic matrix, the investigated reservoir is more water wetted.

A comparison of the oil recovery for both fracture patterns is presented in Figure 5.22 along with cumulative oil production after 1500 days as shown in Figure 5.23. At the early time, the recovery factors for two patterns are the same. However water breakthrough happens earlier for the zipper fracture pattern as shown in Figure 5.24 since the distance between production fractures and injection fractures is closer. After water breakthrough, the recovery gradually increases since the reservoir is more water wetted as discussed above. The
Table 5.7: Input parameters used for obtaining relative permeability and capillary pressure curves

<table>
<thead>
<tr>
<th>Fracture</th>
<th>Organic Matrix</th>
<th>Inorganic Matrix</th>
</tr>
</thead>
<tbody>
<tr>
<td>Parameter</td>
<td>Value</td>
<td>Parameter</td>
</tr>
<tr>
<td>(k_{rof}^*)</td>
<td>0.4</td>
<td>(k_{rw}^*)</td>
</tr>
<tr>
<td>(k_{rwf}^*)</td>
<td>0.8</td>
<td>(k_{rom}^*)</td>
</tr>
<tr>
<td>(n_{wf})</td>
<td>2</td>
<td>(n_{wm})</td>
</tr>
<tr>
<td>(n_{of})</td>
<td>1.5</td>
<td>(n_{om})</td>
</tr>
<tr>
<td>(S_{orf})</td>
<td>0.05</td>
<td>(S_{orm})</td>
</tr>
<tr>
<td>(S_{wrf})</td>
<td>0.1</td>
<td>(S_{wrm})</td>
</tr>
<tr>
<td>(\alpha_f)</td>
<td>0.15</td>
<td>(S_{wxm})</td>
</tr>
<tr>
<td>(\alpha_m)</td>
<td>-50</td>
<td></td>
</tr>
</tbody>
</table>

Figure 5.19: Percentage of the organic matrix block used in the reservoir scale simulation.

Oil recovery from the modified zipper fracture pattern is higher than that of zipper fracture pattern. Therefore, modified zipper fracture pattern is recommended for EOR operations and this pattern is used for the rest of this study. It should also be emphasized that the effect of stress shadowing and fracture interaction is not considered in this study.

**5.2.1 Effect of Salinity on Oil Recovery**

Effect of salinity is accounted through the contribution of the osmotic transport and the wettability variation. Depending on the permeability of the formation, contribution of each
factor is different. The contribution of osmotic transport is more significant for formation with low matrix permeability, or higher membrane efficiency. In this section, the separate contribution of each factor on the oil recovery is investigated.
Figure 5.22: Comparison of oil recovery factor for the zipper and modified zipper fracture patterns.

Figure 5.23: Comparison of the cumulative oil production between zipper and modified zipper fracture patterns.

Figure 5.24: Comparison of the production water salinity for the zipper and modified zipper fracture patterns.
5.2.1.1 Contribution of osmotic transport

The contribution of the osmotic transport on the oil recovery from rock matrix is evaluated for various membrane coefficients in this section as shown in Figure 5.25. The result confirms that osmosis has a positive contribution to oil recovery in reservoir scale. The contribution of osmosis on oil recovery is proportional to the matrix membrane coefficient. It is important to re-emphasize that the recovery from shale matrix by osmosis is relatively small as the result of low membrane efficiency, typically less than 10% (van Oort et al. 1996, Ewy and Stankovich 2000, Mody et al. 2002, Zhang et al. 2008, and Osuji et al. 2008). The recovery can increase up to 1% if the membrane coefficient changes from 0 to 20%. For conventional reservoirs with larger pore sizes, the membrane efficiency is approximately zero. Hence, the contribution of the osmotic transport on oil recovery from this group of reservoirs is negligible.

![](image)

Figure 5.25: Recovery factor for various matrix membrane coefficients.

5.2.1.2 Contribution of wettability alteration

To model the effect of salinity on the wettability alteration and the oil recovery, correlations for obtaining the permeability and capillary pressure at different salinities are used. Al-Shalabi et al. (2014) showed several models for this purpose. The applicability of each model for unconventional formations is still under investigation. For simplicity, the model
proposed by Jerauld et al. (2008) to model the dependence of permeability and capillary pressure on salinity is used in this study. The relative permeability and capillary pressure are obtained as,

\[
\begin{align*}
    k_{\text{rwm}} &= \theta k_{\text{rwm}}^H(S\ast) + (1 - \theta) k_{\text{rwm}}^L(S\ast) \\
    k_{\text{rom}} &= \theta k_{\text{rom}}^H(S\ast) + (1 - \theta) k_{\text{rom}}^L(S\ast) \\
    p_{\text{cwm}} &= \theta p_{\text{cwm}}^H(S\ast) + (1 - \theta) p_{\text{cwm}}^L(S\ast)
\end{align*}
\]  

(5.4)

where the superscripts \(HS\) and \(LS\) are used to represent high salinity and low salinity and variables \(\theta\) and \(S\ast\) are calculated from Equation 5.5:

\[
\begin{align*}
    \theta &= \frac{S_{\text{orm}} - S_{\text{LSorm}}}{S_{\text{HSorm}} - S_{\text{LSorm}}} \\
    S\ast &= \frac{S_{\text{orm}} - S_{\text{orm}}}{1 - S_{\text{wrm}} - S_{\text{orm}}}
\end{align*}
\]  

(5.5)

where \(S_{\text{wrm}}\) and \(S_{\text{orm}}\) are the residual water and residual oil saturation. The residual saturation is salinity dependent.

The data for relative permeability and capillary pressure for shale at low and high salinity is not available in the literature. Synthetic data are used in this research study with 60000 ppm considered to be high salinity (HS) and 1000 ppm considered as low salinity (LS). The salinity dependence of relative permeability and capillary pressure for fractures and matrix using the input parameters listed in Table 5.8 is presented in Figure 5.26, Figure 5.27 and Figure 5.28. The dependence of the residual oil saturation on salinity is also presented in Figure 5.29.

The wettability alteration promotes more water to be imbibed into the rock matrix and more oil in the rock matrix can be recovered delaying the water breakthrough at the production well and increasing oil recovery as shown in Figure 5.30. The simulation results suggest that the contribution of wettability alteration is considerably important. It should be noted that the relative permeability and capillary pressure curves for various salinity values is still not available and the results reported here are based on simulations using the synthetic relative permeability and capillary pressure curves in this study. Further experimental research studies should be conducted to obtain more experimental data improving wettability alteration modeling.
Figure 5.26: Fracture relative permeability and capillary pressure at high and low salinity.

Figure 5.27: Inorganic matrix relative permeability and capillary pressure at high and low salinity.
5.2.2 Effect of Fracture and Well Spacing

The reservoir is configured for two fracture and well spacings in order to investigate the effect of spacing on the oil recovery. The results shown in Figure 5.31 suggests that higher
Figure 5.29: Schematic of salinity dependence of residual-oil saturation.

Figure 5.30: Contribution of wettability alteration on oil recovery.

hydraulic fracture density increases the oil recovery during water injection. However, we need to emphasize that the stress shadowing effect has not been considered in this study. The same stimulated reservoir volume is assume resulting in a small difference in oil recovery between two fracture spacing. With additional hydraulic fractures, the permeability in the stimulated reservoir volume may vary affecting the oil recovery.

Close well spacing is not recommended for water injection enhanced oil recovery in shale formation since water breakthrough happens very early if the well is too close as shown
in Figure 5.32. It should be also noted that fracture network has not been considered in this study. The simulation volume consists of only planar hydraulic fractures and natural fractures. In the reservoir, fracture network may be present and may be created through hydraulic fracturing operations resulting in much earlier water breakthrough than the simulation results reported here.

5.2.3 Effect of Shale Swelling

In addition to the data presented in Table 5.6, the input parameters used for shale swelling model is listed in Table 5.9. It should be noted that these data are currently not available for organic-rich shale formations. More swelling experimental measurements are
being conducted at UNGI Geomechanics Laboratory. Hence, synthetic data have been used in our modeling study presented here. For shale formations with high swelling potential, the permeability near injection hydraulic fractures rapidly decrease resulting in a substantial pressure build up. This may form additional hydraulic fractures. It also causes a lot of challenges from simulation perspective because the variation of matrix block boundary conditions is greater creating the instability in the numerical simulation. Therefore, we used a shale with very low swelling potential for the simulation presented in this primary numerical study. The correlation between swelling strain, Young’s modulus and the incremental water content is presented in Figure 5.33 using the input parameter in Table 5.6.

Table 5.9: Geomechanical parameters used in the reservoir scale simulation

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>$E_o$</td>
<td>3.76</td>
<td>Mpsi</td>
</tr>
<tr>
<td>$\nu$</td>
<td>0.15</td>
<td>-</td>
</tr>
<tr>
<td>$f$</td>
<td>0.3</td>
<td>-</td>
</tr>
<tr>
<td>$K_1$</td>
<td>0.0000708</td>
<td>-</td>
</tr>
<tr>
<td>$K_2$</td>
<td>0.01108</td>
<td>-</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>$K_3$</td>
<td>2.28</td>
<td>Mpsi</td>
</tr>
<tr>
<td>$c_{fk}$</td>
<td>2.02*10^-4</td>
<td>psi^-1</td>
</tr>
<tr>
<td>$c_{fp}$</td>
<td>1.01*10^-4</td>
<td>psi^-1</td>
</tr>
<tr>
<td>$c_{mk}$</td>
<td>8*10^-4</td>
<td>psi^-1</td>
</tr>
<tr>
<td>$c_{mp}$</td>
<td>1*10^-4</td>
<td>psi^-1</td>
</tr>
</tbody>
</table>

Figure 5.33: Variation of Young’s modulus and strains with incremental water saturation.

The recovery factors for the case without shale swelling and with shale swelling are shown in Figure 5.34. This suggests that recovery factor reduces more than 1% as a result of swelling. The main reason for this recovery reduction is the decrease of the fracture
permeability and the amount of oil recovered from rock matrix. In early injection times, the recovery factor is almost the same since the same amount of water is injected in the reservoir. The difference between two cases, with and without swelling, is the pressure build up significantly near the injection well for swelling case. The reduction of oil recovery after water breakthrough is the result of the decrease of mass transfer from shale matrix to fractures due to shale swelling. For shale with higher swelling potential, we should expect a significant reduction of the oil recovery factor. High pressure build up in the injection well significantly reduces the injection index and may result in screen out. Therefore, chemical for preventing shale swelling should be considered for water injection operations in shale formations with swelling potential.

![Figure 5.34: Effect of shale swelling oil recovery factor.](image)

5.3 Limitations of the Study and Future Work

This multi-physics reservoir modeling research study evaluates the potential of water injection enhanced oil recovery from liquid-rich unconventional formations. The main focus is to simulate the multi-physics at various scales in the reservoir by solving the mass transport equations for every matrix block in the reservoir. A mass transport model along with a swelling model are developed and integrated into the reservoir model. The simulation results suggested that low salinity can increase the oil recovery from the matrix due to the contribution of osmotic transport, the variation of the surface properties, and wettability
alteration. However, due to the lack of laboratory experiments to determine the input data for simulations, some synthetic input data are used in this research. Experimental studies should be conducted to obtain inputs for simulation.

Although, the membrane efficiency is a function of solute concentration, pressure, and other physical properties of fluid and rock, constant value for membrane efficiency was used in this primary modeling effort. Different ion types have different effects on the interfacial properties affecting the oil recovery. The effect of fluid can be explained using the membrane efficiency and diffusion coefficient. Solute with smaller hydrated ion diameter and molecular weight often has lower membrane efficiency. However, determination of diffusion coefficient and membrane efficiency for reservoir engineering applications is still an objective of further studies.

Stress shadowing and fracture network are not considered in reservoir scale simulations. A homogeneous reservoir is considered, especially for shale matrix, in this primary modeling study. Heterogeneity at different scales may completely change the simulation results. However, the underlying physics does not change and the developed model can also be modified to account for the complexity of any reservoirs provided that the input data for heterogeneous reservoir are available. Hence, reservoir characterization methods should be employed to obtain better input parameters for the simulation and better represent the reservoir.

The numerical simulation with clay swelling is often unstable, particularly for clay with high swelling potential. A numerical scheme to overcome this problem is recommended in future studies to overcome this challenge.
CHAPTER 6
SUMMARY AND RECOMMENDATIONS

In this chapter, a summary of the research results presented and the recommendations for the field operations and further research are discussed.

6.1 Conclusion and Remarks

The interfacial tension-induced transport at pore scale using an idealized pore model was investigated. Pore scale provides more understanding of transport at pore size. However, the upscaling from this pore scale model to a larger scale flow simulator requires additional work. The potential of water injection enhanced oil recovery from liquid-rich unconventional formations has been investigated in this multi-physics reservoir modeling research study. The main focus is on the development of a model to simulate the multi-physics at different scales in reservoirs. Mass transport and shale swelling models were developed and integrated into the reservoir model. The main conclusions of this research are summarized below.

1. Water enters nano-porous rock by at least two mechanisms, namely capillary imbibition and chemical osmosis. However, by looking at cores submerged in brine, it is difficult to distinguish between the two because capillary imbibition is driven by interfacial tension forces while osmotic filtration is driven by a chemical potential gradient of solvent with respect to pore selectivity, or membrane efficiency. Pore selectivity includes pore throat size and the propensity of the pore surface to hold on to the dissolved ions by electrochemical bonding.

2. The model for imbibition of water (both by capillarity and osmosis) was tested on a very small capillary tube representing a pore. The results from this model emphasize the contribution of interfacial tension-induced transport on water imbibition in oil-wetted rock matrix and is consistent with laboratory observations.
3. The mass transport model developed in this research accounts for advection by three different forces: flow potential gradient, osmosis, and molecular diffusion.

4. Low salinity increases the oil recovery from the matrix due to the contribution of the osmotic transport and the variation of the surface properties, or wettability alteration. Since osmosis is a very slow process, yet more important in low permeability and small matrix block size and high membrane efficiency, the contribution of osmosis is rather in longer time. The actual contribution of osmotic transport on oil recovery is also considerably less than the osmotic potential because the membrane coefficient of shale matrix is small, typically less than 10%. For conventional reservoirs with large pore size and very low membrane efficiency, the contribution of the osmosis is negligible.

5. Because water transport into the pores causes shale swelling (especially in pores coated with clay minerals), the transport model in this thesis incorporates rock frame displacement. The model seems to be a very good tool to model shale swelling.

6. Shale swelling reduces the matrix porosity and permeability forcing more oil to move out of the rock matrix. However, it also reduces the mass exchange between fractures and rock matrix reducing the oil recovery from shale matrix. The reduction of fracture permeability reduces the overall oil recovery factor and the injection index of injection wells.

6.2 Recommendations

There are a large body of research studies that try to explain and qualify osmotic transport, swelling of pores containing clays, and their implication to enhanced oil recovery. While this research study has provided helpful insights, more research is needed, especially in the area of upscaling the capillary tube model to the complex pores in the reservoir. Consequently, further studies need be conducted to examine the methodology of this research, and to extend our results and findings to field applications.
The diffusion coefficient in multi-component system (beyond binary) is very difficult to measure and quantify. There are several complex theoretical techniques to calculate the diffusion coefficient. However, there exist practical methods to use binary equivalents that are easier to use and represent laboratory experiments. These binary approaches should be re-visited and quantified. Furthermore, the diffusion coefficient in high pressure solutions is very small (i.e., $10^{-9}$ m$^2$/s), which is reasonable for engineering modeling approaches.

To maximize the profit from shale oil EOR project by water injection, long horizontal wells with multiple fractures are recommended. Chemical for preventing shale swelling and altering the wettability is also recommended for water injection in formations with high shale swelling potential.

Further effort on the pore characterization and modeling is necessary for more realistic modeling of mass transport phenomena along pores. Advanced imaging techniques should be used for more realistic modeling of the mass transport at pore scale. The surface force of the pore wall should be considered to accurately evaluate the rate of solute transport in the future research studies. Reducing the interfacial tension between oil and water forces oil out of the pores and may have applications in improved and enhanced oil recovery operations. Further research on the mechanism for wettability alteration is essential for effective implementation of EOR projects. A comprehensive investigation of surface forces, surface charge and surface energy, clay swelling should also be conducted before any recommendation of low salinity water injection.

For the reservoir scale modeling, experimental measurements should be conducted to determine the input for the numerical simulation. The following laboratory experiments are needed to determine input data

- Experiments to determine the swelling strain with water content and electrochemical properties of the water injected are highly recommended. Experiments should be conducted at reservoir conditions with the presence of two phases, hydrocarbon and water.
- Experiments to correlate the matrix permeability with failure and disassociation of the shale matrix due to water invasion. Experiments should be conducted at reservoir stress and pressure conditions.

- Experiments to determine the membrane efficiency of the shale matrix. Experimental determination of the pressure-dependence of the membrane efficiency is also recommended. A method for increasing membrane efficiency of the rock matrix can improve the contribution of osmotic pressure on the hydrocarbon recovery from the rock matrix.

- Experiments to obtain the capillary pressure and permeability curves at both high and low salinity water.

Further research on the swelling should consider temperature variation by incorporating the conservation of energy equation. It is also recommended to develop a coupled fluid flow and geomechanics model to account for the rock deformation in reservoir scale.
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APPENDIX A - DERIVATION OF OSMOTIC TRANSPORT EQUATION

We consider the flux of water into a control volume as shown in Figure A.1. The net mass of water flux into the control volume is defined as follows:

\( x \)-direction due to advection is:

\[
\frac{dJ}{dx} = \rho_w v_w dxdydz - \left( \rho_w + \frac{\partial \rho_w}{\partial x} dx \right) \left( v_{wx} + \frac{\partial v_{wx}}{\partial x} dx \right) dydz \approx -\frac{\partial}{\partial x} (\rho_w v_{wx}) dxdydz \quad \text{(A.1)}
\]

\( y \)-direction due to advection is:

\[
\frac{dJ}{dy} = \rho_w v_w dxdz - \left( \rho_w + \frac{\partial \rho_w}{\partial y} dy \right) \left( v_{wy} + \frac{\partial v_{wy}}{\partial y} dy \right) dxdz \approx -\frac{\partial}{\partial y} (\rho_w v_{wy}) dxdydz \quad \text{(A.2)}
\]

\( z \)-direction due to advection is:

\[
\frac{dJ}{dz} = \rho_w v_w dydz - \left( \rho_w + \frac{\partial \rho_w}{\partial z} dz \right) \left( v_{wz} + \frac{\partial v_{wz}}{\partial z} dz \right) dxdy \approx -\frac{\partial}{\partial z} (\rho_w v_{wz}) dxdydz \quad \text{(A.3)}
\]

The total net volume of water flux into the control volume is:

\[
\frac{dJ}{= -\left[ \frac{\partial}{\partial x} (\rho_w v_{wx}) + \frac{\partial}{\partial y} (\rho_w v_{wy}) + \frac{\partial}{\partial z} (\rho_w v_{wz}) \right] dxdydz = \nabla \cdot (\rho_w v_w) dxdydz}
\]

The water flux into the control volume due to osmosis is (Jensen et al. 2009):

\[
\frac{dJ_{osm}}{= -\rho_w \frac{k_w \omega RT}{V_w} \nabla c_s dxdydz} \quad \text{(A.4)}
\]

The van Hoff equation for osmotic pressure (Schultz 1980), \( \Pi = \frac{-\omega RT}{V_w} \nabla c_s \), is used.

The mass change from \( t_o \) to \( t_o + \Delta t \) is:

\[
\frac{\rho_w S_w dxdydz}_{t_o + \Delta t} - \frac{\rho_w S_w dxdydz}_{t_o} = \frac{\partial}{\partial t} (\rho_w S_w dxdydz) \quad \text{(A.5)}
\]

The source/sink term entering or leaving the control volume is: \( \rho_w \tilde{q}_w dxdydz \).
Using the conservation of mass assuming the volume of the control volume \((dxdydz)\) does not change, we obtain:

\[
\left[ -\frac{\partial}{\partial x} (\rho_w v_{w_x}) - \frac{\partial}{\partial x} (\rho_w v_{w_x}) - \frac{\partial}{\partial x} (\rho_w v_{w_x}) \right] dxdydz + \rho_w \hat{q}_w dx dy dz = \frac{\partial}{\partial t} (\phi \rho_w S_w dx dy dz) \tag{A.6}
\]

or

\[- \nabla \cdot (\rho_w \mathbf{v}_w) - \rho_w \frac{k_w}{\mu_w} \frac{\omega RT}{V_w} \nabla c_s + \rho_w \hat{q}_w = \frac{\partial}{\partial t} (\phi \rho_w S_w) \tag{A.7}\]

Using Darcy’s law, Equation A.7 can be written as,

\[
\nabla \cdot \left[ \rho_w \frac{k_w}{\mu_w} \nabla (p_w - \gamma_w D) - \rho_w \frac{k_w}{\mu_w} \left( \frac{\omega RT}{V_w} \nabla c_s \right) \right] + \rho_w \hat{q}_w = \frac{\partial}{\partial t} (\phi \rho_w S_w) \tag{A.8}
\]
APPENDIX B - NUMERICAL SIMULATION

The numerical procedure and discretized equations for numerical solution of governing equations are formulated in this Appendix. First, the governing equations for water and oil in reservoir are solved implicitly to obtain phase pressure, phase saturation, and solute concentration for each grid block. Then, the mass transport equation for each matrix block in the grid block is solved implicitly to obtain saturation, pressure, and solute concentration on refined matrix block. The validation of the numerical simulation is presented in Appendix C.

B.1 Solution of Fluid Flow Equation

The solution of fluid flow equation gives us the pressure of each phase in fractures. First, the pressure of oil phase in fractures is calculated by solving the discretized equation implicitly, then water pressure is obtained through capillary pressure. Water saturation in fracture is computed explicitly using the continuity equation for water.

B.1.1 Phase Pressure in Fractures

First, we solve the fracture total pressure for the pressure of oil phase in fracture. The finite difference form of equation 4.12 is written as,

\[
B_{i,j,k}p_{o,f,i,j,k}^{n+1} + C_{i,j,k}p_{o,f,i-1,j,k}^{n+1} + B_{i,j,k}p_{o,f,i,j-1,k}^{n+1} + E_{i,j,k}p_{o,f,i,j,k}^{n+1} \\
+ F_{i,j,k}p_{o,f,i+1,j,k}^{n+1} + G_{i,j,k}p_{o,f,i,j+1,k}^{n+1} + H_{i,j,k}p_{o,f,i,j,k+1}^{n+1} + C_{T_{i,j,k}}\delta T_{i,j,k} = R_{i,j,k} \tag{B.1}
\]

where

\[
B_{i,j,k} = \frac{\Delta x_{i,j,k}\Delta y_{i,j,k}}{\Delta z_{i,j,k-\frac{1}{2}}} [k_{f,eff} (\lambda_{w,f} + \lambda_{o,f})]_{i,j,k-\frac{1}{2}}^n \tag{B.2}
\]

\[
C_{i,j,k} = \frac{\Delta x_{i,j,k}\Delta z_{i,j,k}}{\Delta y_{i,j-\frac{1}{2},k}} [k_{f,eff} (\lambda_{w,f} + \lambda_{o,f})]_{i,j-\frac{1}{2},k}^n \tag{B.3}
\]
\[ D_{i,j,k} = \frac{\Delta y_{i,j,k} \Delta z_{i,j,k}}{\Delta x_{i-\frac{1}{2},j,k}} \left[ k_{f,\text{eff}} (\lambda_w,f + \lambda_o,f) \right]_{i-\frac{1}{2},j,k}^n \] (B.4)

\[ F_{i,j,k} = \frac{\Delta y_{i,j,k} \Delta z_{i,j,k}}{\Delta x_{i+\frac{1}{2},j,k}} \left[ k_{f,\text{eff}} (\lambda_w,f + \lambda_o,f) \right]_{i+\frac{1}{2},j,k}^n \] (B.5)

\[ G_{i,j,k} = \frac{\Delta x_{i,j,k} \Delta z_{i,j,k}}{\Delta y_{i,j+\frac{1}{2},k}} \left[ k_{f,\text{eff}} (\lambda_w,f + \lambda_o,f) \right]_{i,j+\frac{1}{2},k}^n \] (B.6)

\[ H_{i,j,k} = \frac{\Delta x_{i,j,k} \Delta z_{i,j,k}}{\Delta y_{i,j+\frac{1}{2},k}} \left[ k_{f,\text{eff}} (\lambda_w,f + \lambda_o,f) \right]_{i,j+\frac{1}{2},k}^n \] (B.7)

\[ E_{i,j,k} = - \left\{ \begin{array}{l}
\frac{\Delta y_{i,j,k} \Delta z_{i,j,k}}{\Delta x_{i+\frac{1}{2},j,k}} \left[ k_{f,\text{eff}} (\lambda_w,f + \lambda_o,f) \right]_{i+\frac{1}{2},j,k}^n \\
+ \frac{\Delta y_{i,j,k} \Delta z_{i,j,k}}{\Delta x_{i-j+\frac{1}{2},k}} \left[ k_{f,\text{eff}} (\lambda_w,f + \lambda_o,f) \right]_{i-j+\frac{1}{2},k}^n \\
+ \frac{\Delta x_{i,j,k} \Delta z_{i,j,k}}{\Delta y_{i,j-k+\frac{1}{2},k}} \left[ k_{f,\text{eff}} (\lambda_w,f + \lambda_o,f) \right]_{i,j-k+\frac{1}{2},k}^n \\
+ \frac{\Delta x_{i,j,k} \Delta z_{i,j,k}}{\Delta y_{i,j+k+\frac{1}{2},k}} \left[ k_{f,\text{eff}} (\lambda_w,f + \lambda_o,f) \right]_{i,j+k+\frac{1}{2},k}^n \\
\end{array} \right\} \] (B.8)

\[ C_{T_{i,j,k}} = \frac{1}{\Delta t} V_i \left( 1 - e_{\mu}^n \right) \phi f_{i,j,k}^n \] (B.9)

\[ R_{i,j,k} = \Delta y_{i,j,k} \Delta z_{i,j,k} \left\{ \begin{array}{l}
\left[ k_{f,\text{eff}} \lambda_w,f \right]_{i+\frac{1}{2},j,k}^n \left( \frac{p_{c\text{w},i+1,j,k}^{n+1} - p_{c\text{w},i,j,k}^{n+1}}{\Delta x_{i+\frac{1}{2},j,k}} \right) \\
\left[ k_{f,\text{eff}} \lambda_w,f \right]_{i-\frac{1}{2},j,k}^n \left( \frac{p_{c\text{w},i,j-k+1,k}^{n+1} - p_{c\text{w},i,j-k-1,k}^{n+1}}{\Delta x_{i-\frac{1}{2},j,k}} \right) \\
\left[ k_{f,\text{eff}} \lambda_w,f \right]_{i+\frac{1}{2},j,k}^n \left( \frac{p_{c\text{w},i+1,j,k}^{n+1} - p_{c\text{w},i,j,k}^{n+1}}{\Delta x_{i+\frac{1}{2},j,k}} \right) \\
\left[ k_{f,\text{eff}} \lambda_w,f \right]_{i-\frac{1}{2},j,k}^n \left( \frac{p_{c\text{w},i,j-k+1,k}^{n+1} - p_{c\text{w},i,j-k-1,k}^{n+1}}{\Delta x_{i-\frac{1}{2},j,k}} \right) \\
\end{array} \right\} \]
B.1.2 Phase Saturation in Fractures

After obtaining the pressure of the oil phase in the fracture, the fracture water saturation equation is obtained from the continuity equation of the water phase (Equation 4.35) as,

\[
\begin{align*}
S_{w,f,i,j,k}^{n+1} &= \frac{\Delta t}{\phi_f (1 - \epsilon_v,f)_{i,j,k}} \left[ (\tau_w)_{i,j,k}^n + \left( \frac{q_w}{V_R} \right)_{i,j,k}^n + \phi_f S_{w,f}^n \frac{\epsilon_{v,f}^{n+1} - \epsilon_{v,f}^n}{\partial t} ight] \\
&\quad - [S_{w,f} (c_w + c_o)_{i,j,k}^n (p_{w,f,i,j,k}^{n+1} - p_{w,f,i,j,k}^n) - [S_{w,f} \beta_w]_{i,j,k}^n (T_{o,f,i,j,k}^{n+1} - T_{o,f,i,j,k}^n) + S_{w,f,i,j,k} + 2] \\
&\quad + \Delta t (k_{f,eff} \lambda_{w,f})_{i+\frac{1}{2},j,k}^n [p_{o,f,i,j+1,k}^{n+1} - p_{o,f,i,j,k}^n - p_{cuo,f,i+1,j,k}^n + p_{cuo,f,i,j,k}^n - \gamma_w (D_{i+1,j,k} - D_{i,j,k})] \\
&\quad - \Delta t (k_{f,eff} \lambda_{w,f})_{i-\frac{1}{2},j,k}^n [p_{o,f,i-1,j,k}^{n+1} - p_{o,f,i,j,k}^n - p_{cuo,f,i-1,j,k}^n + p_{cuo,f,i,j,k}^n - \gamma_w (D_{i,j,k} - D_{i-1,j,k})] \\
&\quad + \Delta t [\phi_f (1 - \epsilon_v,f)_{i,j,k}^n \Delta x_{i,j,k} \Delta y_{i,j,k}^2] \\
&\quad - \Delta t (k_{f,eff} \lambda_{w,f})_{i,j-\frac{1}{2},k}^n [p_{o,f,i,j-1,k}^{n+1} - p_{o,f,i,j,k}^n - p_{cuo,f,i,j-1,k}^n + p_{cuo,f,i,j,k}^n - \gamma_w (D_{i,j,k} - D_{i,j-1,k})] \\
&\quad + \Delta t [\phi_f (1 - \epsilon_v,f)_{i,j,k}^n \Delta y_{i,j,k} \Delta z_{i,j,k}^2] \\
&\quad - \Delta t (k_{f,eff} \lambda_{w,f})_{i,j,k+\frac{1}{2}} [p_{o,f,i,j,k+1}^{n+1} - p_{o,f,i,j,k}^n - p_{cuo,f,i,j,k+1}^n + p_{cuo,f,i,j,k}^n - \gamma_w (D_{i,j,k+1} - D_{i,j,k})] \\
&\quad + \Delta t [\phi_f (1 - \epsilon_v,f)_{i,j,k}^n \Delta z_{i,j,k} \Delta z_{i,j,k+\frac{1}{2}}] \\
&\quad - \Delta t (k_{f,eff} \lambda_{w,f})_{i,j,k-\frac{1}{2}} [p_{o,f,i,j,k-1}^{n+1} - p_{o,f,i,j,k}^n - p_{cuo,f,i,j,k-1}^n - p_{cuo,f,i,j,k}^n - \gamma_w (D_{i,j,k} - D_{i,j,k-1})] \\
&\quad + \Delta t [\phi_f (1 - \epsilon_v,f)_{i,j,k}^n \Delta z_{i,j,k} \Delta z_{i,j,k-\frac{1}{2}}] \\
&\quad - \Delta t (V_R (\tau_w + \tau_o))_{i,j,k}^n - (q_w + q_o)_{i,j,k}^n - (V_R \phi_f \epsilon_{t,f})_{i,j,k} \frac{p_{o,f,i,j,k}^n}{\Delta t} \quad \text{(B.10)}
\end{align*}
\]
The oil saturation in fractures is calculated from water saturation in fractures as,

$$S_{o,f_{i,j,k}}^{n+1} = 1 - S_{w,f_{i,j,k}}^{n+1} \quad (B.12)$$

Then, the fracture capillary pressure $p_{cwof_{i,j,k}}^{n+1}$ can be calculated using the water saturation (Equation D.12). The pressure of the water phase is calculated from the pressure of the oil phase in the fracture and the fracture capillary pressure,

$$p_{wf_{i,j,k}}^{n+1} = p_{of_{i,j,k}}^{n+1} - p_{cwof_{i,j,k}}^{n+1} \quad (B.13)$$

### B.1.3 Solute Concentration in Fractures

The next step is to compute the solute concentration in the fracture using equation 4.25,

$$c_{wsf_{i,j,k}}^{n+1} = -\frac{1}{S_{wf_{i,j,k}}^{n+1}} \frac{\Delta t}{\phi_f} \left( \frac{1}{\Delta x_{i,j,k}} \left( (c_{wsf}v_{wf})_{i+\frac{1}{2},j,k} - (c_{wsf}v_{wf})_{i-\frac{1}{2},j,k} \right) \right) + \frac{1}{\Delta y_{i,j,k}} \left( (c_{wsf}v_{wf})_{i,j+\frac{1}{2},k} - (c_{wsf}v_{wf})_{i,j-\frac{1}{2},k} \right) + \frac{1}{\Delta z_{i,j,k}} \left( (c_{wsf}v_{wf})_{i,j,k+\frac{1}{2}} - (c_{wsf}v_{wf})_{i,j,k-\frac{1}{2}} \right) + \frac{1}{S_{wf_{i,j,k}}^{n+1}} \frac{\Delta t}{\phi_f} \left( c_{wsf}q_{w} \right)_{i,j,k} + \left( \frac{S_{nf}^{n}}{S_{nf}^{n+1}} c_{wsf} \right)_{i,j,k} \quad (B.14)$$

where the phase velocities are calculated from Darcy’s law as,

$$v_{wf_{i+\frac{1}{2},j,k}}^{n} = -k_{f,eff} \frac{p_{wf_{i+1,j,k}}^{n+1} - p_{wf_{i,j,k}}^{n+1} - \gamma_{w_{i+\frac{1}{2},j,k}} (D_{i+1,j,k} - D_{i,j,k})}{\Delta x_{i+\frac{1}{2},j,k}} \quad (B.15)$$

$$v_{wf_{i-\frac{1}{2},j,k}}^{n} = -k_{f,eff} \frac{p_{wf_{i,j,k}}^{n+1} - p_{wf_{i-1,j,k}}^{n+1} - \gamma_{w_{i-\frac{1}{2},j,k}} (D_{i,j,k} - D_{i-1,j,k})}{\Delta x_{i-\frac{1}{2},j,k}} \quad (B.16)$$

$$v_{wf_{i,j+\frac{1}{2},k}}^{n} = -k_{f,eff} \frac{p_{wf_{i,j+1,k}}^{n+1} - p_{wf_{i,j,k}}^{n+1} - \gamma_{w_{i,j+\frac{1}{2},k}} (D_{i,j+1,k} - D_{i,j,k})}{\Delta y_{i,j+\frac{1}{2},k}} \quad (B.17)$$

$$v_{wf_{i,j-\frac{1}{2},k}}^{n} = -k_{f,eff} \frac{p_{wf_{i,j-1,k}}^{n+1} - p_{wf_{i,j,k}}^{n+1} - \gamma_{w_{i,j-\frac{1}{2},k}} (D_{i,j,k} - D_{i,j-1,k})}{\Delta y_{i,j-\frac{1}{2},k}} \quad (B.18)$$

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B.2 Solution of Mass Transport Equation in Matrix Block

The mass transport model is solved numerically for every matrix block in reservoir. For small matrix block and the difference between water density and oil density is small, ignoring the effect of gravity, we can simplify the solution to a 1-D problem for both core sample and the matrix block as illustrated in Figure B.1. For the matrix block simulation, we solved the

\[ \begin{align*}
\mathbf{v}_n^{\text{w} f_{i,j,k+\frac{1}{2}}} &= -k_{f,\text{eff}} \lambda \mathbf{w} f_{i,j,k+\frac{1}{2}} \rho^{\text{w} f_{i,j,k+\frac{1}{2}} - \rho^{\text{w} f_{i,j,k}}} - \gamma \mathbf{w} f_{i,j,k+\frac{1}{2}} \left( D_{i,j,k+1} - D_{i,j,k} \right) \\
\Delta z_{i,j,k+\frac{1}{2}} \\
\mathbf{v}_n^{\text{w} f_{i+\frac{1}{2},j,k}} &= -k_{f,\text{eff}} \lambda \mathbf{w} f_{i+\frac{1}{2},j,k} \rho^{\text{w} f_{i+\frac{1}{2},j,k} - \rho^{\text{w} f_{i,j,k}}} - \gamma \mathbf{w} f_{i+\frac{1}{2},j,k} \left( D_{i,j,k} - D_{i,j,k-1} \right) \\
\Delta x_{i+\frac{1}{2},j,k} \\
\mathbf{v}_n^{\text{o} f_{i+\frac{1}{2},j,k}} &= -k_{f,\text{eff}} \lambda \mathbf{o} f_{i+\frac{1}{2},j,k} \rho^{\text{o} f_{i+\frac{1}{2},j,k} - \rho^{\text{o} f_{i,j,k}}} - \gamma \mathbf{o} f_{i+\frac{1}{2},j,k} \left( D_{i,j+1,k} - D_{i,j,k} \right) \\
\Delta y_{i+\frac{1}{2},j,k} \\
\mathbf{v}_n^{\text{o} f_{i,j+\frac{1}{2},k}} &= -k_{f,\text{eff}} \lambda \mathbf{o} f_{i,j+\frac{1}{2},k} \rho^{\text{o} f_{i,j+\frac{1}{2},k} - \rho^{\text{o} f_{i,j,k}}} - \gamma \mathbf{o} f_{i,j+\frac{1}{2},k} \left( D_{i,j+1,k} - D_{i,j,k} \right) \\
\Delta z_{i,j+\frac{1}{2},k} \\
\mathbf{v}_n^{\text{o} f_{i,j-\frac{1}{2},k}} &= -k_{f,\text{eff}} \lambda \mathbf{o} f_{i,j-\frac{1}{2},k} \rho^{\text{o} f_{i,j-\frac{1}{2},k} - \rho^{\text{o} f_{i,j,k}}} - \gamma \mathbf{o} f_{i,j-\frac{1}{2},k} \left( D_{i,j,k} - D_{i,j-1,k} \right) \\
\Delta y_{i,j-\frac{1}{2},k} \\
\mathbf{v}_n^{\text{o} f_{i,j,k+\frac{1}{2}}} &= -k_{f,\text{eff}} \lambda \mathbf{o} f_{i,j,k+\frac{1}{2}} \rho^{\text{o} f_{i,j,k+\frac{1}{2}} - \rho^{\text{o} f_{i,j,k}}} - \gamma \mathbf{o} f_{i,j,k+\frac{1}{2}} \left( D_{i,j+1,k} - D_{i,j,k} \right) \\
\Delta z_{i,j,k+\frac{1}{2}} \\
\mathbf{v}_n^{\text{o} f_{i+\frac{1}{2},j,k}} &= -k_{f,\text{eff}} \lambda \mathbf{o} f_{i+\frac{1}{2},j,k} \rho^{\text{o} f_{i+\frac{1}{2},j,k} - \rho^{\text{o} f_{i,j,k}}} - \gamma \mathbf{o} f_{i+\frac{1}{2},j,k} \left( D_{i,j,k} - D_{i,j-1,k} \right) \\
\Delta x_{i+\frac{1}{2},j,k} \\
\end{align*} \]
governing equation for one eighth of the block as shown in Figure B.1.

Figure B.1: Meshing scheme for matrix block.

The boundary condition for transport and geomechanics equations of the matrix block is determined from the solution of the reservoir scale model. The phase pressure and the solute concentration in the fractures of the grid block containing the matrix block are used as constant pressure boundary condition for each matrix block. So, every time step of the reservoir scale simulation, we will have a new boundary condition for matrix block and boundary conditions for each matrix block are different. The inner boundary condition for the matrix block is no-flow and no-displacement boundary. When fluids, water and oil, are transported along the fracture, wettability determines which phase is in contact with the matrix block. Since the mass exchange model is simulated for every matrix block in the reservoir, the computational load is very high. A parallelization scheme is used to reduce the simulation time. The matrix block-scale simulation for each grid block is run on different core of a multi-core computer.

B.2.1 Phase Pressure in the Matrix

The solution of the mass transport equation is obtained by refining the grid size on each matrix block. The solution of this equation gives us the saturation of fluid, oil and water, and phase pressures in the rock matrix. The total pressure equation for matrix block is solved for oil phase pressure or water phase pressure depending on the wettability of the
matrix block. For simplicity, the numerical solution of the matrix total pressure equation for water-wetted rock is presented here. The solution of this equation for oil-wetted rock is similar. From the matrix total pressure Equation 4.57 we obtain the algebraic equation as,

\[
M_{xb}^{n+1} + M_{yb}^{n+1} + M_{zf}^{n+1} + M_{zf}^{n+1} = M_{RF}\tag{B.27}
\]

where

\[
M_{xb} = \frac{1}{\Delta x_i,j,k} \left( \frac{k_m \lambda_{om}}{\Delta x} + \frac{k_m \lambda_{wm}}{\Delta x} \right)_{i-\frac{1}{2},j,k}^{n}\tag{B.28}
\]

\[
M_{xf} = \frac{1}{\Delta x_i,j,k} \left( \frac{k_m \lambda_{om}}{\Delta x} + \frac{k_m \lambda_{wm}}{\Delta x} \right)_{i+\frac{1}{2},j,k}^{n}\tag{B.29}
\]

\[
M_{yb} = \frac{1}{\Delta y_i,j,k} \left( \frac{k_m \lambda_{om}}{\Delta y} + \frac{k_m \lambda_{wm}}{\Delta y} \right)_{i,j-\frac{1}{2},k}^{n}\tag{B.30}
\]

\[
M_{yf} = \frac{1}{\Delta y_i,j,k} \left( \frac{k_m \lambda_{om}}{\Delta y} + \frac{k_m \lambda_{wm}}{\Delta y} \right)_{i,j+\frac{1}{2},k}^{n}\tag{B.31}
\]

\[
M_{zb} = \frac{1}{\Delta z_i,j,k} \left( \frac{k_m \lambda_{om}}{\Delta z} + \frac{k_m \lambda_{wm}}{\Delta z} \right)_{i,j,k-\frac{1}{2}}^{n}\tag{B.32}
\]

\[
M_{zf} = \frac{1}{\Delta z_i,j,k} \left( \frac{k_m \lambda_{om}}{\Delta z} + \frac{k_m \lambda_{wm}}{\Delta z} \right)_{i,j,k+\frac{1}{2}}^{n}\tag{B.33}
\]

\[
M_m = -\left\{ M_{xb} + M_{xf} + M_{yb} + M_{yf} + M_{zb} + M_{zf} + \frac{1 - \epsilon_{wm}}{\Delta t_m}[\phi_m c_{tm}]_{i,j,k}^{n} \right\}\tag{B.34}
\]

\[
M_{RF} = \frac{1}{\Delta x_i,j,k} \left\{ \left( \frac{k_m \lambda_{om}}{\Delta x} \right)_{i+\frac{1}{2},j,k}^{n} \left[ p_{\text{cwom}_{i+1,j,k}}^{n+1} - p_{\text{cwom}_{i,j,k}}^{n+1} + \gamma_{i,j,k} (D_{i+1,j,k} - D_{i,j,k}) \right] + \right.\]

\[
-\left. \left( \frac{k_m \lambda_{om}}{\Delta x} \right)_{i-\frac{1}{2},j,k}^{n} \left[ p_{\text{cwom}_{i-1,j,k}}^{n+1} - p_{\text{cwom}_{i,j,k}}^{n+1} + \gamma_{i,j,k} (D_{i,j,k} - D_{i-1,j,k}) \right] \right\}\tag{B.35}
\]

\[
\frac{1}{\Delta y_i,j,k} \left\{ \left( \frac{k_m \lambda_{om}}{\Delta y} \right)_{i,j+\frac{1}{2},k}^{n} \left[ p_{\text{cwom}_{i,j+1,k}}^{n+1} - p_{\text{cwom}_{i,j,k}}^{n+1} + \gamma_{i,j,k} (D_{i,j,k+1} - D_{i,j,k}) \right] - \right.\]

\[
\left. \left( \frac{k_m \lambda_{om}}{\Delta y} \right)_{i,j-\frac{1}{2},k}^{n} \left[ p_{\text{cwom}_{i,j-1,k}}^{n+1} - p_{\text{cwom}_{i,j,k}}^{n+1} + \gamma_{i,j,k} (D_{i,j,k} - D_{i,j,k-1}) \right] \right\}\tag{B.36}
\]

\[
+ \frac{1}{\Delta z_i,j,k} \left\{ \left( \frac{k_m \lambda_{om}}{\Delta z} \right)_{i,j,k+\frac{1}{2}}^{n} \left[ p_{\text{cwom}_{i,j,k+1}}^{n+1} - p_{\text{cwom}_{i,j,k}}^{n+1} + \gamma_{i,j,k} (D_{i,j,k+1} - D_{i,j,k}) \right] - \right.\]

\[
\left. \left( \frac{k_m \lambda_{om}}{\Delta z} \right)_{i,j,k-\frac{1}{2}}^{n} \left[ p_{\text{cwom}_{i,j,k-1}}^{n+1} - p_{\text{cwom}_{i,j,k}}^{n+1} + \gamma_{i,j,k} (D_{i,j,k} - D_{i,j,k-1}) \right] \right\}\tag{B.37}
\]
B.2.2 Phase Saturation in Matrix

Water saturation

Matrix water saturation is calculated from the continuity equation for water phase in the matrix 4.5.1 as,

\[
S_{wm,i,j,k}^{n+1} = (S_{wm})_{i,j,k}^n + \frac{\Delta t_m}{[(1 - \epsilon_{wm}) \phi_m]_{i,j,k}^n} - \frac{\Delta t_m}{[(1 - \epsilon_{wm}) \phi_m]_{i,j,k}^{n-1}}
\]

\[
\begin{align*}
&\left\{ \frac{1}{\Delta x_{i,j,k}} \left\{ \left( \frac{k_m \lambda_{wm}}{\Delta x} \right)^n_{i+\frac{1}{2},j,k} \left[ p_{wm,i+1,j,k}^{n+1} - p_{wm,i,j+1,k}^{n+1} - \gamma_{w,i,j,k} (D_{i+1,j,k} - D_{i,j,k}) \right] \right. \\
&\quad - \left( \frac{k_m \lambda_{wm}}{\Delta x} \right)^n_{i-\frac{1}{2},j,k} \left[ p_{wm,i-1,j,k}^{n+1} - p_{wm,i,j-1,k}^{n+1} - \gamma_{w,i,j,k} (D_{i,j,k} - D_{i-1,j,k}) \right] \right\} \\
&\quad + \frac{1}{\Delta y_{i,j,k}} \left\{ \left( \frac{k_m \lambda_{wm}}{\Delta y} \right)^n_{i,j+\frac{1}{2},k} \left[ p_{wm,i,j+1,k}^{n+1} - p_{wm,i,j,k+1}^{n+1} - \gamma_{w,i,j,k} (D_{i,j,k+1} - D_{i,j,k}) \right] \right. \\
&\quad - \left( \frac{k_m \lambda_{wm}}{\Delta y} \right)^n_{i,j-\frac{1}{2},k} \left[ p_{wm,i,j,k-1}^{n+1} - p_{wm,i,j,k}^{n+1} - \gamma_{w,i,j,k} (D_{i,j,k} - D_{i,j,k-1}) \right] \right\} \\
&\quad + \frac{1}{\Delta z_{i,j,k}} \left\{ \left( \frac{k_m \lambda_{wm}}{\Delta z} \right)^n_{i,j,k+\frac{1}{2}} \left[ p_{wm,i,j+1,k}^{n+1} - p_{wm,i,j,k+1}^{n+1} - \gamma_{w,i,j,k} (D_{i,j,k+1} - D_{i,j,k}) \right] \right. \\
&\quad - \left( \frac{k_m \lambda_{wm}}{\Delta z} \right)^n_{i,j,k-\frac{1}{2}} \left[ p_{wm,i,j,k-1}^{n+1} - p_{wm,i,j,k}^{n+1} - \gamma_{w,i,j,k} (D_{i,j,k} - D_{i,j,k-1}) \right] \right\} \\
\end{align*}
\]
The oil saturation in rock matrix is calculated from water saturation in rock matrix as,

\[ S_{om_{i,j,k}}^{n+1} = 1 - S_{wm_{i,j,k}}^{n+1} \]  \hspace{1cm} (B.37)

### B.2.3 Solute Concentration in Rock Matrix

Solute concentration in rock matrix is calculated from continuity equation for solute in matrix (Equation 4.64) as,

\[
\begin{align*}
\frac{c_{sm_{i,j,k}}^{n+1}}{(1 - \epsilon_{vm})(\phi_m)^n_{i,j,k}} &= \frac{\hat{q}_{sm_{i,j,k}} \Delta t}{S_{wm_{i,j,k}}^{n+1} \rho_w} + \frac{S_{wm_{i,j,k}}^{n+1}}{S_{wm_{i,j,k}}^{n+1}} \\
&+ T_{x_{i,j,k}^{+ \frac{1}{2}}} \left[ p_{wm_{i,j+1,k}}^{n+1} - p_{wm_{i,j,k}}^{n+1} - \gamma_w (D_{i,j,k} - D_{i,j,k}) \right] \\
&- T_{x_{i,j,k}^{- \frac{1}{2}}} \left[ p_{wm_{i,j-1,k}}^{n+1} - p_{wm_{i,j,k}}^{n+1} - \gamma_w (D_{i,j,k} - D_{i,j,k}) \right] \\
&+ T_{y_{i,j,k}^{+ \frac{1}{2}}} \left[ p_{wm_{i+1,j,k}}^{n+1} - p_{wm_{i,j,k}}^{n+1} - \gamma_w (D_{i,j,k} - D_{i,j,k}) \right] \\
&- T_{y_{i,j,k}^{- \frac{1}{2}}} \left[ p_{wm_{i,j-1,k}}^{n+1} - p_{wm_{i,j,k}}^{n+1} - \gamma_w (D_{i,j,k} - D_{i,j,k}) \right] \\
&+ T_{z_{i,j,k}^{+ \frac{1}{2}}} \left[ p_{wm_{i,j,k+1}}^{n+1} - p_{wm_{i,j,k}}^{n+1} - \gamma_w (D_{i,j,k} - D_{i,j,k}) \right] \\
&- T_{z_{i,j,k}^{- \frac{1}{2}}} \left[ p_{wm_{i,j,k-1}}^{n+1} - p_{wm_{i,j,k}}^{n+1} - \gamma_w (D_{i,j,k} - D_{i,j,k}) \right]
\end{align*}
\]

\[ \text{for } i, j, k = 1, 2, \ldots, M_i, M_j, M_k \]
\[ \begin{align*} 
- T_{x_{i+\frac{1}{2},j,k}} & \left[ \frac{\omega RT_m}{V_w \Delta x} \right]^n (c_{sm_{i+1,j,k}}^{n+1} - c_{sm_{i,j,k}}^n) + T_{x_{i-\frac{1}{2},j,k}} \left[ \frac{\omega RT_m}{V_w \Delta x} \right]^n (c_{sm_{i,j,k}}^n - c_{s_{i-1,j,k}}^n) \\
- T_{y_{i,j+\frac{1}{2},k}} & \left[ \frac{\omega RT_m}{V_w \Delta y} \right]^n (c_{sm_{i,j+1,k}}^{n+1} - c_{sm_{i,j,k}}^n) + T_{y_{i,j-\frac{1}{2},k}} \left[ \frac{\omega RT_m}{V_w \Delta y} \right]^n (c_{sm_{i,j,k}}^n - c_{s_{i,j-1,k}}^n) \\
- T_{z_{i,j,k+\frac{1}{2}}} & \left[ \frac{\omega RT_m}{V_w \Delta z} \right]^n (c_{sm_{i,j,k+1}}^{n+1} - c_{sm_{i,j,k}}^n) + T_{z_{i,j,k-\frac{1}{2}}} \left[ \frac{\omega RT_m}{V_w \Delta z} \right]^n (c_{sm_{i,j,k}}^n - c_{s_{i,j,k-1}}^n) \\
- C_x & \left[ \frac{\phi_m D_{eff}^n}{\Delta x} \right]_{i+\frac{1}{2},j,k} (c_{s_{i+1,j,k}}^n - c_{s_{i,j,k}}^n) - \left( \frac{\phi_m D_{eff}^n}{\Delta x} \right)_{i-\frac{1}{2},j,k} (c_{s_{i,j,k}}^n - c_{s_{i-1,j,k}}^n) \\
- C_y & \left[ \frac{\phi_m D_{eff}^n}{\Delta y} \right]_{i,j+\frac{1}{2},k} (c_{s_{i,j+1,k}}^n - c_{s_{i,j,k}}^n) - \left( \frac{\phi_m D_{eff}^n}{\Delta y} \right)_{i,j-\frac{1}{2},k} (c_{s_{i,j,k}}^n - c_{s_{i,j-1,k}}^n) \\
- C_z & \left[ \frac{\phi_m D_{eff}^n}{\Delta z} \right]_{i,j,k+\frac{1}{2}} (c_{s_{i,j,k+1}}^n - c_{s_{i,j,k}}^n) - \left( \frac{\phi_m D_{eff}^n}{\Delta z} \right)_{i,j,k-\frac{1}{2}} (c_{s_{i,j,k}}^n - c_{s_{i,j,k-1}}^n) \quad (B.38) 
\end{align*} \]

where

\[ \begin{align*} 
C_x & = \frac{\Delta t}{(1 - \epsilon_{vm}) \phi_m_{i,j,k} \Delta x_{i,j,k}} \frac{\rho_s}{\rho_w} \\
C_y & = \frac{\Delta t}{(1 - \epsilon_{vm}) \phi_m_{i,j,k} \Delta y_{i,j,k}} \frac{\rho_s}{\rho_w} \\
C_z & = \frac{\Delta t}{(1 - \epsilon_{vm}) \phi_m_{i,j,k} \Delta z_{i,j,k}} \frac{\rho_s}{\rho_w} \\
T_{x_{i+\frac{1}{2},j,k}} & = C_x \left[ c_{sm} \frac{k_m \lambda_{wm}}{\Delta x} \left( \omega + \frac{\rho_w c_{sm}}{\rho_s} \right) \right]_{i+\frac{1}{2},j,k} \quad (B.42) \\
T_{y_{i,j+\frac{1}{2},k}} & = C_y \left[ c_{sm} \frac{k_m \lambda_{wm}}{\Delta y} \left( \omega + \frac{\rho_w c_{sm}}{\rho_s} \right) \right]_{i,j+\frac{1}{2},k} \quad (B.43) \\
T_{z_{i,j,k+\frac{1}{2}}} & = C_z \left[ c_{sm} \frac{k_m \lambda_{wm}}{\Delta z} \left( \omega + \frac{\rho_w c_{sm}}{\rho_s} \right) \right]_{i,j,k+\frac{1}{2}} \quad (B.44) 
\end{align*} \]

**B.2.4 Volume Flux Rate**

The volumetric exchange rate is computed at every time step by calculating the flow rate through the node on the boundary as,
where $A$ is area; $q$ is mass flux rate; $n'$ is the step $n'$ of the reservoir scale simulation.

### B.3 Solution of Geomechanics Equations

The geomechanics equation is solved for every single matrix blocks in the reservoir. The meshing scheme for geomechanics equation is shown in Figure B.1. This meshing scheme simplifies our problem to an 1-D problem. For the sake of completeness, the 3D solution is presented. We solve Equation 4.85 using the following discretized equations:

The finite difference equation for equation of motion in x-direction is:

$$
\begin{align*}
\left\{\begin{array}{l}
d_{wm_{i,j,k}^{n+1}}^{j,k} = A_{1,j,k} \left[ \left( k_{wm} \lambda_{wm} \right)^n_{\frac{i}{2},j,k} \frac{p_{wm_{i,j,k}^{n+1}}^{i+1} - p_{wm_{i,j,k}^{n}}^{i}}{\Delta x_{\frac{1}{2},j,k}} \right] - \left( \frac{k_{wm} \omega}{V_{wm}} RT_m \right)^n_{\frac{i}{2},j,k} \frac{c_{wm_{i,j,k}^{n+1}}^{i+1} - c_{wm_{i,j,k}^{n}}^{i}}{\Delta x_{\frac{1}{2},j,k}} \\
d_{om_{i,j,k}^{n+1}}^{j,k} = A_{1,j,k} \left( k_{om} \lambda_{om} \right)^n_{\frac{i}{2},j,k} \frac{p_{om_{i,j,k}^{n+1}}^{i+1} - p_{om_{i,j,k}^{n}}^{i}}{\Delta x_{\frac{1}{2},j,k}} \\
d_{wm_{i,j,1}^{n+1}}^{j,k} = A_{1,i,k} \left( k_{wm} \lambda_{wm} \right)^n_{i,j,1} \frac{p_{wm_{i,j,1}^{n+1}}^{j+1} - p_{wm_{i,j,1}^{n}}^{j}}{\Delta y_{1,j,k}} \\
d_{om_{i,j,1}^{n+1}}^{j,k} = A_{1,i,k} \left( k_{om} \lambda_{om} \right)^n_{i,j,1} \frac{p_{om_{i,j,1}^{n+1}}^{j+1} - p_{om_{i,j,1}^{n}}^{j}}{\Delta y_{1,j,k}} \\
d_{wm_{i,j,1}^{n+1}}^{j,k} = A_{1,i,j} \left( k_{wm} \lambda_{wm} \right)^n_{i,j,1} \frac{p_{wm_{i,j,1}^{n+1}}^{j+1} - p_{wm_{i,j,1}^{n}}^{j}}{\Delta z_{1,j,k}} \\
d_{om_{i,j,1}^{n+1}}^{j,k} = A_{1,i,j} \left( k_{om} \lambda_{om} \right)^n_{i,j,1} \frac{p_{om_{i,j,1}^{n+1}}^{j+1} - p_{om_{i,j,1}^{n}}^{j}}{\Delta z_{1,j,k}} \\
\end{array}\right. \\
\right.
\end{align*}
(B.45)

where $A$ is area; $q$ is mass flux rate; $n'$ is the step $n'$ of the reservoir scale simulation.
\[ X_{mmm} = -\frac{1}{2\Delta x_{i,j,k}} \left[ \left( \frac{C_{11}}{\Delta x} \right)_{i+\frac{1}{2},j,k} - \left( \frac{C_{11}}{\Delta x} \right)_{i-\frac{1}{2},j,k} \right] - \frac{1}{2\Delta y_{i,j,k}} \left[ \left( \frac{C_{44}}{\Delta y} \right)_{i,j+\frac{1}{2},k} - \left( \frac{C_{44}}{\Delta y} \right)_{i,j-\frac{1}{2},k} \right] \]
\[ - \frac{1}{2\Delta z_{i,j,k}} \left[ \left( \frac{C_{66}}{\Delta z} \right)_{i,j,k+\frac{1}{2}} - \left( \frac{C_{66}}{\Delta z} \right)_{i,j,k-\frac{1}{2}} \right] \]

\[ X_{mm} = \frac{1}{2\Delta x_{i,j,k}} \left( \frac{C_{11}}{\Delta x} \right)_{i+\frac{1}{2},j,k} ; \quad X_{mf} = \frac{1}{2\Delta y_{i,j,k}} \left( \frac{C_{44}}{\Delta y} \right)_{i,j+\frac{1}{2},k} ; \quad X_{mf} = \frac{1}{2\Delta z_{i,j,k}} \left( \frac{C_{66}}{\Delta z} \right)_{i,j,k+\frac{1}{2}} \]

\[ Y_{bmb} = \frac{2 (C_{12})_{i-1,j,k} + (C_{44})_{i,j-1,k}}{2 \left( x_{i+\frac{1}{2},j,k} + x_{i-\frac{1}{2},j,k} \right) \left( y_{i,j+\frac{1}{2},k} + y_{i,j-\frac{1}{2},k} \right)} \]

\[ Y_{fmb} = \frac{-2 (C_{12})_{i-1,j,k} - (C_{44})_{i,j+1,k}}{2 \left( x_{i+\frac{1}{2},j,k} + x_{i-\frac{1}{2},j,k} \right) \left( y_{i,j+\frac{1}{2},k} + y_{i,j-\frac{1}{2},k} \right)} \]

\[ Y_{fmm} = \frac{-2 (C_{13})_{i+1,j,k} + (C_{44})_{i+1,j,k}}{2 \left( x_{i+\frac{1}{2},j,k} + x_{i-\frac{1}{2},j,k} \right) \left( y_{i,j+\frac{1}{2},k} + y_{i,j-\frac{1}{2},k} \right)} \]

\[ Y_{fmb} = \frac{-2 (C_{13})_{i+1,j,k} - (C_{66})_{i,j,k+1}}{2 \left( x_{i+\frac{1}{2},j,k} + x_{i-\frac{1}{2},j,k} \right) \left( y_{i,j+\frac{1}{2},k} + y_{i,j-\frac{1}{2},k} \right)} \]

\[ Y_{fmm} = \frac{2 (C_{13})_{i+1,j,k} + (C_{44})_{i,j+1,k}}{2 \left( x_{i+\frac{1}{2},j,k} + x_{i-\frac{1}{2},j,k} \right) \left( y_{i,j+\frac{1}{2},k} + y_{i,j-\frac{1}{2},k} \right)} \]

\[ R X_{i,j,k} = -\frac{(C_{11}\delta e_{sz})_{i+\frac{1}{2},j,k} - (C_{11}\delta e_{sz})_{i-\frac{1}{2},j,k}}{\Delta x_{i,j,k}} \]
\[ + \frac{(C_{12}\delta e_{sy})_{i+\frac{1}{2},j,k} - (C_{12}\delta e_{sy})_{i-\frac{1}{2},j,k}}{\Delta x_{i,j,k}} \]

\[ - \frac{(\alpha_{xx})_{i,j,k}}{\Delta x} \left[ \delta p_{w,m,i+\frac{1}{2},j,k} - \delta p_{w,m,i-\frac{1}{2},j,k} + \delta (S_{o,m,p}c_{wom})_{i+\frac{1}{2},j,k} - \delta (S_{o,m,p}c_{wom})_{i-\frac{1}{2},j,k} \right] \]
\[ - \frac{(\alpha_{yy})_{i,j,k}}{\Delta y} \left[ \delta p_{w,m,i,j+\frac{1}{2},k} - \delta p_{w,m,i,j-\frac{1}{2},k} + \delta (S_{o,m,p}c_{wom})_{i,j+\frac{1}{2},k} - \delta (S_{o,m,p}c_{wom})_{i,j-\frac{1}{2},k} \right] \]
The finite difference equation for equation of motion in y-direction is:

\[
X_{bmm}\delta u_{z_{i-1,j-1,k}} + X_{ffm}\delta u_{z_{i+1,j+1,k}} + X_{fwm}\delta u_{z_{i-1,j+1,k}} + X_{bfm}\delta u_{z_{i+1,j-1,k}} + Y_{mmm}\delta u_{y_{i,j-1,k}} + Y_{fmm}\delta u_{y_{i,j+1,k}} + Y_{mmb}\delta u_{y_{i,j+1,k}} + Y_{fmm}\delta u_{y_{i-1,j,k}} + Y_{mmb}\delta u_{y_{i,j-1,k}} + Z_{mbb}\delta u_{z_{i,j-1,k}} + Z_{mfb}\delta u_{z_{i,j+1,k}} + Z_{mff}\delta u_{z_{i,j-1,k}} + 1 = RY_{i,j,k}
\]  

(B.57)

where:

\[
X_{bbl} = \frac{(C_{44})_{i-1,j,k} + 2(C_{21})_{i,j-1,k}}{2(\Delta x_{i+\frac{1}{2},j,k} + \Delta x_{i-\frac{1}{2},j,k})(\Delta y_{i,j+\frac{1}{2},k} + \Delta y_{i,j-\frac{1}{2},k})}
\]  

(B.58)

\[
X_{bbl} = \frac{(C_{44})_{i-1,j,k} + 2(C_{21})_{i,j-1,k}}{2(\Delta x_{i+\frac{1}{2},j,k} + \Delta x_{i-\frac{1}{2},j,k})(\Delta y_{i,j+\frac{1}{2},k} + \Delta y_{i,j-\frac{1}{2},k})}
\]  

(B.59)

\[
X_{ffm} = \frac{(C_{44})_{i+1,j,k} + 2(C_{21})_{i,j+1,k}}{2(\Delta x_{i+\frac{1}{2},j,k} + \Delta x_{i-\frac{1}{2},j,k})(\Delta y_{i,j+\frac{1}{2},k} + \Delta y_{i,j-\frac{1}{2},k})}
\]  

(B.60)

\[
X_{fwm} = \frac{-(C_{44})_{i+1,j,k} - 2(C_{21})_{i,j-1,k}}{2(\Delta x_{i+\frac{1}{2},j,k} + \Delta x_{i-\frac{1}{2},j,k})(\Delta y_{i,j+\frac{1}{2},k} + \Delta y_{i,j-\frac{1}{2},k})}
\]  

(B.61)

\[
X_{bfm} = \frac{(C_{21})_{i,j+1,k} - 2(C_{44})_{i-1,j,k}}{2(\Delta x_{i+\frac{1}{2},j,k} + \Delta x_{i-\frac{1}{2},j,k})(\Delta y_{i,j+\frac{1}{2},k} + \Delta y_{i,j-\frac{1}{2},k})}
\]  

(B.62)

\[
Y_{bmm} = \frac{1}{2\Delta x_{i,j,k}} \left( \frac{C_{44}}{\Delta x} \right)_{i-\frac{1}{2},j,k}; \quad Y_{fmm} = \frac{1}{2\Delta x_{i,j,k}} \left( \frac{C_{44}}{\Delta x} \right)_{i+\frac{1}{2},j,k}; \quad Y_{mbm} = \frac{1}{2\Delta z_{i,j,k}} \left( \frac{C_{22}}{\Delta y} \right)_{i-\frac{1}{2},j,k}
\]  

(B.63)

\[
Y_{mmm} = -\frac{1}{2\Delta x_{i,j,k}} \left[ \left( \frac{C_{44}}{\Delta x} \right)_{i+\frac{1}{2},j,k} - \left( \frac{C_{44}}{\Delta x} \right)_{i-\frac{1}{2},j,k} \right] - \frac{1}{\Delta y_{i,j,k}} \left[ \left( \frac{C_{22}}{\Delta y} \right)_{i,j+\frac{1}{2},k} - \left( \frac{C_{22}}{\Delta y} \right)_{i,j-\frac{1}{2},k} \right]
\]

\[
- \frac{1}{2\Delta z_{i,j,k}} \left[ \left( \frac{C_{55}}{\Delta z} \right)_{i,j,k+\frac{1}{2}} - \left( \frac{C_{55}}{\Delta z} \right)_{i,j,k-\frac{1}{2}} \right]
\]

(B.64)
\[ Y_{mf} = \frac{1}{2\Delta y_{i,j,k}} \left( \frac{C_{22}}{\Delta y} \right)_{i,j\pm \frac{1}{2},k} ; \quad Y_{mm} = \frac{1}{2\Delta z_{i,j,k}} \left( \frac{C_{55}}{\Delta z} \right)_{i,j,k}^{\pm \frac{1}{2}} ; \quad Y_{mmb} = \frac{1}{2\Delta z_{i,j,k}} \left( \frac{C_{55}}{\Delta z} \right)_{i,j,k}^{\pm \frac{1}{2}} \quad (B.65) \]

\[ Z_{mbb} = \frac{(C_{23})_{i,j-1,k} - (C_{55})_{i,j,k-1}}{2 \left( \Delta y_{i\pm \frac{1}{2},j,k} + \Delta y_{i-\frac{1}{2},j,k} \right) \left( \Delta z_{i,j,k} + \frac{1}{2} \Delta z_{i,j,k-\frac{1}{2}} \right)} \quad (B.66) \]

\[ Z_{mfb} = \frac{-(C_{23})_{i,j+1,k} - (C_{55})_{i,j,k-1}}{2 \left( \Delta y_{i\pm \frac{1}{2},j,k} + \Delta y_{i-\frac{1}{2},j,k} \right) \left( \Delta z_{i,j,k} + \frac{1}{2} \Delta z_{i,j,k-\frac{1}{2}} \right)} \quad (B.67) \]

\[ Z_{mbf} = \frac{-2(C_{23})_{i,j-1,k} - (C_{55})_{i,j,k+1}}{2 \left( \Delta y_{i\pm \frac{1}{2},j,k} + \Delta y_{i-\frac{1}{2},j,k} \right) \left( \Delta z_{i,j,k} + \frac{1}{2} \Delta z_{i,j,k-\frac{1}{2}} \right)} \quad (B.68) \]

\[ Z_{mff} = \frac{2(C_{23})_{i,j+1,k} + (C_{55})_{i,j,k+1}}{2 \left( \Delta y_{i\pm \frac{1}{2},j,k} + \Delta y_{i-\frac{1}{2},j,k} \right) \left( \Delta z_{i,j,k} + \frac{1}{2} \Delta z_{i,j,k-\frac{1}{2}} \right)} \quad (B.69) \]

\[ RY_{i,j,k} = -\frac{(C_{21} \delta \epsilon_{xx})_{i,j\pm \frac{1}{2},k} - (C_{21} \delta \epsilon_{xx})_{i,j\pm \frac{1}{2},k}}{\Delta y_{i,j,k}} \left( C_{22} \delta \epsilon_{sy} \right)_{i,j\pm \frac{1}{2},k}^{\pm \frac{1}{2},k} - \frac{(C_{23} \delta \epsilon_{sz})_{i,j\pm \frac{1}{2},k} - (C_{23} \delta \epsilon_{sz})_{i,j\pm \frac{1}{2},k}}{\Delta y_{i,j,k}} \frac{(C_{22} \delta \epsilon_{sy})_{i,j\pm \frac{1}{2},k} - (C_{22} \delta \epsilon_{sy})_{i,j\pm \frac{1}{2},k}}{\Delta y_{i,j,k}} \begin{array}{c} \delta \rho_{w,mi\pm \frac{1}{2},j,k} - \delta \rho_{w,mi\pm \frac{1}{2},j,k} + \delta (S_{omPcwom})_{i\pm \frac{1}{2},j,k} - \delta (S_{omPcwom})_{i\pm \frac{1}{2},j,k} \\ \delta \rho_{w,mi\pm \frac{1}{2},j,k} - \delta \rho_{w,mi\pm \frac{1}{2},j,k} + \delta (S_{omPcwom})_{i\pm \frac{1}{2},j,k} - \delta (S_{omPcwom})_{i\pm \frac{1}{2},j,k} \end{array} \right) \] \quad (B.70)

The finite difference equation for equation of motion in z-direction is:

\[ X_{bmb} \delta u_{z_{i-1,j,k}} + X_{bmb} \delta u_{z_{i-1,j,k+1}} + X_{fmb} \delta u_{z_{i+1,j,k}} + X_{fmb} \delta u_{z_{i+1,j,k+1}} + Y_{mbb} \delta u_{y_{i-1,j,k}} \]
\[ + Y_{mbf} \delta u_{y_{i,j-1,k+1}} + Y_{mbf} \delta u_{y_{i,j+1,k}} + Y_{mbf} \delta u_{y_{i,j+1,k+1}} + Z_{mbm} \delta u_{z_{i-1,j,k}} + Z_{mbm} \delta u_{z_{i+1,j,k}} \]
\[ + Z_{mbm} \delta u_{z_{i,j-1,k}} + Z_{mbm} \delta u_{z_{i,j+1,k}} + Z_{bmm} \delta u_{z_{i,j-1,k}} + Z_{bmm} \delta u_{z_{i,j-1,k}} + Z_{mbm} \delta u_{z_{i,j,1,k}} + Z_{mbm} \delta u_{z_{i,j,1,k}} = RZ_{i,j,k} \quad (B.71) \]

where:

\[ X_{bmb} = \frac{(C_{66})_{i+1,j,k} + 2(C_{31})_{i,j,k-1}}{2 \left( \Delta x_{i\pm \frac{1}{2},j,k} + \Delta x_{i-\frac{1}{2},j,k} \right) \left( \Delta x_{i,j,k} + \frac{1}{2} \Delta x_{i,j,k-\frac{1}{2}} \right)} \quad (B.72) \]

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\[ X_{bm} = \frac{(C_{66})_{i,j} - (C_{31})_{i,j}}{2 \left( \Delta x_{i,j} + \Delta z_{i,j} \right) \left( \Delta z_{i,j} + \Delta z_{i,j} \right)} \]  

\[ X_{fm} = \frac{(C_{66})_{i,j} + (C_{31})_{i,j}}{2 \left( \Delta x_{i,j} + \Delta z_{i,j} \right) \left( \Delta z_{i,j} + \Delta z_{i,j} \right)} \]  

\[ Y_{mb} = \frac{(C_{55})_{i,j} - (C_{32})_{i,j}}{2 \left( \Delta y_{i,j} + \Delta z_{i,j} \right) \left( \Delta z_{i,j} + \Delta z_{i,j} \right)} \]  

\[ Y_{mf} = \frac{(C_{55})_{i,j} + (C_{32})_{i,j}}{2 \left( \Delta y_{i,j} + \Delta z_{i,j} \right) \left( \Delta z_{i,j} + \Delta z_{i,j} \right)} \]  

\[ Z_{bm} = \frac{1}{2 \Delta x_{i,j} \left( \frac{C_{55}}{\Delta y} \right)_{i,j}} \quad \text{;} \quad Z_{fm} = \frac{1}{2 \Delta x_{i,j} \left( \frac{C_{66}}{\Delta x} \right)_{i,j}} \quad \text{;} \quad Z_{mb} = \frac{1}{2 \Delta y_{i,j} \left( \frac{C_{55}}{\Delta y} \right)_{i,j}} \]  

\[ Z_{mf} = \frac{1}{2 \Delta y_{i,j} \left( \frac{C_{55}}{\Delta y} \right)_{i,j}} \quad \text{;} \quad Z_{mm} = \frac{1}{2 \Delta z_{i,j} \left( \frac{C_{33}}{\Delta z} \right)_{i,j}} \quad \text{;} \quad Z_{mf} = \frac{1}{2 \Delta z_{i,j} \left( \frac{C_{33}}{\Delta z} \right)_{i,j}} \]  

\[ Z_{m} = \frac{1}{2 \Delta x_{i,j} \left[ \left( \frac{C_{66}}{\Delta x} \right)_{i,j} - \left( \frac{C_{66}}{\Delta x} \right)_{i,j} \right] - \frac{1}{2 \Delta y_{i,j} \left[ \left( \frac{C_{55}}{\Delta y} \right)_{i,j} - \left( \frac{C_{55}}{\Delta y} \right)_{i,j} \right] - \frac{1}{2 \Delta z_{i,j} \left[ \left( \frac{C_{33}}{\Delta z} \right)_{i,j} - \left( \frac{C_{33}}{\Delta z} \right)_{i,j} \right]} \]  

\[ RZ_{i,j} = \frac{(C_{21} \delta \epsilon_{ex})_{i,j} - (C_{21} \delta \epsilon_{ex})_{i,j}}{\Delta z_{i,j}} \]
\[
\begin{align*}
&\frac{(C_{22}\delta\varepsilon_{xy})_{i,j,k+\frac{1}{2}} - (C_{22}\delta\varepsilon_{xy})_{i,j,k-\frac{1}{2}}}{\Delta z_{i,j,k}} - \frac{(C_{23}\delta\varepsilon_{sz})_{i,j,k+\frac{1}{2}} - (C_{23}\delta\varepsilon_{sz})_{i,j,k-\frac{1}{2}}}{\Delta z_{i,j,k}} \\
&= \frac{-\left(\alpha_{xz}\right)_{i,j,k}}{\Delta x} \left[\delta p_{w,m_{i+\frac{1}{2},j,k}} - \delta p_{w,m_{i-\frac{1}{2},j,k}} + \delta (S_{o,m_{p_{cwom}}})_{i+\frac{1}{2},j,k} - \delta (S_{o,m_{p_{cwom}}})_{i-\frac{1}{2},j,k}\right] \\
&+ \frac{-\left(\alpha_{yz}\right)_{i,j,k}}{\Delta y} \left[\delta p_{w,m_{i,j+\frac{1}{2},k}} - \delta p_{w,m_{i,j-\frac{1}{2},k}} + \delta (S_{o,m_{p_{cwom}}})_{i,j+\frac{1}{2},k} - \delta (S_{o,m_{p_{cwom}}})_{i,j-\frac{1}{2},k}\right] \\
&+ \frac{-\left(\alpha_{zz}\right)_{i,j,k}}{\Delta z} \left[\delta p_{w,m_{i,j,k+\frac{1}{2}}} - \delta p_{w,m_{i,j,k-\frac{1}{2}}} + \delta (S_{o,m_{p_{cwom}}})_{i,j,k+\frac{1}{2}} - \delta (S_{o,m_{p_{cwom}}})_{i,j,k-\frac{1}{2}}\right]
\end{align*}
\] (B.82)

The staggered grid system is used in the numerical solution. The flow related variables such as phase pressure \((p_{n+1}^{i,j,k})\) and phase saturation \((S_{n+1}^{i,j,k})\) are obtained at the center of the grid cells. While the geomechanical related variables \((\delta u_{n+1}^{x_{i,j,k}}, \delta u_{n+1}^{y_{i,j,k}}, \delta u_{n+1}^{z_{i,j,k}})\) are obtained at the edge of the node. No displacement is considered for the grid block at the center of the matrix block. The pressure at the boundary of the matrix block is considered to be constant at every time step of the reservoir scale simulation. The effective stress acting on the outer boundary node of the matrix block is constant and equal to the fracture pressure. Since two phases, water and oil, co-exist in the fracture, an average fracture pressure equation is used. Hence, the outer condition is written in the incremental form as,

\[
\begin{align*}
\delta\sigma_{m,effect}\left[\begin{array}{c}
\frac{\partial u_{x}}{\partial x}
+ (C_{11}\delta\varepsilon_{x} + C_{12}\delta\varepsilon_{sy} + C_{13}\delta\varepsilon_{sz}) = \delta p_{f} = \delta (S_{o,f}p_{o} + S_{w,f}p_{w}) \\
\frac{\partial u_{y}}{\partial y}
+ (C_{21}\delta\varepsilon_{x} + C_{22}\delta\varepsilon_{sy} + C_{23}\delta\varepsilon_{sz}) = \delta p_{f} = \delta (S_{o,f}p_{o} + S_{w,f}p_{w}) \\
\frac{\partial u_{z}}{\partial z}
+ (C_{31}\delta\varepsilon_{x} + C_{32}\delta\varepsilon_{sy} + C_{33}\delta\varepsilon_{sz}) = \delta p_{f} = \delta (S_{o,f}p_{o} + S_{w,f}p_{w})
\end{array}\right]
\end{align*}
\] (B.83)

This boundary conditions can be written in the discretized equation as,

x-direction:

\[
\begin{align*}
\frac{(C_{11})}{\Delta x} \left(\delta u_{n+1}^{x_{2,j,k}} - \delta u_{n+1}^{x_{1,j,k}}\right) + \frac{(C_{12})}{\Delta y} \left(\delta u_{n+1}^{y_{1,j+1,k}} - \delta u_{n+1}^{y_{1,j,k}}\right) + \\
\frac{(C_{13})}{\Delta z} \left(\delta u_{n+1}^{z_{1,j,k+1}} - \delta u_{n+1}^{z_{1,j,k}}\right) + (C_{11}\delta\varepsilon_{x} + C_{12}\delta\varepsilon_{sy} + C_{13}\delta\varepsilon_{sz})_{1,j,k} = \delta p_{f_{1,j,k}}
\end{align*}
\] (B.84)
y-direction:

\[
\left( \frac{C_{21}}{\Delta x} \right)_{i+\frac{1}{2},1,k} \left( \delta u_{x(i+1,k)}^{n+1} - \delta u_{x,i,k}^{n+1} \right) + \left( \frac{C_{22}}{\Delta y} \right)_{i,\frac{3}{2},k} \left( \delta u_{y,2,k}^{n+1} - \delta u_{y,i,k}^{n+1} \right) +
\left( \frac{C_{23}}{\Delta z} \right)_{i,1,k+\frac{1}{2}} \left( \delta u_{z,i,k+1}^{n+1} - \delta u_{z,i,k}^{n+1} \right) + (C_{21}\delta \epsilon_{sx} + C_{22}\delta \epsilon_{sy} + C_{23}\delta \epsilon_{sz})_{i,1,k} = \delta p_{f,i,k} \tag{B.85}
\]

z-direction:

\[
\left( \frac{C_{31}}{\Delta x} \right)_{i+\frac{1}{2},j,1} \left( \delta u_{x(i+1,j)}^{n+1} - \delta u_{x,i,j}^{n+1} \right) + \left( \frac{C_{32}}{\Delta y} \right)_{i,j+\frac{1}{2},k} \left( \delta u_{y,j+1,k}^{n+1} - \delta u_{y,i,j,k}^{n+1} \right) +
\left( \frac{C_{33}}{\Delta z} \right)_{i,j,\frac{3}{2}} \left( \delta u_{z,i,j,2} - \delta u_{z,i,j,1} \right) + (C_{31}\delta \epsilon_{sx} + C_{32}\delta \epsilon_{sy} + C_{33}\delta \epsilon_{sz})_{i,j,1} = \delta \bar{p}_{f,i,j,1} \tag{B.86}
\]
APPENDIX C - NUMERICAL SOLUTION VALIDATION

The numerical code was validated using the analytical solution for fluid flow simulation and geomechanical simulation. Fluid flow numerical code is validated against the analytical solution of fluid flow in hydraulically fractured reservoir and 1-D Buckley Leverett displacement of Newtonian fluid. Coupled fluid flow and geomechanics numerical code was validated against the analytical solution of 1-D consolidation.

C.1 Single Phase Flow in a Hydraulically Fractured Well

Fluid flow in reservoir numerical code is validated against the analytical solution of single phase flow in a hydraulically fractured well presented by Gringarten et al. (1974). In this problem, the wellbore with a vertical fracture totally penetrating a horizontal, homogeneous, and isotropic reservoir initially at constant pressure is produced at constant rate. Gringarten et al. (1974) derived an equation for the dimensionless pressure at the wellbore as,

\[
p_D = \sqrt{\pi t_D}
\]

(C.1)

where dimensionless pressure \(p_D\) and dimensionless time \(t_D\), are defined as,

\[
\begin{align*}
  p_D &= \frac{k_m h \Delta p}{2 \pi q u B} \\
  t_D &= \frac{k_m l}{\phi c \mu x_f^2}
\end{align*}
\]

(C.2)

where \(\Delta p\) is pressure drop.

The input parameters in Table C.1 are used for numerical simulation. The results given in Figure C.1 confirm the accuracy of the numerical solution for fluid flow.

C.2 1-D Buckley Leverett Displacement

The numerical code is validated against the analytical solution of 1-D Buckley Leverett displacement of Newtonian fluid in porous media. The input parameters used in the simulation are summarized in Table C.2. The results given in Figure C.2 again confirm the accuracy of the numerical solution for fluid flow.
Figure C.1: Comparison between the numerical results and the analytical solution for single phase fluid flow in hydraulically fractured well.

Table C.1: Input parameters used in the model for single phase flow in a hydraulically fractured well

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
<th>Unit</th>
<th>Parameter</th>
<th>Value</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>Reservoir thickness ((h))</td>
<td>200</td>
<td>ft</td>
<td>Compressibility ((c_t))</td>
<td>6 x 10^{-6}</td>
<td>psi^{-1}</td>
</tr>
<tr>
<td>Initial pressure ((p_i))</td>
<td>5000</td>
<td>psi</td>
<td>Viscosity ((\mu))</td>
<td>0.3</td>
<td>cp</td>
</tr>
<tr>
<td>Production rate ((q))</td>
<td>10</td>
<td>bbl/day</td>
<td>Porosity ((\phi))</td>
<td>0.06</td>
<td>-</td>
</tr>
<tr>
<td>Fracture half-length ((x_f))</td>
<td>505</td>
<td>ft</td>
<td>Permeability ((k_m))</td>
<td>0.05</td>
<td>md</td>
</tr>
</tbody>
</table>

Table C.2: Input parameter used in Buckley Leverett displacement simulation

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
<th>Unit</th>
<th>Parameter</th>
<th>Value</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>Grid size ((\Delta x, \Delta y, \Delta z))</td>
<td>200x5x5</td>
<td>ft^{3}</td>
<td>Initial pressure ((p_i))</td>
<td>5000</td>
<td>psi</td>
</tr>
<tr>
<td>Reservoir dimension</td>
<td>200x5x5</td>
<td>ft^{3}</td>
<td>Production pressure</td>
<td>5000</td>
<td>psi</td>
</tr>
<tr>
<td>Inclination angle</td>
<td>0</td>
<td>deg.</td>
<td>Compressibility ((c_t))</td>
<td>0</td>
<td>psi^{-1}</td>
</tr>
<tr>
<td>Permeability ((k_m))</td>
<td>1000</td>
<td>md</td>
<td>Oil viscosity ((\mu_o))</td>
<td>2.4</td>
<td>cp</td>
</tr>
<tr>
<td>(k_{or}^*(S_{or}))</td>
<td>0.75</td>
<td>-</td>
<td>Water viscosity ((\mu_w))</td>
<td>0.6</td>
<td>cp</td>
</tr>
<tr>
<td>(k_{wr}^*(S_{wr}))</td>
<td>0.75</td>
<td>-</td>
<td>Porosity ((\phi))</td>
<td>0.15</td>
<td>-</td>
</tr>
<tr>
<td>(S_{wr}, S_{or})</td>
<td>0.2</td>
<td>-</td>
<td>Injection Rate</td>
<td>30.5</td>
<td>ft^{3}/day</td>
</tr>
<tr>
<td>(n_o, n_w)</td>
<td>2</td>
<td>-</td>
<td>Oil density</td>
<td>48</td>
<td>lbm/ft^{3}</td>
</tr>
<tr>
<td>Initial water saturation</td>
<td>0.2</td>
<td>-</td>
<td>Water density</td>
<td>63</td>
<td>lbm/ft^{3}</td>
</tr>
</tbody>
</table>
C.3 1-D Consolidation

The geomechanics model is validated against the analytical solution of 1-D consolidation problem by Jaeger et al. (2007) for comparison. In this problem, a porous column is fully saturated with fluid and is subjected to a constant axial load as shown in Figure C.3. The loaded stress instantaneously induces the rock deformation and pore pressure increase in the column. Fluid is allowed to drain out of the column from top and the pore pressure increase is allowed to dissipate. An analytical solution (Jaeger et al. 2007) for the dissipation of pore pressure increase is used to verify the numerical results. As the result of axial stress, the pore pressure increases along the porous column. Pressure profile along the porous column can be calculated as,

\[
p(z, t) = p_o \sum_{n=1,3,5,\ldots}^{\infty} \frac{4}{n\pi} \sin \left( \frac{n\pi z}{2h} \right) \exp \left( -\frac{n^2\pi^2 k_m t}{4\mu s h^2} \right) \tag{C.3}
\]

where \( h \) is porous column height; \( k_m \) is permeability; \( \mu \) is fluid viscosity; \( z \) is position; \( t \) is time. Storage coefficient \( (S) \) and incremental pressure \( (p_o) \) are calculated as,

\[
\begin{align*}
S &= \frac{1}{M} + \frac{\alpha^2}{\lambda + 2G} \\
p_o &= \frac{\alpha M \sigma_{ax}}{\lambda + 2G + \alpha^2 M}
\end{align*}
\tag{C.4}
\]
where $\alpha$ is the Biot coefficient; $M$ is Biot modulus; $\sigma_{ax}$ is the loading stress at the top of the column.

The pore pressure increase quickly vanishes due to fluid drainage and finally the pore pressure in the column returns to the initial values.

The input data is presented in Table C.3 show that the normalized pressure predicted agrees well with the analytical solution. The modeling results for displacement at the top of the column is shown in Figure C.3. The results confirm the accuracy of the numerical code for coupled geomechanics and fluid flow.

Table C.3: Input for 1-D consolidation

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
<th>Unit</th>
<th>Parameter</th>
<th>Value</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>Grid size</td>
<td>1x1x200</td>
<td>-</td>
<td>Compressibility ($c_t$)</td>
<td>$2.2 \times 10^{-6}$</td>
<td>psi$^{-1}$</td>
</tr>
<tr>
<td>Reservoir thickness ($h$)</td>
<td>328</td>
<td>ft</td>
<td>Viscosity ($\mu$)</td>
<td>0.89</td>
<td>cp</td>
</tr>
<tr>
<td>Initial pressure ($p_i$)</td>
<td>0</td>
<td>psi</td>
<td>Porosity ($\phi$)</td>
<td>0.15</td>
<td>-</td>
</tr>
<tr>
<td>Young modulus</td>
<td>$2 \times 10^6$</td>
<td>psi</td>
<td>Applied stress</td>
<td>1000</td>
<td>psi</td>
</tr>
<tr>
<td>Poisson’s ratio</td>
<td>0.21</td>
<td>-</td>
<td>Permeability ($k_m$)</td>
<td>100</td>
<td>md</td>
</tr>
<tr>
<td>Fluid compressibility</td>
<td>$6 \times 10^{-6}$</td>
<td>psi$^{-1}$</td>
<td>Biot’s coefficient</td>
<td>0.71</td>
<td>-</td>
</tr>
</tbody>
</table>

Figure C.3: A comparison of the numerical results and analytical solution for 1D compaction.
D.1 Permeability Averaging

For pore and matrix block, often two consecutive grids have different permeability. The permeability of the boundary need to be calculated from the permeability of the two consecutive grids. The average permeability equations for pore and the matrix are presented in this section.

D.1.1 Permeability Averaging for Pore Scale Modeling

Permeability averaging is needed since the dimensions of the grid cells vary along the geometry and the permeability is calculated on the boundary of the node.

\[ Q = -A \frac{k}{\mu} \frac{\partial p}{\partial z} \Rightarrow \Delta p = 8 \int_{x_i}^{x_{i+1}} \frac{-\mu Q}{\pi r^4} dz \]  
\[ (D.1) \]

where \( r \) can be calculated as (see Figure D.1),

\[ r = \frac{D_i}{2} - \frac{D_i - D_{i+1}}{2L} z \]  
\[ (D.2) \]

![Figure D.1: Permeability averaging.](image)

We obtain the equation for pressure drop as,
\[ \Delta p = \frac{8Q\mu}{\pi} \int_{x_i}^{x_{i+1}} \frac{-1}{\left( \frac{D_i}{2} - \frac{D_i - D_{i+1}}{2L} z \right)^4} dz = \frac{128}{3\pi} \frac{\mu Q L}{D_i - D_{i+1}} \left( \frac{1}{D_{i+1}^3} - \frac{1}{D_i^3} \right) \quad (D.3) \]

The pressure drop can be calculated using average permeability \( k_{i+\frac{1}{2}} \) as,

\[ Q = -A_{i+\frac{1}{2}} \frac{k_{i+\frac{1}{2}}}{\mu} \Delta p \Rightarrow \Delta p = -\frac{Q L \mu}{k_{i+\frac{1}{2}} A_{i+\frac{1}{2}}} = -\frac{16QL\mu}{k_{i+\frac{1}{2}} \pi (D_i + D_{i+1})^2} \quad (D.4) \]

Then the averaged permeability can be calculated as,

\[ k_{i+\frac{1}{2}} = \frac{3}{8} \frac{D_i^3 D_{i+1}^3}{[D_i^2 + D_i D_{i+1} + D_{i+1}^2]} (D_i + D_{i+1})^2 \quad (D.5) \]

**D.1.2 Permeability Averaging for Matrix Block**

We consider two blocks next to each other with permeabilities \( k_i \) and \( k_{i+1} \) and the lengths \( \Delta x_i \) and \( \Delta x_{i+1} \). The area of the cross section is \( A = h^2 = (L - 2x)^2 \). Substituting this into equation for pressure, we obtain:

\[ Q = -A \frac{k}{\mu} \frac{\partial p}{\partial x} = -(L - 2x)^2 \frac{k}{\mu} \frac{\partial p}{\partial x} \Rightarrow \Delta p = \frac{Q\mu}{k} \frac{\Delta x}{L (L - 2\Delta x)} \quad (D.6) \]

Pressure drop between along the two consecutive blocks is:

\[ \Delta p = \frac{Q\mu}{k_a} \frac{\Delta x_i + \Delta x_{i+1}}{L (L - 2\Delta x_i - 2\Delta x_{i+1})} = \Delta p_i + \Delta p_{i+1} \quad (D.7) \]

Then, we obtain the equation for average permeability as,

\[ k_a = \frac{(\Delta x_i + \Delta x_{i+1}) k_i k_{i+1} (L - 2\Delta x_i)}{\Delta x_i k_{i+1} (L - 2\Delta x_i - 2\Delta x_{i+1}) + \Delta x_{i+1} k_i L} \]

**D.2 Relative Permeability**

The relative permeability equation of the oil and the water phases in the fracture and the matrix are specified based on the Corey model as follows:

For the water phase in the fractures:
\[
\begin{cases}
k_{rwf} = 0, & \text{if } S_{wf} < S_{wrf} \\
k_{rwf} = k_{rwf}^* \left( \frac{S_{wf}-S_{wrf}}{1-S_{orf}-S_{wrf}} \right)^{n_{wf}}, & \text{if } S_{wrf} < S_{wf} < 1 - S_{orf} \\
k_{rwf} = k_{rwf}^*, & \text{if } S_{wf} > 1 - S_{orf}
\end{cases}
\] (D.8)

For the oil phase in the fractures:

\[
\begin{cases}
k_{rof} = 0, & \text{if } S_{of} < S_{orf} \\
k_{rof} = k_{rof}^* \left( \frac{S_{of}-S_{orf}}{1-S_{orf}-S_{wrf}} \right)^{n_{of}}, & \text{if } S_{orf} < S_{of} < 1 - S_{orf} \\
k_{rof} = k_{rof}^*, & \text{if } S_{of} > 1 - S_{orf}
\end{cases}
\] (D.9)

For the water phase in the rock matrix:

\[
\begin{cases}
k_{rwm} = 0, & \text{if } S_{wm} < S_{wrm} \\
k_{rwm} = k_{rwm}^* \left( \frac{S_{wm}-S_{wrm}}{1-S_{orm}-S_{wrm}} \right)^{n_{wm}}, & \text{if } S_{wrm} < S_{wm} < 1 - S_{orm} \\
k_{rwm} = k_{rwm}^*, & \text{if } S_{wm} > 1 - S_{orm}
\end{cases}
\] (D.10)

For the oil phase in the rock matrix:

\[
\begin{cases}
k_{rom} = 0, & \text{if } S_{om} < S_{orm} \\
k_{rom} = k_{rom}^* \left( \frac{S_{om}-S_{orm}}{1-S_{orm}-S_{wrm}} \right)^{n_{om}}, & \text{if } S_{orm} < S_{om} < 1 - S_{orm} \\
k_{rom} = k_{rom}^*, & \text{if } S_{om} > 1 - S_{orm}
\end{cases}
\] (D.11)

D.3 Capillary Pressure

The capillary pressure in the fracture is specified as follows:

\[
\begin{cases}
p_{cwof}(S_{w,f}) = p_{cwof}(S_{wrf}), & \text{if } S_{wrf} < S_{w,f} \\
p_{cwof}(S_{w,f}) = \alpha_f \ln \left( \frac{1-S_{orf}-S_{wrf}}{S_{w,f}-S_{wrf}+0.0001} \right), & \text{if } S_{wrf} < S_{w,f} < 1 - S_{orf} \\
p_{cwof}(S_{w,f}) = 0, & \text{if } S_{w,f} > 1 - S_{orf}
\end{cases}
\] (D.12)

The capillary pressure in the matrix is specified as follows:
\[
\begin{cases}
p_{cwom}(S_{w,m}) = p_{cwof}(S_{wrm}), & \text{if } S_{wm} < S_{wrm} \\
p_{cwom}(S_{w,m}) = \alpha_m 1n \left( \frac{1-S_{wmx}-S_{orm}}{S_{w,m}-S_{wrm}+0.0001} \right), & \text{if } S_{w,xm} < S_{wm} < 1 - S_{orm} \\
p_{cwom}(S_{w,m}) = \alpha_m 2n \left( \frac{1-S_{wmx}-S_{wrm}}{1-S_{w,m}-S_{orm}+0.0001} \right), & \text{if } S_{w,xm} > S_{wm} > S_{wrm}
\end{cases}
\]

where

\[S_{wmx} = 1 - S_{omx}\]  \hspace{1cm} (D.14)

\[\alpha_{m2} = -\frac{S_{wmx} - S_{wrm}}{1 - S_{wmx} - S_{orm}} \alpha_{m1}\]  \hspace{1cm} (D.15)