A SIMULATION STUDY OF INJECTED CO₂ MIGRATION IN THE FAULTED RESERVOIR

by

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IN THE FAULTED RESERVOIR

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ABSTRACT

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The injection and underground storage of carbon dioxide, CO₂, can reduce anthropogenic (human-generated) emissions of greenhouse gases into the atmosphere. Accordingly, the CO₂ sequestration into a deep saline aquifer is a subject of intensive study with current reservoir simulators incorporating dissolution, dispersion of CO₂ in water, and chemical reactions of CO₂ with existing phases and host rock. However, there is little information in the literature on the numerical analysis of the structural aspect of CO₂ sequestration. The purpose of this simulation study is to understand the effects of geomechanical structures, especially faults, on the behavior of injected CO₂.
The GEM (Generalized Equation-of-State Model) Compositional Reservoir Simulator is used to observe how fault-related structure impacts behavior of injected CO₂ in the saline formation. Three main tasks are categorized as follows:

1) Comparison of the analytical approach for fluid distribution, based on Buckley-Leverett theory, with the simulation results; 2) Simulation study which illustrates the impact of fault properties on the behavior of carbon dioxide phase in a CO₂ and a H₂O (brine) saturated reservoir; 3) Simulation study which shows the effect of leakage through the fault (due to geologic imperfections) during the CO₂ migration.

These fault-scale interactions can play an important role in determining CO₂ and storage depending on whether the faults act as barriers, conduits or combined barrier-conduits. The simulator outputs reveal that each property of the fault as a barrier and also a conduit can restrict the migration of CO₂ through the reservoir as a consequence of compartmentalization (barrier) and bypassing (conduit).

This study concludes that the properties of a fault and the interactions between the fault and the reservoir matrix can play a critical role in quantifying the behavior of CO₂ after injection ends. A fault within the target formation can have a positive or negative effect on the capture of the buoyancy-driven CO₂ with residual trapping mechanism depending on its geometry and/or petrophysical
property. Accordingly, when it comes to the injection and storage of CO₂, an accurate prediction of the fault conductivity and petrophysical properties of the reservoir would be required to optimize the rate of injection and the storage capacity of the reservoir for the permanent capture of CO₂.
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Chapter 1: INTRODUCTION

Storage of carbon dioxide (CO$_2$) in deep saline aquifers has been suggested as one method to reduce greenhouse gases in the atmosphere. Trapping and sealing CO$_2$ in deep brine formations underground requires a sufficiently impermeable caprock layer to prevent upward migration from the target reservoir. Accordingly, the risk of CO$_2$ leakage has been one of the main issues for CO$_2$ sequestration to be a reliable carbon dioxide management solution. However, caprock layers may contain imperfections, such as faults or fracture zones, which can act as a conduit for leakage of CO$_2$ from depth to other underground assets or to the near surface. In addition, continuous CO$_2$ injection causes changes in the stress field that could potentially alter the conductivity of a fault by applying effective normal stress on the fault plane.

1.1 Research Objectives

Various approaches have been proposed to measure and interpret the behavior of carbon dioxide gas due to changes of petrophysical and geomechanical properties in reservoir systems. Moreover, to reduce, even eliminate, the risk of CO$_2$ leakage many studies have focused on representing effects of geologic imperfections, including a fault in a reservoir. Typically, flow simulation models represent a fault as an aggregation of surfaces between grid blocks, which involves specific fault properties. To include the impacts of faults,
Manzocchi et al. (1999) suggested that fault zone properties can be incorporated in flow simulators using fault transmissibility multiplier. The static geological approximation of fault transmissibility is useful to simulate the reservoir, where no dynamic data are available due to the natural uncertainty of fault zone structure and content. Therefore, to determine the value of transmissibility multiplier requires the physical observation of fault permeability and thickness, which implies that this modeling work is not theoretical estimation of fault properties; instead, it is based on empirical data. Also, Pasala et al. (2003) measured the impact of fault permeability/porosity structures on the migration of CO₂ by varying the range of permeability. His simulation results prove that the fault zone properties, especially permeability, in the reservoir can influence the flow of CO₂ through the aquifer as a consequence of bypassing (conduits, high-permeability) or compartmentalization (barriers, low-permeability). Likewise, faults interact with the properties of a given reservoir so that coupling factors are required. In addition, several studies have tried to simplify and represent real properties of a fault in a simulator. Pruess (2005) observed the behavior of CO₂ under the system which allows the interaction between multiphase flows and heat transfer. He concludes that buoyant-driven CO₂ plumes will show non-monotonic behavior due to the feedback between fluid flow and conductive heat transfer.

In order to represent efficiently the influence of geologically discontinuous structures on the overall reservoir condition, the previously
described methods have been developed. Nevertheless, not enough study has been done regarding the effect of fault's properties on the flow response for some aspects of CO$_2$ storage, especially buoyancy driven flow. Therefore, the purpose of this study is to summarize and evaluate geometric and petrophysical factors mainly associated with faults, which should be taken into account in predicting the behavior of CO$_2$ flow during carbon dioxide sequestration process in deep saline aquifers.

1.2 Review of Categories

First, an overview of risk related to CO$_2$ injection and storage process is presented to describe the main issues: the factors to be considered and the reason this study is necessary. Second, a summary of features of the simulator, General Equation-of-State Model Compositional Reservoir Simulator (GEM) by CMG group, is introduced to provide physical and numerical information essential to understanding the GEM process. The third part discusses the general impact of faults on the CO$_2$ geological storage and migration process, and introduces the concept of fault transmissibility multipliers in the simulation model. The fourth part illustrates the application of GEM, and shows results of the simulation study to identify how diverse types of geologic features affect the behavior of CO$_2$ migration: declined vs. inclined fault and low-permeability (sealing) vs. high-
permeability (conductive) fault. In addition, the outputs are analyzed to estimate the accuracy of the simulation by comparing simulation work with an analytical approach based on Darcy's law and Buckley-Leverett theory (Buckley and Leverett, 1942). The final part summarizes the conclusions of this research work, and details recommendations for future research.
Chapter 2: TRAPPING AND LEAKAGE OF CARBON DIOXIDE

2.1 CO2 Trapping Mechanisms and Leakage

Injected and stored CO2 in geological reservoirs might potentially migrate out of the reservoir through the subsurface and finally to atmosphere. In the case of CO2 storage in deep saline aquifers, the potential for CO2 leakage will depend on the well and cap rock (seal) integrity and the trapping mechanism, which can be categorized into the following four categories:

1) Hydrodynamic trapping: injected CO2 is primarily trapped as a gas or supercritical fluid. In this case, CO2 can be considered as free gas; and, will rise up due to buoyancy effect until it approaches the geologic seals, typically cap rock, in which CO2 will accumulate (general trapping mechanism).

2) Residual saturation trapping: CO2 can be stored as an immobile form in deep saline aquifers due to the petrophysical property of flow phases (Kumar et al., 2004). Capillary forces restrict the behavior of the CO2 flow, and CO2 will be left behind as trapped (residual) saturation. Therefore, the substantial volume of buoyancy-driven CO2 plumes is immobilized by residual gas saturation before it hits the low-permeable (sealing) boundaries of the reservoir.

3) Solubility trapping: CO2 has high solubility in water as well as in oil; accordingly, solubility trapping is also significant trapping mechanism in deep saline aquifers, depleted oil and gas fields. In the process of injecting in the
aquifer, CO₂ is mainly present as supercritical fluid before it perfectly dissolves. After CO₂ is completely dissolved, leakage is no longer possible, since free CO₂ will not exist any more.

4) Mineral trapping: CO₂ can react with minerals and organic matters in the geologic formations to become a portion of the solid matrix. However, the extent to which injected CO₂ reacts with minerals present in either sandstone or carbonate reservoir is relatively low. Simulation works on the Utsira formation model at Sleipner revealed that less than 1% precipitates as carbonate minerals. Likewise, the effect of mineralization of CO₂ is small compared to the other forms of CO₂ storage; however, it may contribute to reduce the amount of free gas at long times. (Ozah et al., 2005)

The permeability and capillary entry pressure of the overburden formations are also critical elements of leakage since they determine the retention time of CO₂ in the subsurface. Generally, only reservoirs below 800 meters are considered for CO₂ sequestration because at this depth CO₂ becomes supercritical, a state in which the density of CO₂ allows optimal storage capacity (Van der Meer, 2005).
Various models have been introduced to predict the future movement of CO$_2$ through the overburden. Numerical simulation of CO$_2$ diffusion through the 700 meters overburden above the Utsira formation at Sleipner shows that it will take more than 500,000 years for CO$_2$ to reach the sea floor (Lindeberg and Bergmo, 2003). Another study indicates that the release of CO$_2$ from an aquifer at 1000 meters depth in the Northeastern part of the Netherlands takes about 5500 years breakthrough time to reach the surface (Holloway, 2001).
2.1.1 Mechanism of CO₂ Leakage

Migration of injected CO₂ can occur by several mechanisms from the reservoir through the subsurface. These mechanisms can be organized with reference to the target formation as follows:

*Depleted oil and gas fields*

The hydrocarbon reservoir has been considered to be a safe site for CO₂ capture and storage because this reservoir type is mostly impermeable to hold oil/gas for millions of years without abrupt, huge releases. Therefore, most hydrocarbon reservoirs are likely to store CO₂ safely. However, wells in the reservoir can be paths of CO₂ migration; plus, the cap rock failure would allow CO₂ to escape from the reservoir. In addition, CO₂ can move via spill points¹ or dissolve into the fluid flow in the reservoir rock beneath the CO₂ accumulation to surrounding formations.

1) CO₂ leakage through or along wells: after the injection process CO₂ leakage can be caused by casing or cementing defects due to improper design or construction, corrosion of the casing and deterioration of current plugs by CO₂ and/or brine. The leakage phenomenon occurs through or along abandoned wells or improperly constructed operative wells, which are used for extraction/injection of CO₂ or water.

---

¹ The structurally lowest point in a trap that can retain hydrocarbons. Once a trap has been filled to its spill point, further storage of hydrocarbons will not occur for the lack of reservoir space.
Abandoned wells can be a serious pathway of CO\textsubscript{2} migration since depleted gas/oil reservoirs are generally punctured by numerous non-operative exploration and production wells. Especially, unidentified and poorly plugged wells are potential point sources of CO\textsubscript{2} leakage; therefore, they require proper control and maintenance.

Corrosion causes slow diffusion of CO\textsubscript{2} through the cement or steel casing at a rate of 20cm/1000years (Seinen \textit{et al.}, 1994). However, it is uncertain how the well bore integrity is affected by CO\textsubscript{2} and brine considering a sequestration timescale of 100's to 10000's of years. In the case of long timescales, abandoned wells serve as preferential leakage pathways; thus, they represent a significant long-term risk (Celia and Bachu, 2003).

2) A cap rock failure:

- Capillary leakage occurs when the pressure difference of fluid phase and the water phase in the pores adjacent to the cap rock is higher than the capillary entry pressure of the cap rock. However, generally capillary leakage mechanism is not considered seriously because the capillary entry pressure of the cap rock has been sufficient to retain hydrocarbons and the pressure can be measured by means of core testing (Jimenez and Chalaturnyk, 2003).

- A difference in CO\textsubscript{2} concentration due to pressure decays inside the reservoir can cause diffusion of CO\textsubscript{2} through the cap rock. However, this
mechanism is likely not a threat to cap rock failure because it is controlled by the long-term processes, such as tectonic activities. (Jimenez and Chalaturnyk, 2003).

- A man-made fracture, referred to as hydraulic fracturing, is also a factor of CO₂ leakage. When injecting CO₂ into the reservoir, fracturing of the seal can occur as a consequence of the pressure fluctuations, so-called "over-pressuring" (Wildenborg et al., 2002). In addition, the earlier production/injection processes to exploit hydrocarbon reservoirs can create fractures.

Fractures can be sealed in time by precipitation of newly formed minerals; on the other hand, they can be re-opened as a result of changes in stresses and/or pressures during CO₂ sequestration (Jimenez and Chalaturnyk, 2003). In order to prevent the growth of fractures, the maximum injection pressure should be kept below the level at which the cap rock may shear (Over et al., 1999). The risk of leakage through fracturing is low as long as the storage pressure does not exceed the initial reservoir pressure. However, over a specific level of pressure the CO₂ leakage can happen, depending on depth, pore pressure, rock properties and sedimentary (tectonic) history.

- Fracturing and the volume increase of rocks by shear deformation (dilatant shear deformation) play a significant role in CO₂ diffusion in the cap rock,
which create preferential flow pathways and increase the cap rock permeability by opening throats. However, shear deformation also results in low permeability of cap rock; thus, it can block or change the preferential pathway of CO$_2$ migration (Jimenez and Chalaturnyk, 2003). These structural deformations can affect the CO$_2$ leakage positively or negatively depending on the circumstantial conditions.

- CO$_2$ can react chemically with the cap rock, especially calcium carbonate rocks, and dehydrate clay shales of the cap rock. This dissolution procedure can produce high-permeability zones in the cap rock, such as caverns or sink hole in limestone bed.
- CO$_2$ can migrate through open (non-sealing) faults, which extend into the cap rock.
- Seismic disturbance can cause cap rock failure (Saripalli et al., 2003).

Among the above mechanisms leakage along and/or through wells, faults and fractures are considered to be the most serious leakage pathways; especially, CO$_2$ migration due to the geological cap rock failure is less controllable than leakage from the near-well failures. Until now, few measurements of CO$_2$ leakage via above mechanisms have been performed.

**Deep saline aquifers**

In general, the best storage reservoirs are at depths of greater than 3000 feet below the surface, have several hundred feet of porous and permeable sands, and
are overlain by at least one, and preferably more, thick and continuous seals (Benson and Myer, 2002). Leakage in deep saline aquifers has similar mechanisms as discussed above. One major difference with hydrocarbon reservoirs is that general saline aquifers do not contain cap rocks or seals, which have stood the test of time. In the case of aquifers, economic interests are much less significant than hydrocarbon reservoirs; therefore, the number of wells in aquifers is relatively low. Accordingly, the probability of CO₂ leakage is less than other cases. However, exploration and production wells have often been drilled through deep saline aquifers; so, they must be potential leakage pathways.

Another difference is that CO₂ storage in aquifers induces temporary pressure increase in the reservoir, because the space to store CO₂ becomes available as a result of compression of the fluids and rock in the reservoir, or displacement of formation water into adjacent formations or to the surface (Holloway, 2001).

Leakage from a typical deep saline aquifer has been modeled to estimate leakage rates from wellhead and cap rock failure, which is used as input for risk assessment. Results show that a failed cap rock implies the highest risk of leakage to all environmental media (Saripalli et al., 2003). A leakage rate of 0.1% of the whole volume stored per year corresponds to the estimated flux from a continuous fracture aperture of 2000 microns. Through high-permeable zone in the cap rock the leakage rate is calculated at 0.5% of the total volume stored per year. Spatial
frequency of cap rock failures within the area of review was estimated at 0.01 for both a fractured cap rock and high-permeable zones, assuming 1% of the cap rock area spread over an area of review of 50 kilometers radius is fractured; and, another 1% is highly permeable. Even though the estimated frequency of 0.00002 for a major wellhead failure based on statistical data of underground gas storage accidents in the USA and Canada is much lower, the consequences (CO₂ flux) of such event are larger (Saripalli et al., 2003). Moreover, in other regions, the frequency of well failures might be much higher.

Unminable coal seams

The large amount of the injected CO₂ can be absorbed to the coal matrix, replacing methane adsorbed to the coal matrix (coal bed methane), since CO₂ is preferentially adsorbed by coal relative to methane. This means that if coal seams have retained methane for millions of years, they will probably hold CO₂ for another thousands of years as well, assuming that CO₂ is sequestered at reservoir pressure. But, if overpressure occurs during injection, the risk of leakage is higher.

The methane content of the target coal seams offers an indication of the sealing capacity of the overburden. When a coal seam is unsaturated with methane due to degassing, the partial content of methane may not be detected on the coal seam. Insight in degassing and the sealing capacity of the overburden can be provided by information on the burial history. For each targeted coal seam for
CO₂ sequestration, the burial history needs to be studied to draw conclusion upon the overburden integrity.

However, several aspects related to the interaction between CO₂ and coal seams still require more studies. Especially, the physical and chemical reaction as well as its impact on the coal seam during the CO₂ injection procedure needs further research. One of the general reactions, swelling of the coal matrix, might cause a decrease in the permeability. In addition, swelling can induce changes of the stress on the overlying and/or underlying rock strata in non-ideal coal seams (thin, low permeable and highly faulted), which might result in faulting and migration pathways out of the coal seam (Gale, 2004).

**2.1.2 Local effects of CO₂ leakage**

CO₂ can put a serious, even fatal, effect on humans, animals and ecosystems. For instance, long-term exposure to high CO₂ levels, above 20~30%, might cause death by suffocation to humans and most air-breathing animals (Benson and Myer, 2002). In addition, sudden release of CO₂ would cause CO₂-saturated environment in a short time; and, this catastrophic emission of CO₂ is generally from an overturn of the lake, the hypolimnion\(^2\) of which became oversaturated with CO₂. This collapse is caused by a slow leakage of CO₂ from magma into the deep lake waters (Holloway, 2001). This represents that the health hazard of CO₂

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\(^2\) The hypolimnion is the bottom and most dense layer of water in a thermally-stratified lake.
releases depends mainly on the natural incident rather than the initial size of the release. The fact that CO$_2$ is heavier than other components in the air implies that leakage of CO$_2$ poses a lethal threat when CO$_2$ accumulates in confined areas, such as valleys or cellars. That is, released CO$_2$ remains concentrated rather than disperse due to topography of the ground (Holloway, 2001).

CO$_2$ under the earth, which migrates upwards through the geological imperfections, may also affect the quality of ground and surface water, soil and mineral resources; thus, it pollutes environmental and ecological circumstance on the earth. Fresh, potable groundwater, located in 100–200 meters of the subsurface, could be contaminated by even a small amount of CO$_2$ leakage. An increase of CO$_2$ concentration results in a decrease in pH, which causes calcium dissolution with an increase in the hardness of water (Holloway, 2001). The leakage of CO$_2$ also causes a contamination of surface water; thus, a decrease of pH affects the aquatic ecosystem, especially stagnant or stably stratified waters (Benson and Myer, 2002).

2.1.3 Global Effect of CO$_2$ Leakage

The CO$_2$ sequestration technology can be rendered ineffective depending on the CO$_2$ leakage rate; thus, the crucial point is to determine an acceptable leakage rate for the stabilization of greenhouse gas concentration in the atmosphere.

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Typically, it is non-circulatory and remains cold throughout the year.
Obviously, the reasonable rate of leakage depends on stabilization targets and the extent and timing of CO₂ sequestration. Accordingly, numerous approaches have been introduced to estimate the leakage rate associated with various parameters. As for an example of these studies, Lindeberg and Bergmo (2003) show a model, which represents physical and geological features realistically, to estimate required residence time of CO₂ in the reservoir. According to his calculation, injected CO₂ requires at least 10,000 years to reside in the target reservoir. Even though a certain range of leakage can be acceptable, most studies have claimed that the leakage rate should be kept lower than 0.1%.

2.2 CH₄ Leakage

Injected CO₂ in depleted hydrocarbon reservoirs can cause the leakage of methane or light alkane, which are omnipresent components in the reservoirs, coal beds and moderately common in deep saline aquifers. Generally, CH₄ can disperse faster than CO₂; therefore, its leakage locally has an effect on shallow water quality and can be a fatal threat in the case of accumulation in confined spaces.

2.3 Seismicity

The injection of fluid into a sedimentary layer or a fractured reservoir causes changes of existing mechanical states. Even if large amounts of fluid are injected with high pressure, this artificial process cannot modify the earth-scale tremor
itself. However, liquid injection may lead to the change of underground stress fields, which result in triggering earth tremors (Over et al., 1999). Enhanced oil recovery process is generally regarded as a source of reservoir-induced seismicity due to the change of reservoir pressures (Holloway, 2001). The leakage risk associated with seismicity depends on the condition of the target reservoir; for instance, the stability of the fractured reservoir can be easily affected just by the small change of pressures.

What is worse, reservoir-induced seismicity can increase the risk of CO₂ leakage or damage to structures; therefore, a seismic hazard assessment requires a careful examination of the conditions at the sequestration site. The investigation should contain historical seismicity, structural study of the area, evaluation of the critical fluid pressure for failure and pre-injection seismic monitoring of the area to define "zero-state" seismicity (Holloway, 2001).

2.4 Ground Movement

Man-made pressure changes lead the earth's surface to sink or rise, which damage structures on the earth. In a CO₂ reservoir, the uplift will not take place as long as the geostatic pressure is higher than the tectonic pressure. However, any geological reason can induce the reduction of the grain pressure, which acts between individual rock particles. This decrease causes uplifting or down-faulting of the surface. Another reason of subsidence is the chemical reaction between
aqueous CO₂ and the reservoir rock, which results in dissolution of reservoir rock, so-called chemical compaction. This phenomenon can be discovered especially in the case of carbonate rocks with high porosity (Holloway, 2001).

2.5 Displacement of Brine

The basic process, the CO₂ injection in the target sink, can cause the displacement of brine (saline groundwater). This phase change may result in undesirable effects, for instance, an increase in salinity of drinking water or a rise of the water table, which means that displace brine will infiltrate and pollute the groundwater (Benson, 2005). Thus, to prevent the underground contamination requires the consideration of CO₂-mixed brine effects on the reservoir.

2.6 Implication of This Study

Likewise, the trapping and leakage of CO₂ must be considered to perform the appropriate CO₂ capture and storage process. However, few studies pay attention to how the structural aspect of the CO₂ storage site will affect the CO₂ behavior. Therefore, this simulation study focuses on the effect of geological structures, especially a fault, on the behavior of CO₂ plume within a saline aquifer.

All simulation works are based on the buoyancy-driven CO₂ migration after injection. As CO₂ migrates upward due to buoyancy, it can be trapped by previously introduced mechanisms. In this simulation study, we consider only
residual saturation trapping. Plus, the reservoir properties, such as permeability and dipping, can determine the preferential behavior of CO₂ plumes. The presence of a fault will restrict or support CO₂ migration depending on the fault’s properties. As well, the interaction between reservoir conditions and fault properties plays a significant role in permanent capture of CO₂ with improving the efficiency of residual saturation trapping.
Chapter 3: FEATURES OF GEM SIMULATOR

This chapter introduces significant features of GEM (Generalized Equation-of-State Model) simulator, which are used in this simulation work. GEM is a compositional reservoir simulator from CMG based on Equation-of-State (EOS) (Nghiem and Li, 1989) to model complex reservoirs by considering the flow of three-phase, multi-component fluids. It is based on the flexible application of each formulation to define the specific grid block and time step. This method allows GEM simulator to represent the interaction among various components of the reservoir; and, to simulate combined structures efficiently. Especially, in this simulation study, the interaction between faults and the matrix plays an important role in determining the migration of injected or stored CO₂. The GEM simulator provides extensive optional tools to combine the properties of faults with the existing reservoir condition. The purpose of this chapter is to explain the diverse features of GEM used in this simulation study.

In Section 3.1, fundamental parameters and equations regarding the general equation-of-state model are reviewed. Section 3.2 introduces how to model the interaction among the phases. Next, the simulator keywords to represent the properties of faults in the reservoir are discussed in Section 3.3. Finally, the Section 3.4 shows the function of refined grid blocks for simulating the
propagation of CO2 in detail; also, it discusses the efficiency of refined grid block method.

### 3.1 General Equation of State (EOS)

The GEM simulator uses Peng-Robinson equation of state (EOS) to predict the composition and density of oil and gas phases. In this application, the EOS is used to calculate the gas and aqueous phase that flow when CO2 and H2O components mix, so the oil phase is actually the aqueous phase.

The binary interaction coefficient for the CO2-H2O pair, $BIC_{CO2-H2O}$, was tuned to match the CO2 solubility in brine with experimental data (Kumar et al., 2004). Also, volume shift parameters, $VSP_{CO2}$ and $VSP_{H2O}$, were tuned to match the CO2-saturated brine density and brine density with experimental data (Kumar et al., 2004). The Peng-Robinson equation of state is as follows:

\[
P = \frac{RT}{V_m - b} - \frac{aa}{V_m^2 + 2bV_m - b^2}
\]

where

\[
a = \frac{0.45724R^2T_c^2}{P_c}
\]

\[
b = \frac{0.07780RT_c}{P_c}
\]

\[
a = \left[ 1 + \left( 0.37464 + 1.54226\omega - 0.26993\omega^2 \right) \left( 1 - T_r^{0.5} \right)^2 \right]
\]

\[
T_r = \frac{T}{T_c}
\]
The CO₂ solubility in brine can be matched with experimental data by using the binary interaction coefficients. Among several GEM keywords to represent binary interaction, $PVC3$ is used to calculate the interaction between hydrocarbon-hydrocarbon component pairs. The volume shift parameter is used to match experimental density data. In addition, coefficients in Pedersen's viscosity model (Pedersen et al., 1984) are used to compute the viscosity of each phase.

$$\frac{\mu_{\text{mix}}(P, T)}{\mu_o(P_o, T_o)} = \left(\frac{T_{c,\text{mix}}}{T_{c,o}}\right)^{-1/6} \left(\frac{P_{c,\text{mix}}}{P_{c,o}}\right)^{-2/3} \left(\frac{MW_{\text{mix}}}{MW_o}\right)^{-1/2} \left(\frac{a_{\text{mix}}}{a_o}\right)$$

(3.2)

In the above equation, the subscript "mix" means the mixture property, and the subscript "o" refers to the reference substance property; especially, the reference substance for the Pedersen's theory is methane.

The mixture critical temperature and pressure are calculated using mixing rules that are a function of the component critical temperatures and pressures, and mole fractions. Also, the molecular weight of the mixture is determined from:

$$MW_{\text{mix}} = \text{coef}_1 \left(MW_w \text{coef}_1 - MW_n \text{coef}_1\right) + MW_n$$

(3.3)

where $MW_w = $ weight fraction averaged molecular weight

$MW_n = $ mole fraction averaged molecular weight

The rotational coupling coefficient can be calculated as follows:

$$\alpha = 1 + \text{coef}_3 \left(\rho_r \text{coef}_3 \cdot MW \text{coef}_3\right)$$

(3.4)
In the above two equations, the coefficients $coef_1$ through $coef_5$ are default values introduced by Pedersen et al. (1984).

If the calculated phase density is below the defined reference density on the GEM simulator, it is identified as gas (CO$_2$) phase; otherwise, as oil (brine) phase. The related GEM keywords for computing the equation-of-state are $BIN$, $VSHIFT$, $PEDERSEN$, $VISCOR$, $VISCOEFF$, $PHASEID$ and $DEN$.

### 3.2 Phase Relationship

This section describes the equations and variables used in the numerical simulation of GEM and the way of approaching for solving these equations. Using the adaptive-implicit method (Collins et al., 1986, Thomas and Thrurnau, 1983) allows the flow equations be divided because it encompasses both the explicit-transmissibility method and the fully-implicit method as particular cases. The equations, variables and solution method introduced in the following are variations of the approach of Collins et al. (1986).

**Flow Equations**

The following finite-difference equations for the components in the oil and gas phases (equation 3.6), and for the water component (equation 3.7) are from a material balance:
\[ \psi_i = \Delta T_0 \gamma_i^m \left( \Delta p_{i,o}^{n+1} - \gamma_o^{m} \Delta D \right) + \Delta T_g \gamma_{ig}^m \left( \Delta p_{i,g}^{n+1} + \Delta p_{ig}^{m} - \gamma_g^{m} \Delta D \right) \\
+ q_i^m - \frac{V}{\Delta t} \left[ N_i^{n+1} - N_i^n \right] = 0 \quad (i = 1, \ldots, n_v) \tag{3.6} \]

\[ \psi_{n_{e+1}} = T_w \left( \Delta p_{n_{e+1}} - \Delta p_{cwo}^m - \gamma_w^m \Delta D \right) + q_{n_{e+1}}^m - \frac{V}{\Delta t} \left[ N_{n_{e+1}}^{n+1} - N_{n_{e+1}}^n \right] = 0 \tag{3.7} \]

where \( T_m = \frac{A}{\Delta x} \frac{k_{m}}{m} \rho_m = \text{molar transmissibility of phase } m \ (m = o, g, w) \)

It is assumed that no mass transfer exists between the hydrocarbon and water phases. This is another reason for using the oil phase to act as aqueous phase and the gas phase to act as CO₂. In this way, mass transfer between the phases in an aquifer is correctly represented. The superscripts \( n \) and \( n+1 \) denote respectively the old and current time level. The superscript \( m \) refers to \( n \) for explicit grid blocks and \( n+1 \) for fully implicit grid blocks. In GEM, the term explicit refers to grid blocks with explicit transmissibilities where only pressure is treated implicitly.

The \( N \)'s are related to porosities, phase molar densities, saturations and compositions as follows:

\[ N_i = \phi \left( \rho_o S_o y_{io} + \rho_g S_g y_{ig} \right) \tag{3.8} \]

\[ N_{n_{e+1}} = \phi \rho_w S_w \tag{3.9} \]

*Phase-Equilibrium Equations*
Overall composition of a mixture is in the two phase region at a given \( p \) and \( T \), then the phase compositions and splits can be obtained by solving the thermodynamic-phase-equilibrium equation; 
\[
g_i = \ln f_{ig} - \ln f_{io} = 0 \quad (i = 1,\ldots,n_c)
\] (3.10)
for \( N_{ig} \), the moles of component \( i \) in the gas phase. The moles of component \( i \) in the oil phase, \( N_{io} \), can be obtained from
\[
N_{io} = N_i - N_{ig}
\] (3.11)

**Saturation Equation**

The saturations are related to \( N_i \) and \( m (m = o, g, w) \) through the following equation:
\[
S_w = \frac{N_{i_{w+1}}}{\phi \rho_{w}}
\] (3.12)
\[
S_o = (1 - S_w) \frac{N_o/\rho_o}{N_o/\rho_o + N_g/\rho_g}
\] (3.13)
\[
S_g = (1 - S_w) \frac{N_g/\rho_g}{N_o/\rho_o + N_g/\rho_g} = 1 - S_o - S_w
\] (3.14)

**Mole or Volume Consistency Equations**

From the definition of \( N_i \) \((i = 1,\ldots,n_c + 1)\), the following equation can be derived:
\[
\psi_p = \sum_{i=1}^{n_c+1} N_i^{n+1} \left( \rho_o S_o + \rho_g S_g + \rho_w S_w \right)^{n+1} = 0
\] (3.15)
Equation (3.15) forces the consistency between the $N_i$'s and the densities, saturations, and porosities. Equation (3.15) can also be rewritten as follows:

$$\psi_p^t = V \sum_{i=1}^{n+1} N_i^{n+1} - V \phi^{n+1} = 0$$  \hspace{1cm} (3.16)$$

The first term in Equation (3.16) indicates the volume occupied by the fluids (oil, gas, water) and the second term is the pore volume. Thus, Equation (3.16) forces the consistency between the fluid volume and the pore volume. A similar equation is referred to as volume balance equation by Acs et al. (1985) and Watt (1986).

The related GEM keywords for computing the properties of each phase or component are $SO$, $SW$, $SG$, $RHOO$, $RHOG$, $DENO$, $DENW$, $DENG$ and $SATP$.

### 3.3 Fault Characteristics

Geological faults are the result of relative movement of adjacent volumes of rock. The “fault zone” refers to the specific part of the reservoir that is under the impact of fault connections. In this zone, lateral flow between fault blocks does not follow the usual geological strata. Therefore, it is required to group grid blocks into fault blocks, and to take the inter-block communication into account when modeling a faulted reservoir.

Fault properties affect the flow of fluids, especially the trapping mechanism of CO$_2$ because faults can act as barriers or conduits for the fluid flow.
in the reservoir. The concept of transmissibility can represent these properties of fault. When computing transmissibilities for lateral inter-block flow in a faulted reservoir, a special connection, so-called "fault connection" should be implemented.

A fault connection accounts for depth when creating a connection and would create connections between blocks which physically contact. The GEM simulator uses following numerical relationship assuming four real connections:

$$ IVAL = \text{nilow} + 2 \times \text{nihigh} + 4 \times \text{nlow} + 8 \times \text{nhigh} \quad (3.17) $$

where $\text{nilow, nihigh, nlow, nhigh} = 0$ if standard connection

$$ \text{nilow, nihigh, nlow, nhigh} = 1 \text{ if fault connection} $$

Here, $i$ refers to the $i$ direction; and, $j$ refers to the $j$ direction. low refers to flow between block $i$ (or $j$) and $i-1$ (or $j-1$); while, High refers to flow between block $i$ (or $j$) and block $i+1$ ($j+1$).

Accordingly, if $IVAL = 0$ all connections are standard, which means the connection between grid blocks will remain in the numerical order, even if the domain is titled condition; and, if $IVAL = 15$ all connections contain a fault connection property, which implies that grid blocks will have a new connection that is determined by relative displacement along the fault and dip of the reservoir. The following example for $i$ direction is helpful to understand the fault connection:
The related keywords of GEM simulator are **FAULT, FAULTARRAY, TRANSF, IDIR, JDIR** and **KDIR**.
Chapter 4: REPRESENTING FLOW FEATURE OF FAULTS

Generally, faults play a significant role in the distribution of fluids in the geologic formation. Thus, a fault-containing reservoir represents more ambiguity and complexity to estimate the dynamic properties of fluid flows than pure (non-faulted) reservoir does. Therefore, one of the most significant purposes in this simulation work is to observe the effect of geologic discontinuity, especially fault, on the dynamics of buoyancy-driven CO₂ plume. The fault-derived geological heterogeneity leads to more complex fluid interactions depending on fault geomechanical and/or petrophysical properties of a fault.

4.1 Fault Characteristics in the Simulation Work

Every simulation work requires simplified model to represent typical properties of the real object. Accordingly, geomechanical and petrophysical properties of a fault also need to be simplified to study their effects on the CO₂ migration. The basic concept of fault modeling is to show abrupt changes of relative depths of geologic layers due to faulting activities and to clarify effects of this discontinuity of layers on the fluid dynamics in the reservoir. Generally, faults have two sorts of major impact on the fluid flow (Manzocchi et al., 1999). The first critical effect of faulting is the juxtaposition of different flow units, which results in altering connectivity of sedimentary layers. It causes the disconnection between highly
permeable zones (sealing effect) and/or juxtaposition of high-permeable fault zone against low-permeable flow unit (channeling effect). These heterogeneous properties can be modeled by using simple geometry assuming a fault as a single strand or a group of grid blocks; however, the precise influence of fault displacements on reservoir connectivity is complicated because the faulting effect should be understood with the interaction between the fault zone and the surrounding zone. Moreover, a fault contains its own heterogeneous properties, which means that modeling a fault as an aggregation of blocks will be more reasonable than as a single strand. Plus, the time-dependent tectonic deformation along the fault plane results in changes of hydraulic properties; and, it causes the presence of larger fault zone in the Earth's crust. These relatively large-scale connectivity effects which can be analyzed with Allan diagrams using sequence/throw juxtaposition diagrams or with aggregate connectivity plots (Cerveny et al., 2004).

Secondly, the petrophysical properties of the fault-rock itself influence a fluid flow, usually represented by using transmissibility multipliers mainly associated with permeability and thickness of the fault zone. In the following section, a geologically driven method for determining fault transmissibility multipliers as a function of known properties of the reservoir model will be outlined and discussed based on Manzocchi's studies. The discussion includes verbatim sentences from Manzocchi et al. (1999) between which I interspersed
my comments on the application of their ideas to this study. The method of using transmissibility multipliers mainly aims to consider the influence of fault properties in the stratigraphically deposited plane. Inevitably, this method requires calibration and correction to reduce the error between numerically simplified analysis and dynamic reservoir data. Even though dynamic (time-dependent) data related to fault properties are not available in the reservoir, transmissibility multipliers can be numerical devices in the simulation study because we can observe main physical factors: fault permeability and thickness. Indeed, dynamic information contains various error ranges of fault properties, which means that we need to average them assigned to the typical fault type or adapt all data into every fault condition corresponding to time-variation. However, this numerical analysis of using transmissibility multipliers is based on a static geological prediction assuming no dynamic tectonic and/or geologic activities.

Figure 4.1: Conceptual up-scaling hierarchy. a) At the sub-meter scale, the fault-rock permeability is a function of its shale content. b) At the sub-grid-block scale, the fault zones are considered heterogeneous in permeability and thickness. c) At
the grid-block scale each grid-block connection is assigned a uniform transmissibility (Figure from Manzocchi et al., 1999)

The conceptual model we consider for the determination of fault transmissibility multipliers is shown on Figure 4.1 see Manzocchi et al. (1999) for further details. Figure 4.1a describes a fault conceptually as a volume of a particular thickness and shale content, which mainly control the fault permeability. The shale content of the fault zone is calculated as a function of the faulted sequence using the Shale Gouge Ratio method (described in the following section 4.2) introduced by Yielding et al. (1997). Figure 4.1b illustrates a fault zone with an intermediate-scale. Fault thickness and permeability are assumed to be log-normally distributed with 75% of the values covering two orders of magnitude around the median value. The correlation-lengths of this heterogeneity are assumed to be substantially smaller than the simulation grid-block size. Figure 4.1c describes appropriately up-scaled simulation grid blocks in which the transmissibility multiplier is assigned to fault-face of each grid-block. Each grid block of the heterogeneous fault zone represents the average value of permeability and thickness; therefore, it is numerically reasonable to assume that grid blocks involve uniform transmissibility. Consequently, we can simulate typical fault properties by alteration of transmissibility multipliers; for instance, to allocate sealing fault blocks with small, even zero, transmissibility multipliers and conductive fault blocks with larger values. Furthermore, CO₂ leakage through the
geologic seal can be modeled simply by allocating different transmissibility multipliers on specific grid blocks.

The following two sections (4.2 and 4.3) explain the main petrophysical and geometric properties of a fault to derive transmissibility multiplier: fault permeability and thickness.

4.2 Fault Zone Permeability

The trapping and leakage through the geologic imperfection can be estimated corresponding to the fault permeability. The low-permeable (sealing) fault results in trapping, while the high-permeable (conductive) fault causes leakage through it. Despite inaccuracy of using static data in determining fault zone permeability, several methodologies have emerged to analyze the seal capacity of faults in sandstone/shale sequences. It is efficient way to use proxy-properties to make inferences about the behavior of a fault, through empirical correlations with other faults of known behavior in the same hydrocarbon province.

The Shale Gouge Ratio (SGR) is one of the most widely used algorithms to predict approximately fault zone permeability from the clay/shale content of the faulted lithologies and fault throw (Yielding et al., 1997). The SGR serves as an estimate for the proportion of clay in the fault gouge, and requires a stratigraphical column that is discretized in intervals with an assigned value for
volume of clay. The following Figure 4.2 shows the conceptual model of SGR calculation:

![Conceptual model of SGR calculation](image)

**Fig. 4.2:** Conceptual model describing scheme and values used to calculate the Shale Gouge Ratio (SGR) (Yielding et al., 1997)

\[
SGR = \frac{\sum(V_{\text{clay}} \cdot \Delta z)}{\tau}
\]  

(4.1)

To simulate the fault zone numerically by using SGR, we need to assume that SGR is equivalent to the shale content \((V_{\text{shale}})\) of fault gouge because we cannot estimate directly the precise shale content of the fault zone; however, we can calculate the SGR for the subsurface fault zone. The minimum SGR on the fault surface is assumed to have the lowest capillary entry pressure, which implies that fluids can flow more easily through the fault.
Figure 4.3 summarizes permeability data for various reservoirs and outcrop fault-rock samples (Antonellini and Aydin 1994; Knai 1996; Gibson 1994, Ottesen Ellevset et al. 1998).

Figure 4.3: Log permeability (md) vs. volumetric shale fraction for fault-rock. Large data-points are permeability measurements from core and outcrop samples from a variety of locations (Gibson 1994). Filled circles: cataclastic deformation bands. Open circles: solution deformation bands. Filled squares: clay gouge. Small data-points are probe-permeability measurements of deformation bands (open circles) and slip surfaces (crosses) from sandstones in SE Utah (Antonellini and Aydin 1994). Boxes are summaries of data from the Sleipner Field (Ottesen Ellevset et al., 1998). (i) Cataclastic deformation bands. (ii) Framework phyllosilicate fault rocks. (iii) Shale smears. The line labelled "K" represents average values, based on core samples from the Heidrun Field, used in a full-field flow simulation (Knai 1996). The curves (Equation 4.2) represent the relationship used in this work for permeability as a function of SGR (assumed equivalent to the fault-rock volumetric shale fraction) and displacement. Curves are given for $D=1$ mm (dashed line), $D=10$ cm, $D=1$m, $D=10$ m and $D=1$ km (heavy line) (Figure and caption from Manzocchi et al., 1999).
In the above relationship, we can discover that fault-zone permeability tends to decrease with increasing shale content; but, some permeability values at particular shale content vary quite largely. The major trend of this relationship (decrease of influence of faulting with increase of shale content) is caused by different deformation types with various shale contents. In pure sandstone representing low shale content, the slip surface has extremely low permeability, which results in increase of the cataclastic\(^3\) intensity with displacement. On the other hand, deformation bands in more shaley sandstone are less cataclastic, as displacement is accommodated by small-scale smearing of the phyllosilicate (e.g. Antonellini and Aydin, 1994), and the shale content of a fault plays a main role in controlling fault permeability.

The curves on the Figure 4.3 represent an empirical prediction of fault zone permeability as a function of shale content and displacement. Accordingly, the SGR-values, which vary between 0 and 1, calculated along the fault are then converted to fault permeability using the following correlation:

\[
\log k_f = -4SGR - \frac{1}{4} \log(D)(1 - SGR)^5
\]

(4.2)

where \( k_f \) = fault permeability, md

\( D \) = fault displacement, m

---

\(^3\)“Cataclastic” refers to the shearing and/or granulation of minerals due to high stresses resulted from the faulting.
In general, the value of fault permeability obtained is the median value of a log-normal permeability distribution covering about two orders of magnitude. However, at the low shale content, which means that SGR approaches zero, the above relationship does not provide a reliable estimate of permeability due to the variation of empirical data.

4.3 Fault Zone Thickness

In addition to permeability, thickness is needed to model a fault in a simulation. In the case of a conductive (high-permeable) fault, the thickness is one of the most significant factors affecting the CO₂ migration through the fault. The fault thickness, which is defined as the zone in which permeability is altered as a result of fault movement, can be estimated from fault throw under the assumption that there exists a linear relationship between fault thickness and fault throw, which has been established from field observations. Hull (1988) discovered an approximately linear relationship between fault zone displacement and fault rock thickness (tᵢ) over several decades of scale-range with thickness values distributed over about two orders of magnitude for a particular displacement. As shown in the Figure 4.4, the median fault thickness values can be calculated using Equation 4.3 by superimposing several fault outcrop data including compiled data by Hull (1988), faults in mixed sandstone/shale sequences in Sinai (Knott et al. 1996), SE Utah (Foxford et al., 1998) and Lancashire, UK (Walsh et al. 1998).
The standard deviation for log \( t_f \) is 0.9. Equation 4.3 tends to underestimate the thickness of small-scale faults as shown in Figure 4.4. However, the presence of such a small scale fault does not affect dynamics of the phase model so that fault displacements less than 1m can be neglected in the simulation study.

Figure 4.4: Log thickness vs. log displacement (both in meters). Summaries of out-crop measurements are given as envelopes containing measurements from a variety of sources (Hull 1988), from faults in Nubian Sandstone in Western Sinai (Knott et al., 1996), from the Moab fault in SE Utah (Foxford et al., 1998) and from faults in a Westphalian sandstone/shale sequence from Lancashire, UK (Walsh et al., 1998). 200 log-normally-distributed thickness data (small diamonds) have been generated at various displacements with median value following the relationship \( t_f = D/66 \). The harmonic averages of these data (large circles) follow the relationship \( t_f = D/170 \) (Figure and caption from Manzocchi et al., 1999).
4.4 Fault Zone Properties at Grid Block Scale

In the simulation work, we need to set a reasonable size of grid blocks because in-situ reservoir condition is too complicated to be represented by a single domain. Therefore, the grid block scale must be small enough to model an actual condition properly. However, fault zone properties are variable and unpredictable over short distances. Foxford et al. (1998) characterized the 40 km well-exposed Moab Fault in S.E. Utah over short sections at various locations. He concluded that it is impossible to extrapolate predictions of the fault zone structure over distances greater than about 10 m. Other studies, despite their limited evidence, suggest that fault zone permeability is at least as heterogeneous as thickness (e.g. Figure 4.3, Antonellini and Aydin 1994).

The simulation model for representing a fault structure requires neglecting the extremely small fault structure. The representative elementary volume (REV) of a correlated random field is generally applied to obtain reasonable fault scaling. The REV value is about four times larger than the range of the semivariogram defining the field (Anguy et al., 2004); for instance, if the correlation length of fault zones is assumed to be in the order of 10 – 20 m, then the REV is in the order of 40 – 80 m. To represent a fault properly in the reservoir simulation model, we need to assume a typical REV for real fault zones; and, the value would be smaller than a reservoir grid-block. The typical simulation model is
based on 100 m wide grid-blocks; thus, the correlation length of a fault should be small enough to be a portion of the simulation domain. Based on this assumption, the area-weighted arithmetic and harmonic averaging method is used to derive the representative fault permeability and thickness.

Both thickness and permeability are assumed to vary over the area of a grid-block according to a log-normal distribution. The median value of a log-normal distribution is the mean of the normal distribution of the log-variable. In the case of a log-normal distribution with a log-variable mean $\mu$ and standard deviation $\sigma$, the arithmetic average of the distribution is $10^{(\mu+\sigma^2/2)}$, and the harmonic average is $10^{(\mu-\sigma^2/2)}$. By using both Equation 4.2 and 4.3 with $\mu = 0.9$, we can predict the median values of permeability and thickness. This standard deviation is equivalent to about 75% of the values lying within ± one order of magnitude of the median, and 90% lying within ± 1.5 orders of magnitude (Figure 4.4). By using $\mu = \log\left(D/66\right)$ and $\sigma = 0.9$ we can calculate the harmonic average thickness ($t_{fh}$) as a function of displacement:

$$t_{fh} = \frac{D}{170}$$

(4.4)

Also, from $\mu = -4SGR - \frac{1}{4} \log(D)(1 - SGR)^5$ and $\sigma = 0.9$ we can derive the arithmetic average permeability ($k_{fa}$) as a function of SGR and displacement:
From the Equations 4.4 and 4.5, we can derive average values of the fault zone thickness and permeability appropriate for incorporation in a reservoir flow simulator based on the assumptions about fault zone structure and properties, which have been described above.

**4.5 Fault Zone Properties in the Simulation Model**

Fluid phases in a numerical simulation can be represented as a function of transmissibilities between grid blocks. Normally, transmissibility of each grid-block can be obtained by dividing the permeability by the distance separating block centers, which ignores grid-block dips. In addition, fault properties (seal and/or conduit) of each grid block in a fault zone can be represented by using transmissibility multipliers, which operate on transmissibility between adjacent grid blocks. That is, lower values of transmissibility multiplier (less than 1) indicate sealing faults; while, relatively higher values (more than 1) represent conductive faults. Figure 4.5 illustrates the transmissibility multiplier, $Trans_i$, between two blocks separated by a transmissibility multiplier and a discrete thickness of fault-rock.

\[
\log k_{fa} = 0.4 - 4SGR - \frac{1}{4} \log(D)(1 - SGR)^5
\]  
(4.5)
Figure 4.5: The transmissibility between two grid-blocks separated by (a) a transmissibility multiplier and (b) a discrete thickness of fault-rock (Figure and caption from Manzocchi et al., 1999)

Accordingly, the transmissibility multiplier is derived as a function of the dimensions and permeability of the grid-blocks and the thickness and permeability of the fault:

$$T = \left[ 1 + t_f \left( \frac{2/k_f - 1/k_i - 1/k_j}{L_i/k_i + L_j/k_j} \right) \right]^{-1}$$  \hspace{1cm} (4.6)

where  

- $T$ = transmissibility multiplier
- $t_f$ = fault thickness
- $L$ = grid block length
- $k$ = fault permeability

For a case where $L_i = L_j = L_m$ and $k_i = k_j = k_m$ (‘m’ refers to ‘matrix’), transmissibility multiplier, $T$, becomes:

$$T = \left[ 1 + t_f \left( \frac{k_m - k_f}{k_f} \right) \right]^{-1}$$  \hspace{1cm} (4.7)
which is equivalent to the transmissibility factor defined by Walsh et al. (1998). For a specific case where $L_i \neq L_j$ and/or $k_i \neq k_j$, Equation 4.7 can be used as a multiplier on the permeability of one of the grid-blocks adjacent to the fault, effectively assigning the entire thickness of fault-rock to this cell. This provides the same transmissibility across the fault as applying Equation 4.7 to the interface between the two grid-blocks, but also modifies the transmissibility on the other side of the grid-block to which the permeability multiplier has been assigned. Therefore, the transmissibility multiplier provides a numerically more robust representation of the fault than the permeability multiplier.

Likewise, we can model numerically the property of a fault-structure, such as low-permeable or high-permeable, by using transmissibility multipliers, which allow each grid block to represent individually its own property. In the GEM simulator transmissibility on each grid-block is assigned using keyword: TRANSI, TRANSJ, TRANSK, and, especially, it is available to account for fault-based reservoir model with TRANSF. To represent a fault each face of one grid block can involve different transmissibility multiplier to express every single connection on a certain grid-block face with IDIR+/-, JDIR+/-, and KDIR+/-. Basically, the default value of transmissibility multiplier is 1 as an initial setting of the GEM simulator. Thus, multipliers can be used to modify different types of fault conditions: zero value of transmissibility means that there is no communication between grid blocks in the specific direction (perfectly sealing fault); on the other
hand, larger value (>1) indicates that there can be more interaction between grid blocks (highly conductive fault). Accordingly, each grid block represents the basic unit, which consists of a fault being allocated with a specific petrophysical property. The following Figure 4.6 explains how the multipliers apply to grid blocks for simulating faulted reservoir model, which contains a dip in a whole reservoir domain:

Figure 4.6: Connection type between grid blocks: this scheme shows 2D model to simulate a reservoir, which contains a declined fault. (a) The dark cells involve conductive (high-permeability) fault properties; thus, transmissibility multipliers of each cell face are 100. The black arrows mean more fluent communication between grid blocks. (b) The dark cell involves sealing (low-permeability) fault properties; thus, transmissibility multipliers of each cell face are zero. In contrast to case (a), case (b) does not have arrows, which indicates no communication through the contact area.
Chapter 5: SIMULATION ANALYSIS AND DISCUSSION

To simulate the faulted reservoir model, GEM, CMG’s compositional reservoir simulator was used in this study. The simulation work focuses on three key points: gas migration, gas storage and gas leakage in the given reservoir condition. Especially, the main idea of this simulation study is the buoyancy-driven flow of CO₂ after it has been injected or stored in deep, saline aquifers with geologically discontinuous structures: faults and fractures. Therefore, specific petrophysical characteristics of the reservoir are selected to represent well-defined discontinuities; and, parameters are varied to evaluate sensitivity.

In Section 5.1, the base case model is introduced to show the behavior of stored CO₂ at reservoir condition. The simulation studies of Section 5.2 and 5.3 use more complicated models, which combine geological discontinuity (fault) with the base model to estimate the effect of faults on the CO₂ migration

5.1 Description of Tilted Two-Dimensional Base Case

As a basic model, the immiscible displacement of CO₂-rich gas and water (brine) phases is simulated to explain the migration of stored CO₂ in the saline aquifer. Gravity force plays the most significant role in the fluid flow when there is no injection or production in the given reservoir. Thus, the base case assumes that CO₂ is present in the aquifer as an initial condition, and that no further injection
occurs. Also, anisotropy of parameters is varied to study the directional tendency of CO₂ migration.

5.1.1 Aquifer Description

This basic case simulation grid dimensioning are 400 ft × 100 ft × 2 ft. This grid was used to establish a wide volume of CO₂ migration along which buoyant instabilities could develop. The simulation used 10,000 grid-blocks; and, each grid block size is 2 ft × 2 ft × 2 ft. To study the effect of buoyancy force along the bedding plane, the domain was tilted to a dip angle of five degrees. In addition, there are no injection nor production wells in this model. The boundary of the domain is closed. Accordingly, there is no external force to drive fluid flow except buoyancy. CO₂ injection is not simulated. Instead, the injected CO₂ is assumed initially to occupy a region in the lower part of the aquifer, whose range of area is 1st to 100th grid block in j-direction (horizontal) and 40th to 50th grid block in k-direction (vertical). The scheme of the base case model is Figure 5.1:
Figure 5.1 Scheme of the Aquifer for Base Case. The red portion indicates the zone initially occupied by CO₂, and the blue part means water (brine)-saturated zone.

It is assumed that the base case does not include any fault; thus, the base model represents only fluid migration in the matrix. Table 5.1 summarizes various reservoir property values used in the two-dimensional base case.

<table>
<thead>
<tr>
<th>General Property of Whole Aquifer</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Width, ft</td>
<td>400</td>
</tr>
<tr>
<td>Thickness, ft</td>
<td>100</td>
</tr>
<tr>
<td>Depth at top of the center of the reservoir, ft</td>
<td>5300</td>
</tr>
<tr>
<td>Temperature, °F</td>
<td>140</td>
</tr>
<tr>
<td>Salinity, ppm</td>
<td>100,000</td>
</tr>
<tr>
<td>Initial pressure at the top seal of an aquifer, psi</td>
<td>2295</td>
</tr>
<tr>
<td>Constant boundary pressure at 5300 ft depth, psi</td>
<td>2295</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Specific Property</th>
<th>Matrix</th>
</tr>
</thead>
<tbody>
<tr>
<td>Permeability, md</td>
<td>1</td>
</tr>
<tr>
<td>Horizontal to vertical permeability ratio</td>
<td>1</td>
</tr>
<tr>
<td>Transmissibility</td>
<td>1</td>
</tr>
<tr>
<td>Horizontal to vertical transmissibility ratio</td>
<td>1</td>
</tr>
<tr>
<td>Porosity, fraction</td>
<td>0.15</td>
</tr>
</tbody>
</table>
Table 5.1: Summary of Aquifer Properties for the Base Case

5.1.2 Component Properties

The base case model aims to represent the interaction between two components, carbon dioxide (CO₂) and water (H₂O), by using PR-EOS (Peng-Robinson Equation of State). H₂O forms a liquid phase with dissolved CO₂ that is recognized as 'oil phase' by the simulator; while, CO₂ forms a gas phase with a small mole fraction of H₂O that is labeled as 'gas phase' by the simulator. The properties of each component are shown in the following Table 5.2 and 5.3:

<table>
<thead>
<tr>
<th>Component Name</th>
<th>CO₂</th>
<th>H₂O</th>
</tr>
</thead>
<tbody>
<tr>
<td>Critical Pressure (atm)</td>
<td>72.809</td>
<td>217.7546</td>
</tr>
<tr>
<td>Critical Temperature (°K)</td>
<td>304.1278</td>
<td>647.0944</td>
</tr>
<tr>
<td>Critical Volume (m³/kmole)</td>
<td>0.094</td>
<td>0.056</td>
</tr>
<tr>
<td>Molecular Weight (g/gmole)</td>
<td>44.01</td>
<td>18.015</td>
</tr>
<tr>
<td>Acentric Factor</td>
<td>0.22394</td>
<td>0.344</td>
</tr>
<tr>
<td>Parachor</td>
<td>78</td>
<td>52</td>
</tr>
<tr>
<td>Boiling Temperature (°F)</td>
<td>-109.21</td>
<td>212</td>
</tr>
</tbody>
</table>

Table 5.2: Component Properties (Kumar et al., 2004)

<table>
<thead>
<tr>
<th>Volume Shift Parameter</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>CO₂</td>
<td>0.234867</td>
</tr>
<tr>
<td>H₂O</td>
<td>0.024668</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Binary Interaction Coefficients</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>K_{CO₂-H₂O}</td>
<td>-0.0576003</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Coefficients for Pederson's Correlation (Viscosity)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Coefficient 1</td>
</tr>
<tr>
<td>Coefficient 2</td>
</tr>
<tr>
<td>Coefficient 3</td>
</tr>
<tr>
<td>Coefficient 4</td>
</tr>
<tr>
<td>Coefficient 5</td>
</tr>
</tbody>
</table>
Table 5.3: Parameters to Model Fluid Behavior (Kumar et al., 2004)

5.1.3 Rock Fluid Data

Rock-fluid data include rock property, especially relative permeability values of the matrix. The matrix relative permeability input data are calculated by using the following equations:

For $S_g < S_{gcr}$:

$$k_{rg} = 0$$

(5.1)

For $S_g > 1 - S_{wcon}$:

$$k_{rw} = 0$$

(5.2)

For $S_g \geq S_{gcr}$:

$$k_{rg} = k_{rg}' \left( \frac{S_g - S_{gcr}}{1 - S_{wcon} - S_{wir}} \right)^{N_g}$$

(5.3)

For $S_g \leq 1 - S_{wcon}$:

$$k_{rw} = k_{rw}' \left( 1 - \frac{S_g - S_{gr}}{1 - S_{wcon} - S_{gr}} \right)^{N_w}$$

(5.4)

where $S_g$ = gas saturation
$S_{gr}$ = residual gas saturation
$S_{gcr}$ = critical gas saturation
$S_{wcon}$ = connate water saturation during a gas flood
$S_{wir}$ = irreducible water saturation
$k_{rg}'$ = relative permeability to gas at connate water saturation (gas end point relative permeability)
\[ k'_{rw} = \text{relative permeability to water at residual gas saturation (water end point relative permeability)} \]

\[ N_g = \text{gas relative permeability exponent} \]

\[ N_w = \text{water relative permeability exponent in the gas-water curve} \]

The term “irreducible water saturation (\(S_{wir}\))” represents the initial water existence in the pore spaces; while “connate water saturation during a gas flood (\(S_{wcon}\))” indicates the water saturation that considers fluctuation due to the displacement between phases. Therefore, in the case of zero-residual-gas-saturation formation the water saturation will keep its initial value; therefore, we can neglect “\(S_{wir}\)” and define the “residual gas saturation (\(S_{gr}\))” as the real initial saturation in the reservoir. However, in the base model this term is being used with the same value of the residual saturation because the saturation corresponds to the end point relative permeability of a flowing phase in the matrix. Plus, this simulation study assumes no distinction between critical and residual saturation as well as between irreducible and residual saturation for each phase. The following Figure 5.2 shows the relative permeability curve for gas and water phase of the matrix. The curve represents "drainage" process which means that non-wetting phase (CO\(_2\) gas) displaces wetting phase (brine) resulting in decrease of the wetting phase saturation at the boundary of CO\(_2\) plumes.
Figure 5.2: Relative Permeability Curve for the Matrix for Base Case. Residual gas saturation is zero, and there is no hysteresis.

Typical parameters of the above relative permeability curve used for the base case simulation are listed on the following Table 5.4:

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Residual gas saturation, $S_{gr}$</td>
<td>0</td>
</tr>
<tr>
<td>Critical gas saturation, $S_{gcr}$</td>
<td>0</td>
</tr>
<tr>
<td>Maximum gas saturation, $S_{gmax}$</td>
<td>0.9</td>
</tr>
<tr>
<td>Constate water saturation, $S_{wcon}$</td>
<td>0.1</td>
</tr>
<tr>
<td>Irreducible water saturation, $S_{wir}$</td>
<td>0</td>
</tr>
<tr>
<td>Gas end point relative permeability, $k_{rg}$</td>
<td>0.75</td>
</tr>
<tr>
<td>Water end point relative permeability, $k_{rw}$</td>
<td>1</td>
</tr>
<tr>
<td>Water relative permeability exponent, $N_w$</td>
<td>2</td>
</tr>
<tr>
<td>Gas relative permeability exponent, $N_g$</td>
<td>2.5</td>
</tr>
</tbody>
</table>

Table 5.4: Parameters of Relative Permeability Curve for the Base Case Model
5.1.4 Base Model Properties

The initial overall, so-called 'global' in the GEM simulator, concentration of CO₂ is zero and that of H₂O is one. In the base case CO₂ is initially present only in the down-dip half of the 40\textsuperscript{th} to 50\textsuperscript{th} bottom layers with 100 \% saturation value. Elsewhere the domain is fully saturated with H₂O (brine) as shown in Figure 5.3. The color bar at the side of the saturation profile represents the value of gas saturation. The aim of the base model is to explain how the stored CO₂ migrates depending on the properties of the aquifer, such as permeability anisotropy. The initial condition is intended to approximate the result of injecting CO₂ at the bottom of an aquifer.

![Image of CO₂ Storage Model](image)

Figure 5.3: Initial CO₂ Saturation profile of the simulation model. The color bar located on the right side of the illustration represents the gas saturation index (the initial gas saturation is 100 \%).
The simulation model considers brine as "oil" phase in GEM as mentioned in the Section 5.1.2; thus, the water phase saturation ($S_w$) is zero. Initial reservoir pressure is 2295 psia, which is calculated by using a hydrostatic gradient of 0.433 psi/ft. In this simulation study, "gas" is assumed as "supercritical fluid"; therefore, pure CO$_2$ is under supercritical state at the temperature and pressure of the aquifer. However, supercritical state CO$_2$ cannot be regarded as in-situ fluid because this model accounts for the solubility of water component in the gas phase.

**5.1.5 Numerical Method and Time Step**

The GEM simulator adapts numerous criteria to optimize the convergence of Newtonian iterations, and to limit the pressure and saturation changes in a given time step. Table 5.5 introduces the parameters used in the simulation study.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Normal pressure change, psi</td>
<td>100</td>
</tr>
<tr>
<td>Maximum saturation change, fraction</td>
<td>0.15</td>
</tr>
<tr>
<td>Maximum global composition change, fraction</td>
<td>0.15</td>
</tr>
<tr>
<td>Tolerance criterion for the convergence of the Newtonian iteration, psi</td>
<td>0.514884</td>
</tr>
<tr>
<td>Maximum number of GMRES$^4$ steps</td>
<td>20</td>
</tr>
<tr>
<td>Maximum number of GMRES iterations</td>
<td>200</td>
</tr>
</tbody>
</table>

Table 5.5 Numerical Method and Time Step Control Parameters

$^4$ Generalized Minimal Residual Method, One of iteration methods generates a sequence of orthogonal vectors, which are retained at every step; therefore, "RESTART" option can be possible in GEM.
The total simulation time of 10,000 years is relatively large compared to the typical time for oil recovery processes; thus, deciding a reasonable time step is required to achieve proper simulation results. At the beginning of simulation, there is limitation associated with changes in saturation and pressure in one time step. Accordingly, during the first 50 years, the time step sizes are kept small to achieve a quick convergence. After a few hundred years, there is little change of fluids' state in the reservoir; thus, larger time steps are used.

5.2 Analytical Solution for Buoyant Flow of CO₂

To analyze the basic behavior of CO₂ migration I assume the following Buckley-Leverett flow conditions; (1) Both fluids and the porous medium are incompressible (2) Capillary pressure gradient is negligible (3) One-dimensional flow and displacement is along the x coordinate of a semi-infinite linear flow system with a constant cross-sectional area (A). Among the above assumptions, the incompressibility of fluids and formation is critical to deriving the Buckley-Leverett solution. In the case of gas and water displacement this assumption may pose certain limitation to the resulting solution, when a flow system has large pressure gradients. However, in many cases, this incompressibility assumption still provides acceptable approximations because the viscosity of the gas phase in normal conditions is ~2 orders of magnitude lower than the water phase. This characteristic prevents high-pressure gradients from building up. In this
simulation model, the confining reservoir pressure of the domain is fixed to 2295 psia.

The behavior of immiscible displacement in porous media depends on viscous and gravity forces. Generally, one-dimensional flows may be unidirectional or countercurrent; plus, flow can take place in either open or closed systems. Viscous-dominated flows typically appeared in open systems and are characterized by uni-directional flow. In contrast, gravity-dominated flows may occur in either open or closed systems, and involve either uni-directional or countercurrent flow. The driving force for countercurrent flow is gravity and phase density differences.

5.2.1 Analysis of Simple 2-D Base Case

Consider the flow of two immiscible fluids (one wetting and another non-wetting phase) in a homogeneous, isothermal and isotropic porous medium. The governing equation for the flow of phase $i$ is from Darcy's law as follows:

$$ u_i = -\frac{kk_i}{\mu_i} \left( \frac{dp}{dx} + \rho_i g \sin \alpha \right) $$ \hspace{1cm} (5.5)

where $\alpha$ = dip angle (positive for upward flow)

$$ u_i = \sum_{i=w,g} u_i $$ \hspace{1cm} (5.6)

In the above equation, the subscript $t$ means total flux of flows; and, $w$ and $g$ denote water and gas phases. Alternatively, the equation 5.5 can be written
where $k = \text{average permeability}, \quad k = \frac{A_{\text{total}}}{k_{\text{vertical}} + \frac{A_{\text{horizontal}}}{k_{\text{horizontal}}}}$

The subscripts $i$ and $j$ are restricted to mobile phases. The continuity equation for phase $i$ is

$$\phi \frac{\partial S_i}{\partial t} = -\frac{\partial u_i}{\partial x} \quad (5.8)$$

In the case of this simulation study, the model is assumed to be closed to fluid injection and withdrawal; thus, the total flux is zero. The equation 5.7 becomes

$$u_i = \frac{kk_j (\rho_j - \rho_i) g \sin \alpha}{\mu_j \left(1 + \frac{k_{ij} \mu_i}{k_{ri} \mu_j}ight)} = \frac{k (\rho_j - \rho_i) g \sin \alpha}{\mu_j + \mu_i} \quad (5.9)$$

$$u_i = \frac{4.9 \times 10^{-4} kk_j \Delta \gamma \sin \alpha}{\mu_j (M + 1)} : M = \frac{k_{ij} \mu_i}{\mu_j k_{ri}} \quad \text{(oil field unit)} \quad (5.10)$$

The reservoir study is based on two-dimensional flows of fluids; thus, it is necessary to analyze flow vertical and parallel to the bedding plane. The scheme of vector analysis of the fluid flux is shown as following Figure 5.4:
Figure 5.4 Analysis of vertical and parallel components of the total fluid flow velocity. The density of fluid 1 is less than the density of fluid 2.

For the parallel component of the total flux of gas (CO₂) phase,

\[ u_{g,\text{parallel}} = \frac{k \left( \rho_w - \rho_g \right) g \sin \alpha}{\mu_w + \frac{\mu_g}{k_{rw}/k_{rg}}} \]  

(5.11)

For the vertical component of the total flux of gas (CO₂) phase,

\[ u_{g,\text{vertical}} = \frac{k \left( \rho_w - \rho_g \right) g \sin 90^\circ}{\mu_w + \frac{\mu_g}{k_{rw}/k_{rg}}} \]  

(5.12)

The flux can be referred to the Darcy velocity of fluid, which represents its rates of flow per unit of surface at right angles to the direction of flow (Walsh and Moon, 1991). The Darcy velocity differs from the interstitial velocity \( (v_g) \) of fluid because of the action of porosity and saturation:

\[ u_g = \phi S_g v_g \]  

(5.13)

where \( S_g \) = average value of gas saturation from the fractional flow curve
Therefore, the distance and direction of CO$_2$ migration can be estimated as follows:

1) Distance

\[ d_g = v_i \cdot t \]  \hspace{1cm} (5.14)

where  \( d_g \) = distance of gas phase migration, ft

\[ v_i = \sqrt{v_{g,parallel}^2 + v_{g,vertical}^2 - 2v_{g,parallel}v_{g,vertical} \cos \left(90^\circ + \alpha\right)} \], \( ft/day \)

\( t = \) total time, \( day \)

2) Direction

The direction of CO$_2$ migration can be calculated by using the second cosine law. The analytical scheme is shown as follows:

![Figure 5.5: Analytical scheme for estimating the direction by using vector components](image)

\[ \cos \theta = \frac{v_i^2 + v_{parallel}^2 - v_{vertical}^2}{2v_i v_{parallel}} \] \hspace{1cm} (the 2$^{\text{nd}}$ cosine law)

\[ \theta = \cos^{-1} \left( \frac{v_i^2 + v_{parallel}^2 - v_{vertical}^2}{2v_i v_{parallel}} \right) \]  \hspace{1cm} (5.15)
Likewise, we can estimate the typical characteristics of CO₂ migration such as distance and direction by applying above equations. The following chapter 5.3 will introduce the simulation results, and we can determine whether this solution is applicable or not.

5.2.2 Validation of Using Buckley-Leverett Theory in Analysis

In this section we review the basic equation of fractional flow theory because we can derive the frontal gas saturation and average gas saturation from the fractional flow curve; and then, comparing these specific values with simulated saturation profile will prove how reasonable it is to apply the analytical solution.

In this theoretical analysis, the fluids are assumed to be incompressible; thus, the continuity equation for each phase yields the following equations:

\[
\frac{\partial q_w}{\partial x} = -\phi A \frac{\partial S_w}{\partial t} \quad (5.16)
\]

\[
\frac{\partial q_g}{\partial x} = -\phi A \frac{\partial S_g}{\partial t} \quad (5.17)
\]

where \( S_w + S_g = 1 \)

By combining equation 5.16 and 5.17,

\[
\frac{\partial}{\partial x} (q_w + q_g) = 0 \quad (5.18)
\]

Accordingly, the total flow rate is derived as follows:

\[
q_t = q_w + q_g = \text{constant} \quad (5.19)
\]
In view of this result, we can define the water phase fraction \( f_w \) of the flow system:

\[
f_w = \frac{q_w}{q_t}
\]  

(5.20)

Similarly, the gas phase fraction \( f_g \) is defined as follows:

\[
f_g = \frac{q_g}{q_t} = 1 - f_w
\]  

(5.21)

Therefore, the fractional flow of gas phase is expressed by following relationship:

\[
f_g = \frac{1 - \frac{k_{rw} A}{q_i \mu_w} \left( \rho_w - \rho_g \right) g \sin \alpha}{1 + \frac{k_{rw} \mu_g}{\mu_w k_{rg}}} \]  

(5.22)

\[
f_g = \frac{1 - 0.001127 k_{rw} A \left( 0.433 \Delta \gamma \sin \alpha \right)}{1 + \frac{k_{rw} \mu_g}{\mu_w k_{rg}}} \quad \text{(oil field unit)}
\]  

(5.23)

where

- \( k \) = average permeability, \( \text{md} \)
- \( A \) = area, \( \text{ft}^2 \) (\( A = A_{\text{vertical}} + A_{\text{horizontal}} \))
- \( q_t \) = total flow rate, \( \text{bbl/day} \)
- \( \mu_w, \mu_g \) = water (brine) and gas (CO₂) viscosity, \( \text{cp} \)

For deriving the fractional flow, we use following Equation 5.24 for non-dipping aquifer with co-current, instead of Equation 5.23.

\[
f_g = \left( 1 + \frac{k_{rw} \mu_g}{\mu_w k_{rg}} \right)^{-1}
\]  

(5.24)
Using Equation 5.24 may not be reasonable because this simulation model involves the counter current flow, which will be discussed in section 5.6. Also, the gravity term of Equation 5.23 is not zero, and the total flow rate \( q_t \) is zero in this closed domain. Nevertheless, to predict buoyant front displacement behavior with Equation 5.24 can be meaningful to analyze the CO\(_2\) plume behavior.

![Fractional Flow Curve for Gas Phase](image)

**Figure 5.6**: Fractional flow of the gas phase (dip angle, \( \alpha = 5^\circ \)), including average and frontal value

From the above curve, the frontal and average CO\(_2\) saturation can be estimated assuming that the displacement satisfies the Buckley-Leverett conditions. The frontal saturation \( (S_{gf}) \) is the saturation at which the straight line passing through the point \( S_g = S_{gr} \) and \( f_g = 0 \) is tangent to the fractional flow curve. On the other hand, the intersection of the tangent line with the line \( f_g = 1 \) provides the constant average gas saturation \( (S_{gav}) \). The frontal saturation
determines the actual distance of CO$_2$ migration at the simulation. It implies that the frontal edge of CO$_2$ plume should not be chosen to determine the rate of CO$_2$ migration.

5.3 Discussion of Simulation Results for the Base Case

5.3.1 Base Case with Isotropic Permeability

As mentioned in the description of model properties, the base model involves dip; thus, the buoyancy force has a non-zero component in the direction of the bedding plane. For the isotropic case ($k_v/k_h = 1$) with dip, gravity force plays a significant role in the CO$_2$ migration. We can anticipate CO$_2$ gas will flow primarily toward the surface; thus, the flow does not reach any of the closed boundaries because initially CO$_2$ is stored only in the down-dip half of the bottom layers. Figures 5.7 ~ 5.15 show the gas (CO$_2$) saturation in the tilted aquifer with isotropic permeability ($k_v = k_h = 1 \text{md}$) at increasing times:

![Figure 5.7: Gas Saturation Profile in an isotropic formation (Base Case) 1 month later](image)
Figure 5.8: Gas Saturation Profile in an isotropic formation 1 year later

Figure 5.9: Gas Saturation Profile in an isotropic formation 3 years later

Figure 5.10: Gas Saturation Profile in an isotropic formation \((k_v/k_h=1)\) 5 years later. The yellow arrow represents the directional distance \((d)\) of CO₂ migration, and the orange arc indicates the angle \((\theta)\) between the directional flow and bedding plane.
We can estimate typical characteristics, distance and direction of fluid flow, by analyzing the simulation output associated with the CO₂ distribution. The distance is measured from the initial edge of CO₂ plume to the boundary involving the frontal saturation \((S_{gf} = 0.4)\). Table 5.6 shows both values from the simulation output and the analytical solution:

<table>
<thead>
<tr>
<th>Characteristic</th>
<th>Analytical Solution</th>
<th>Simulation Output</th>
</tr>
</thead>
<tbody>
<tr>
<td>Distance (d), ft</td>
<td>34.9756</td>
<td>27.88</td>
</tr>
<tr>
<td>Direction (θ), deg</td>
<td>80.08</td>
<td>77</td>
</tr>
</tbody>
</table>

Table 5.6: Comparison of typical properties of CO₂ distribution after 5 years from the simulation result and the analytical solution

The values from each approach for the base case are quite similar; thus, the analytical solution based on Buckley-Leverett theory is reasonable to estimate CO₂ behavior. This is a useful result, but it is not obvious. As shown later, there is no flow or countercurrent flow of water in the CO₂ plume, which does not satisfy the condition of the Buckley-Leverett theory.

Figure 5.11: Gas Saturation Profile in an isotropic formation 15 years later
Figure 5.12: Gas Saturation Profile in an isotropic formation 20 years later

Figure 5.13: Gas Saturation Profile in an isotropic formation 200 years later

Figure 5.14: Gas Saturation Profile in an isotropic formation 600 years later
5.3.2 Effect of Anisotropic Permeability

Anisotropy of reservoir properties affects strongly the flow trend of the buoyant phase. As vertical to horizontal permeability ratio ($k_v/k_h$) becomes smaller, it causes preferential CO$_2$ flow paths to be parallel to the bedding plane. Also, in the tilted aquifer anisotropy combined with a dip influences buoyant displacement.
For these anisotropic formations ($k_v/k_h = 0.1$ and 0.01), the path of CO$_2$ migration tends to be more aligned to the bedding plane. In these simulation studies, CO$_2$ rising toward the surface encounters the no-flow side boundary, which forces CO$_2$ to move vertically. Then, CO$_2$ reaches the top seal of the reservoir model; and, begins to establish an accumulation of large and potentially mobile saturation.

First, the following simulation outputs show CO$_2$ flow paths in domains dipping $5^\circ$ with permeability anisotropy ($k_v = 0.1k_h = 0.1\, md$):

![Figure 5.16: Gas Saturation Profile for anisotropic formation ($k_v/k_h = 0.1$) 1 year later](image1)

Figure 5.16: Gas Saturation Profile for anisotropic formation ($k_v/k_h = 0.1$) 1 year later

![Figure 5.17: Gas Saturation Profile for anisotropic formation ($k_v/k_h = 0.1$) 20 years later](image2)

Figure 5.17: Gas Saturation Profile for anisotropic formation ($k_v/k_h = 0.1$) 20 years later
Figure 5.18: Gas Saturation Profile for anisotropic formation \((k_v/k_h=0.1)\) 60 years later. The yellow arrow represents the directional distance of CO\(_2\) migration, and the orange arc indicates the angle between the directional flow and the bedding plane.

In this anisotropic model, we can also estimate typical characteristics, distance and direction of fluid flow, by analyzing the simulation output associated with the CO\(_2\) distribution. The below table shows both values from the simulation output and the analytical solution:

<table>
<thead>
<tr>
<th>Characteristic</th>
<th>Analytical Solution</th>
<th>Simulation Output</th>
</tr>
</thead>
<tbody>
<tr>
<td>Distance ((d)), ft</td>
<td>57.38</td>
<td>57.52</td>
</tr>
<tr>
<td>Direction ((\theta)), deg</td>
<td>46.09</td>
<td>41.15</td>
</tr>
</tbody>
</table>

Table 5.7: Comparison of typical properties of CO\(_2\) distribution after 60 years from the simulation result and the analytical solution for \(k_v/k_h=0.1\)
Figure 5.19: Gas Saturation Profile for anisotropic formation \((k_v/k_h = 0.1)\) 100 years later

Figure 5.20: Gas Saturation Profile for anisotropic formation \((k_v/k_h = 0.1)\) 200 years later

Figure 5.21: Gas Saturation Profile for anisotropic formation \((k_v/k_h = 0.1)\) 1000 years later
Figure 5.22: Gas Saturation Profile for anisotropic formation ($k_v/k_h= 0.1$) 7000 years later

Next, the Figure 5.23 through 5.31 explain how the larger anisotropy of permeability, ($k_v = 0.01k_h = 0.01 md$) affects the CO$_2$ migration. We can expect that the smaller ratio of vertical to horizontal permeability will cause more lateral movement than vertical.

Figure 5.23: Gas Saturation Profile for anisotropic formation ($k_v/k_h= 0.01$) 1 year later
Figure 5.24: Gas Saturation Profile for anisotropic formation (\(k_v/k_h = 0.01\)) 20 years later

Figure 5.25: Gas Saturation Profile for anisotropic formation (\(k_v/k_h = 0.01\)) 100 years later

Figure 5.26: Gas Saturation Profile for anisotropic formation (\(k_v/k_h = 0.01\)) 200 years later. The yellow arrow represents the directional distance of CO\(_2\) migration, and the orange arc indicates the angle between the directional flow and the bedding plane.
The smaller ratio of vertical to horizontal permeability ($k_v/k_h$) results in more lateral CO$_2$ migration (smaller angle between flow and bedding plane). We can estimate typical characteristics, distance and direction of fluid flow, by analyzing the simulation output associated with the CO$_2$ distribution. The below table shows both values from the simulation output and the analytical solution:

<table>
<thead>
<tr>
<th>Characteristic</th>
<th>Analytical Solution</th>
<th>Simulation Output</th>
</tr>
</thead>
<tbody>
<tr>
<td>Distance (d), ft</td>
<td>122.55</td>
<td>123.27</td>
</tr>
<tr>
<td>Direction ($\theta$), deg</td>
<td>6.46</td>
<td>4.63</td>
</tr>
</tbody>
</table>

Table 5.8: Comparison of typical properties of CO$_2$ distribution after 200 years from the simulation result and the analytical solution for $k_v/k_h=0.01$

The values from each approach are quite similar; thus, the analytical solution based on Buckley-Leverett theory is reasonable to estimate CO$_2$ behavior.

Figure 5.27: Gas Saturation Profile for anisotropic formation ($k_v/k_h=0.01$) 375 years later
As the above Figure 5.28 has shown, more anisotropy between horizontal and vertical permeability causes more movement of CO₂ parallel to the bedding plane; therefore, CO₂ accumulates and moves upward along the boundary after approaching the edge of the reservoir.

Figure 5.29: Gas Saturation Profile for anisotropic formation (kᵥ/kₜ = 0.01) 700 years later
As shown above, the smaller ratio of vertical and horizontal permeability \((k_v/k_h)\) causes the direction angle, \(\theta\) of CO\(_2\) plume migration to be closer to zero, the plume moves up dip along the bedding plane. It is because the smaller value of the vertical permeability causes slower vertical movement of CO\(_2\). The last simulation results show remarkably different behavior of CO\(_2\) that is the CO\(_2\) plume approaches the side boundary first, instead of the upper surface. That means that anisotropy of the reservoir property plays a crucial role in controlling the fluid distribution.
The following Figure 5.32 and 5.33 show both velocity vectors of gas and water phases 400 years later when the vertical movement of CO₂ begins along the boundary:

Figure 5.32: Flux vectors of the gas phase after 500 years of Figure 5.28 representing the effect of anisotropy (k_v/k_h= 0.01). The yellow arrow shows the major direction of the gas flux inside the CO₂ plume, and the red one indicates the gas flux controlling the vertical CO₂ flow.
Figure 5.33: Flux vector of the water phase after 500 years corresponding to gas phase velocity in Figure 5.32. The yellow arrow represents the major direction of the water flux inside the CO₂ plume, and the red one indicates the water flux due to gas displacement.

After gas phase approaches the vertical reservoir boundary, only the vertical movement of the gas phase controls the CO₂ migration (this estimation is supported by the fact that we cannot discover water flux vectors in the vertical CO₂ plume along the edge). In addition, on the lateral aspect of fluxes the water phase moves oppositely to the gas (CO₂) phase, which means that in principle we cannot apply the analytical solution based on Buckley-Leverett theory to analyze fluid distribution in this part of the domain. The theory assumes co-current flow, but Figure 5.32 and 5.33 show counter current flow or no flow of the water phase.
The fact that the theory works well is a subject for further investigation in future work.

### 5.4 Two-Dimensional Base Case Combined with Discontinuity

In this section, the CO$_2$ migration in a faulted reservoir was simulated by assigning to appropriate grid block the petrophysical properties associated with fault characteristics. Such a geological discontinuity can induce the flow (leakage) of "potentially mobile CO$_2$" in the structural trap at large saturation. In the process of the structural trap, the stored CO$_2$ will remain in the trap permanently as long as the geological seal remains intact.

The location of an angled fault cannot be accurately represented in a Cartesian grid, which is based on rectilinear grid blocks.

![Angled fault in the Cartesian grid blocks. The coordinates in each grid block represents the vertical and horizontal order of blocks. Three numbers of a coordinate indicates i, j and k direction.](image)

<table>
<thead>
<tr>
<th>i</th>
<th>j</th>
<th>k</th>
<th>Fault</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.5.3</td>
<td>1.6.3</td>
<td>1.7.3</td>
<td>1.8.3</td>
</tr>
<tr>
<td>1.5.4</td>
<td>1.6.4</td>
<td>1.7.4</td>
<td>1.8.4</td>
</tr>
<tr>
<td>1.5.5</td>
<td>1.6.5</td>
<td>1.7.5</td>
<td>1.8.5</td>
</tr>
<tr>
<td>1.5.6</td>
<td>1.6.6</td>
<td>1.7.6</td>
<td>1.8.6</td>
</tr>
</tbody>
</table>
As shown in the above Figure 5.34, the Cartesian grid block method cannot represent the tilted fault simply by putting fault properties in the cubic grid blocks. Therefore, I use 'Transmissibility Multipliers' (Manzocchi et al., 1999) on every contact face of each grid block to represent a declined or inclined fault in the simulation work. In GEM, \(TRANSF\) is used to represent petrophysical properties of a fault and \(IDIR+/-, JDIR+/-\) and/or \(KDIR+/-\) determine a direction of the flow through a fault. This geologically-driven method allows the combined effect of permeability and thickness to be captured in the flow simulator. Previous Section 4.2 explains how transmissibility multiplier acts on the interaction between grid blocks in the faulted aquifer model.

As shown in the Figure 5.34, specific range of grid blocks should be assigned appropriate transmissibilities to represent the inclined fault; therefore, smaller grid blocks enable us to simulate more realistically the angled geologic discontinuity. Additionally, the type of fault, high-permeability (conduits) or low-permeability (barriers), can be controlled by setting transmissibility multipliers high (more than 1) or low (zero). Moreover, we define two categorizes, declined (negative dip to horizontal plane) and inclined (positive dip to horizontal plane) fault. Thus, we can estimate how the direction of the fault can affect on the CO\(_2\) accumulation and migration mechanism.
5.4.1 Fault Acting as a Barrier

Typically, low-permeable faults, so-called 'sealing' faults, result from 'deformation band-type' formation, which is the geological deformation process of reducing permeability with shear-induced grain-size reduction in bands. The treatment of these kinds of faults in flow simulation for CO₂ sequestration has become more geologically driven and more quantitative. Accordingly, we can model sealing faults by setting transmissibility multipliers as zero for all directions (TRANSF= 0 for IDIR+/-, JDIR+/-, and KDIR+/-); therefore, assumed faults in the model can act as a barrier of CO₂ migration.

Reservoir with a Declined Sealing Fault

First, the simulation work focuses on how the declined fault, which has negative slope relative to the dip of bedding plane, affects CO₂ migration under the anisotropic reservoir condition. The ration of vertical permeability to horizontal permeability is 0.01; thus, the horizontal flow parallel to the bedding will be greater than the vertical movement. Other reservoir properties are as in the base case.
Figure 5.35: Gas Saturation Profile for anisotropic formation with declined sealing fault 1 year later \((k_v = 0.01 k_h = 0.01\text{ md})\). The yellow line represents the fault geometry.

Figure 5.36: Gas Saturation Profile for declined sealing fault 20 years later

Figure 5.37: Gas Saturation Profile for declined sealing fault 65 years later
Figure 5.38: Gas Saturation Profile for declined sealing fault 100 years later

Figure 5.39: Gas Saturation Profile for declined sealing fault 200 years later

Figure 5.40: Gas Saturation Profile for declined sealing fault 400 years later
Figure 5.41: Gas Saturation Profile for declined sealing fault 700 years later

Figure 5.42: Gas Saturation Profile for declined sealing fault 1000 years later

Figure 5.43: Gas Saturation Profile for declined sealing fault 7000 years later

We can discover that the declined fault plays a significant role as one of typical geological traps. In this case, the sealing fault forms a CO₂-trap-zone.
combined with the pre-existing boundaries of the reservoir. Furthermore, from the above series of gas saturation profiles, the most remarkable phenomenon is the accumulation of CO₂ before the vertical CO₂ migration along the sealing fault. In detail, the flow vector analysis Figure 5.44 indicates there would be counter current flow between phases inside the CO₂ plume. Counter current flow means that applying the Buckley-Leverett theory need not be valid. The following Figure 5.44 and 5.45 illustrate flux vectors of both gas and oil (brine) phases at year 2080 (100 years later):

Figure 5.44: Gas Saturation Profile with Gas Flux Vector after 100 years. The yellow arrow represents the direction of the gas flux.
Figure 5.45: Gas Saturation Profile with Water Flux Vector after 100 years. The blue arrow represents the direction of the water flux.

*Reservoir with an Inclined Sealing Fault*

Next, the simulation work explains how the inclined fault, representing a positive slope relative to the dip of bedding plane, affects the CO$_2$ migration and fluids' distribution. Generally, in the case of an inclined fault, the seal integrity cannot act as a geological trap; instead, it alters the path of the CO$_2$ migration (or leakage). To show this effect clearly, I put the inclined fault into the middle of CO$_2$-stored-zone; thus, this model causes separate CO$_2$ movements (frontal and behind parts) with time-step. This initial condition would not arise in a real reservoir, but it is convenient for showing the effect.
Figure 5.46: Gas Saturation Profile for anisotropic formation ($k_v/k_h = 0.01$) with inclined sealing fault 1 year later. The yellow straight line represents the fault location.

Figure 5.47: Gas Saturation Profile for inclined sealing fault 20 years later

Figure 5.48: Gas Saturation Profile for inclined sealing fault 100 years later
Figure 5.49: Gas Saturation Profile for inclined sealing fault 200 years later

Figure 5.50: Gas Saturation Profile for inclined sealing fault 300 years later

Figure 5.51: Gas Saturation Profile for inclined sealing fault 500 years later
As the above figures show, the left part (behind portion) of stored CO₂ moves upward along the sealing fault, and then accumulates at the upper part of given
reservoir. On the other hand, the right part (frontal portion) shows a normal trend of fluid migration, which is observed from outputs of the base case, cf. Figure 5.25. If the reservoir has smaller anisotropy, we can expect that CO$_2$ on the left side of the fault will show a preferential movement toward the upper boundary as shown in the basic condition; while, CO$_2$ in the right side will migrate along the sealing fault. Therefore, when it comes to analysis of CO$_2$ migration, we should consider reservoir properties as well as the distribution of geologic structure. The following Figures 5.55 and 5.56 show the impact of anisotropy on the CO$_2$ flow distribution. Those simulation results are from the reservoirs, which involve the same parameters (transmissibility, fault geometry and dip) as Figure 5.48 except the value of anisotropy ($k_v/k_h$) are larger:

Figure 5.55: Enlarged Gas Saturation Profile of Figure 5.48 for anisotropic formation ($k_v/k_h=0.01$) with inclined sealing fault 100 years later. The yellow line indicates the inclined sealing fault and the brown line represents the top surface boundary of the aquifer.
Figure 5.56: Enlarged Gas Saturation Profile for anisotropic formation \((k_v/k_h=0.1)\) with inclined sealing fault 100 years later. The yellow line indicates the inclined sealing fault and the brown line represents the top surface boundary of the aquifer.

The Figure 5.55 represents smaller anisotropy \((k_v/k_h=0.01)\) than the simulation in Figure 5.56 \((k_v/k_h=0.1)\), and we can easily figure out that the smaller value of \(k_v\) enforce more lateral flow. Consequently, in the case of smaller anisotropy model (Figure 5.55), the frontal part moves like the previous base case while the behind part rises toward the surface along the fault. In contrast, the larger anisotropy model (Figure 5.56) shows the frontal \(CO_2\) rises up along the sealing fault, and then reaches the top seal of the aquifer.

5.4.2 Fault Acting as a Conduit

Faults can provide channels for basement fluids to move across laterally continuous barriers to vertical fluid migration. Structural deformation of rocks during faulting and folding can enhance permeability with open joints. Higher transmissibility multiplier values \((TRANSF=100\) for \(IDIR-, JDIR-\) and \(KDIR+/\))
allow a specific series of grid blocks with inclination to represent high-permeability fault characteristics; thus, the assumed fault can affect CO$_2$ migration as a conduit (so-called "channeling effect").

**Reservoir with a Declined Conductive Fault**

In contrast to the sealing fault, this conductive fault cannot perform the structural trapping of CO$_2$ because the trap mechanism is based on the impermeable and convergent geologic structures. Instead, this simulation model can represent CO$_2$ leakage phenomena along and through the fault; thus, we can simply predict that the distribution of CO$_2$ will be concentrated on the fault structure.

First, the simulation model involves a declined fault that previous works for the sealing fault case proved to play a significant role in the structural trapping. In this simulation, all parameters are those of the base case except for the assignment of large transmissibility multipliers ($TRANSF$= 100) to grid blocks representing the fault ($IDIR$, $JDIR$ and $KDIR^{+/-}$). Also, the anisotropy is set to $k_v/k_h= 0.01$: 
Figure 5.57: Gas Saturation Profile for declined conductive fault 1 month later, $k_v/k_h = 0.01$. The yellow line represents the fault structure.

Figure 5.58: Gas Saturation Profile for declined conductive fault 20 years later

Figure 5.59: Gas Saturation Profile for declined conductive fault 45 years later
Figure 5.60: Gas Saturation Profile for declined conductive fault 100 years later

Figure 5.61: Gas Saturation Profile for declined conductive fault 200 years later

Figure 5.62: Gas Saturation Profile for declined conductive fault 300 years later
Figure 5.63: Gas Saturation Profile for declined conductive fault 400 years later

Figure 5.64: Gas Saturation Profile for declined conductive fault 600 years later

Figure 5.65: Gas Saturation Profile for declined conductive fault 1000 years later
As shown the above, CO₂ does not build up within the fault, phase flows quickly through the fault due to relatively larger transfer capacity of the fault. Actually, I expected that CO₂ distribution might appear largely along the fault zone. However, CO₂ did not migrate through the fault because the buoyant driving along the bedding plane due to dipping condition affects the major flow of the gas phase rather than fault’s geometry. As a result, despite the high-permeability (conductive) fault condition, CO₂ propagation tends to be parallel to the bedding plane not aligned to the fault zone.

*Reservoir with an Inclined Conductive Fault*

The next model contains an inclined fault that is located in the middle of CO₂-stored area. The combination between fault’s geometric property and reservoir’s dipping with anisotropic condition plays a crucial role in CO₂ distribution.
Figure 5.67: Gas Saturation Profile for inclined conductive fault 1 year later. 
\( k_v/k_h = 0.01 \). The yellow dot-line represents the fault.

Figure 5.68: Gas Saturation Profile for inclined conductive fault 10 years later

Figure 5.69: Gas Saturation Profile for inclined conductive fault 30 years later
Figure 5.70: Gas Saturation Profile for inclined conductive fault 65 years later

Figure 5.71: Gas Saturation Profile for inclined conductive fault 200 years later

Figure 5.72: Gas Saturation Profile for inclined conductive fault 400 years later
In these simulation results, we can discover that CO₂ flows dominantly through the convective fault, and accumulates at the top seal of the aquifer. This
phenomenon is exactly what we expected in the case of the high-permeability fault condition, which can be regarded as “CO₂ leakage.” In contrast to the previous case (declined fault model), the geometry of the fault (inclined condition) interplays with the petrophysical properties of the fault zone; and, positively affects CO₂ migration through the large-transfer-capacity geologic channel.

5.5 Effects of Residual Gas Saturation

The migration velocity up-dip of the layer of gas beneath the caprock can be crudely estimated from Darcy's law as shown in the section 5.2.1. Two major factors limit the distance that the carbon dioxide can migrate as a free gas phase. The first is the dissolution of the carbon dioxide in brine, and the second is trapping of residual gas saturation (S_{gr}) when the gas saturation falls to S_{gr}. As CO₂ migrates through the formation, some of it is captured and permanently remained in the pore space, which is referred to “residual CO₂ trapping” (Obdam et al., 2002). When the rate of this trapping is relatively high and CO₂ is injected at the bottom of a sufficiently thick formation, all of the injected CO₂ can be trapped by the mechanism, even before it reaches the top boundary of the formation. Likewise, the residual trapping mechanism plays a significant role in capturing CO₂ to be immobile.
However, in the simulation studies presented above, the residual CO$_2$ trapping is not considered. In this section the influence of residual gas saturation ($S_{gr}$) on the plume/fault interaction is investigated.

### 5.5.1 Rock-Fluid Data

From the mathematical relationship between the gas saturation and relative permeability of each phase introduced in the section 5.1.3 the relative permeability curve involving hysteresis for representing residual gas saturation is shown as the following Figure 5.76:

![Relative Permeability Curve](image)

Figure 5.76: Relative permeability curve involving residual gas saturation of $S_{gr}=0.2$

Table 5.9 lists the pertinent relative permeability parameters used for this case.
Table 5.9: Parameters of the Relative Permeability Curve with Hysteresis

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Residual gas saturation, $S_{gr}$</td>
<td>0.2</td>
</tr>
<tr>
<td>Critical gas saturation, $S_{gcr}$</td>
<td>0</td>
</tr>
<tr>
<td>Maximum gas saturation, $S_{gmax}$</td>
<td>0.9</td>
</tr>
<tr>
<td>Connate water saturation, $S_{wcon}$</td>
<td>0.1</td>
</tr>
<tr>
<td>Gas end point relative permeability, $k_{rg}$</td>
<td>0.716</td>
</tr>
<tr>
<td>Water end point relative permeability, $k_{rw}$</td>
<td>1</td>
</tr>
<tr>
<td>Water relative permeability exponent, $N_w$</td>
<td>2</td>
</tr>
<tr>
<td>Gas relative permeability exponent, $N_g$</td>
<td>2.5</td>
</tr>
</tbody>
</table>

The following Figure 5.77 shows the fractional flow curve:

![Gas Fractional Flow Curve for Drainage](image)

Figure 5.77: Fractional flow curve for gas phase drainage (dip angle, $\alpha = 5^\circ$), involving residual gas saturation ($S_{gr}=0.2$)

From the above Figure 5.77, the value of the frontal gas saturation is 0.42 for drainage curve and the value of the average gas saturation during the gas flood is 0.57.
5.5.2 Base Case with Residual Gas Saturation

*Isotropic reservoir condition*

As shown in the previous section 5.3, in the case of isotropic permeability, the vertical CO₂ migration was much more dominant than the parallel movement. Figure 5.78 through Figure 5.85 show how the isotropic condition affect the fluid flow combined with residual saturation.

![Figure 5.78: Gas Saturation Profile involving residual gas saturation 2 months later](image1)

![Figure 5.79: Gas Saturation Profile involving residual gas saturation 1 year later, k_v/k_h=1](image2)
Figure 5.80: Gas Saturation Profile involving residual gas saturation 5 years later, $k_v/k_h=1$

Figure 5.81: Gas Saturation Profile involving residual gas saturation 10 years later, $k_v/k_h=1$

Figure 5.82: Gas Saturation Profile involving residual gas saturation 15 years later, $k_v/k_h=1$
Figure 5.83: Gas Saturation Profile involving residual gas saturation 20 years later, $k_v/k_h=1$

Figure 5.84: Gas Saturation Profile involving residual gas saturation 100 years later, $k_v/k_h=1$

Figure 5.85: Gas Saturation Profile involving residual gas saturation 600 years later, $k_v/k_h=1$
From the above simulation results, we can easily figure out that all of grid blocks which CO₂ passes though show residual gas saturation: the blue color indicates 0.2 of gas saturation, which is the value of residual gas saturation, S_{gr}.

Consequently, this case represents quite similar trend of upward CO₂ migration compared with the base case due to isotropic condition; however, the explicit difference is that the amount of CO₂ approaching to the top seal is much less. The main reason is that the residual gas saturation results in trapping CO₂ permanently, so less of the initially present CO₂ is available to reach the impermeable surface boundary.

**Anisotropic reservoir condition**

Anisotropic permeability causes more lateral movement of CO₂. To identify the impact of anisotropy more clearly, a smaller permeability ratio (k_v/k_h) is applied by setting the input values of vertical (k_v) and horizontal (k_h) permeabilities as 0.01 md and 1 md. Accordingly, this case will show how the residual gas saturation will affect the migration of CO₂ combined with the anisotropy of permeability.

First of all, by using the analytical solution, which is introduced in the section 5.2, we can estimate the propagation of CO₂ under the specific reservoir condition. Then, the accuracy of the analytical solution can be validated by comparing estimated values with the simulation result. The behavior of CO₂
plume is varied depending on locally-induced conditions, especially counter-current flows. The effect of counter current flows will be discussed in the following sections regarding the flow vector analysis. The following table shows the distance and direction of CO₂ migration with a specific time step.

<table>
<thead>
<tr>
<th>Time step, years</th>
<th>Distance (d), ft</th>
<th>Direction (θ), degree</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Analytical Solution</td>
<td>Simulation Output</td>
</tr>
<tr>
<td>20</td>
<td>8.627</td>
<td>9.055</td>
</tr>
<tr>
<td>100</td>
<td>43.134</td>
<td>52.154</td>
</tr>
<tr>
<td>300</td>
<td>129.401</td>
<td>154.04</td>
</tr>
<tr>
<td>400</td>
<td>172.536</td>
<td>195.84</td>
</tr>
</tbody>
</table>

Table 5.10: Typical values of CO₂ distribution from the analytical solution, Equations 5.14 and 5.15, and the simulation results.

Following Figures 5.86 through 5.93 show the gas saturation profiles that are resulted from the dipping and anisotropic (\( k_v = 0.01 k_h = 0.01 \text{ md} \) ) reservoir model for different time steps:

![Figure 5.86: Gas Saturation Profile involving residual gas saturation 1 year later, \( k_v/k_h=0.01 \) ](image)

Figure 5.86: Gas Saturation Profile involving residual gas saturation 1 year later, \( k_v/k_h=0.01 \)
Figure 5.87: Gas Saturation Profile for dipping anisotropic formation ($k_v/k_h=0.01$) involving residual gas saturation 20 years later. The yellow arrow indicates the direction and distance of CO$_2$ migration.

Figure 5.88: Gas Saturation Profile for dipping anisotropic formation ($k_v/k_h=0.01$) involving residual gas saturation 100 years later. The yellow arrow represents the direction and distance of CO$_2$ migration.
Figure 5.89: Gas Saturation Profile for dipping anisotropic formation ($k_v/k_h=0.01$) involving residual gas saturation 300 years later. The yellow arrow represents the direction and distance of CO$_2$ migration.

Figure 5.90: Gas Saturation Profile for dipping anisotropic formation ($k_v/k_h=0.01$) involving residual gas saturation 400 years later. The yellow arrow represents the direction and distance of CO$_2$ migration.
Figure 5.91: Gas Saturation Profile involving residual gas saturation 500 years later, $k_r/k_S=0.01$

Figure 5.92: Gas Saturation Profile involving residual gas saturation 800 year later, $k_r/k_S=0.01$

Figure 5.93: Gas Saturation Profile involving residual gas saturation 7000 years later, $k_r/k_S=0.01$
The remarkable characteristics of this simulation model are the appearance of residual gas trapping on the trace of the CO₂ migration and smaller amount of CO₂ buildup at the surface boundary. By comparing Figure 5.92 with Figure 5.31, the previous model contains most CO₂ at the surface; while, the current model has sparsely distributed CO₂ due to residual gas saturation.

Likewise, hydrodynamic trapping can occur in saline formations that do not have a closed trap, but where fluids can migrate slowly over long distances. When CO₂ is injected into a deep formation, it displaces brine water and then moves upwards buoyantly due to the contrast of density. Even after approaching the top or the edge of the formation, CO₂ continues to migrate as a separate phase until it is trapped by residual gas saturation or in local physical traps within the sealing formation.

5.5.3 Combined Effect of Fault and Residual Gas Saturation

As shown above, accounting for residual gas saturation has significant consequence for trapping. Therefore, we need to investigate how residual saturation would affect the CO₂ migration combined with faulting conditions. The physical trapping below low-permeability seals (cap rock), including structural and stratigraphical traps, is the principal means to store CO₂ in the formation. Especially, faults can act as permeability barriers or as preferential pathways for fluid flow depending on geological circumstances.
First, a sealing fault will be considered. The reservoir is anisotropic (the ratio of vertical to horizontal permeability is 0.01). We will see that this makes it possible to maximize the effectiveness of a structural CO₂ trapping mechanism (fault-trapping).

**Reservoir with a Declined Sealing Fault**

The sealing declined fault can compose the structural trap with surrounding boundaries. Accordingly, we can predict that CO₂ flow will be blocked by the seal’s integrity, and then will migrate along the fault upwards. As a result, all of CO₂ will be accumulated at the down-dip area of the aquifer. The grid blocks that represent a sealing fault have zero value of transmissibility multiplier \((\text{TRANSF}=0 \text{ for } IDIR^+/-, JDIR^+/- \text{ and } KDIR^+/-)\).

Figure 5.94: Gas Saturation Profile for tilted anisotropic formation \((k_v/k_h=0.01)\) having residual gas saturation \((S_{gr}=0.2)\) with a declined sealing fault, 20 years later. The yellow straight line represents the fault geometry.
Figure 5.95: Gas Saturation Profile with residual gas and structural trapping 200 years later

Figure 5.96: Gas Saturation Profile for dipping anisotropic formation ($k_v/k_h=0.01$) involving residual gas saturation with a declined sealing fault 400 years later. The red arrows represent the major velocity trend for CO$_2$ flow. The early flow is blocked by the seal integrity. A buildup of CO$_2$ occurs, and then CO$_2$ migrates upward along the sealing fault.
Figure 5.97: Gas Saturation Profile for residual gas and structural trapping, 600 years later

Figure 5.98: Gas Saturation Profile for residual gas and structural trapping, 1000 years later

Figure 5.99: Gas Saturation Profile for residual gas and structural trapping 7000 years later
As shown on the above simulation results, the early CO₂ buildup occurs along the fault zone where the gas phase is blocked by a zero-permeability seal. A later CO₂ buildup appears at the upper surface due to the combination between buoyancy force and structural traps. In addition, the accumulation after buoyant migration at the top of the formation is smaller than when which is clearly shown by comparing Figure 5.99 with Figure 5.43 in the section 5.4.1.

Reservoir with an Inclined Sealing Fault

The next model represents the inclined faulting that crosses through the CO₂ storage zone. The grid blocks involving the property of the low-permeability fault zone have zero value of transmissibility multipliers \((TRANSF = 0, \ IDIR+/-, \ JDIR+/- \text{ and } KDIR+/-)\).

Figure 5.100: Gas Saturation Profile for dipping anisotropic formation \((k_v/k_h=0.01)\) involving residual gas saturation \((S_{gr}=0.2)\) with an inclined sealing fault 1 year later
Figure 5.101: Gas Saturation Profile with residual gas and structural trapping 20 years later

Figure 5.102: Gas Saturation Profile with residual gas and structural trapping 100 years later

Figure 5.103: Gas Saturation Profile with residual gas and structural trapping 200 years later
Figure 5.104: Gas Saturation Profile with residual gas and structural trapping 400 years later. The red arrows indicate the flow behavior of the separated gas phases by low-permeability (sealing) fault. The right part is independent on the fault property; while, the left portion is affected by the fault.

Figure 5.105: Gas Saturation Profile with residual gas and structural trapping 700 years later
In this simulation model, the sealing fault is in the middle of stored CO$_2$; therefore, CO$_2$ distribution is separated into frontal and behind portion by the seal. The behavior of the frontal part shows immiscible displacement based on Buckley-Leverett theory; on the other hand, the behind part is blocked by the seal integrity, and migrates upwards along the fault. These results are quite similar as the section to 5.4.1, associated with no-residual-trapping case, has shown. The frontal CO$_2$ in this model does not have the buildup along the vertical boundary,
and the accumulation of the behind CO₂ is also much less than that of the previous model mainly due to residual gas trapping. It is clearly explained by comparing Figure 5.107 with Figure 5.54 in the section 5.4.1.

On the other hand, if a fault has high permeability and transmissibility, the fault may act as a 'conduit,' which implies this geologic structure can provide a preferential path for the CO₂ migration. Therefore, we can predict that most of CO₂ flow appears inside the convective fault zone.

*Reservoir with a Declined Conductive Fault*

First, we investigate dynamics of the reservoir model involving a declined fault. The grid blocks that represents high-permeable (conductive) fault has higher values of transmissibility multiplier in j and k direction ($TRANSF= 100$ for $IDIR-$, $JDIR-$ and $KDIR+/-$).

![Gas Saturation Profile for tilted anisotropic formation (k_v/k_h=0.01) involving declined conductive fault 1 year later. The yellow dot-line represents the fault structure.](image)

Figure 5.108: Gas Saturation Profile for tilted anisotropic formation ($k_v/k_h=0.01$) involving declined conductive fault 1 year later. The yellow dot-line represents the fault structure.
Figure 5.109: Gas Saturation Profile for declined conductive fault 20 years later

Figure 5.110: Gas Saturation Profile for declined conductive fault 60 years later

Figure 5.111: Gas Saturation Profile for declined conductive fault 100 years later
Figure 5.112: Gas Saturation Profile for dipping anisotropic formation (\(k_v/k_h=0.01\)) involving residual gas saturation with a declined conductive fault 200 years later. The red arrows represent the separated flow behaviors resulted from the high-permeability fault. The small arrow indicates the direction of CO\(_2\) accumulation due to high-permeability of the fault zone; thus, actual gas flux direction may be more complex, and we will discuss it in the following section.

Figure 5.113: Gas Saturation Profile for declined conductive fault 300 years later
Figure 5.114: Gas Saturation Profile for declined conductive fault 400 years later

Figure 5.115: Gas Saturation Profile for declined conductive fault 500 years later

Figure 5.116: Gas Saturation Profile for declined conductive fault 700 years later
The remarkable phenomenon in Figure 5.109 through 5.112 that is CO₂ crosses quickly the high-permeability fault zone, and then makes a buildup along the fault to some extent. The conductive fault provides another pathway for the gas phase. However, some of CO₂ still shows the buoyant migration parallel to the bedding plane and the accumulated gas also moves laterally after CO₂ builds up to some extent as illustrated by Figure 5.113. Therefore, we can conclude that the buoyant driving force due to a dip plays a crucial role in determining the major behavior of
CO₂ flow. In addition, the declined conductive fault will offer more benefit of residual trapping by expanding the area vertically through which CO₂ plumes migrate through due to buoyancy.

Reservoir with an Inclined Conductive Fault

In the case of the inclined high-permeability faulting, we can predict that the fault zone may be the channel for preferential CO₂ flow toward the surface (leakage) because the combination between inclined fault geometry and the tilted bedding condition will maximize fluid migration. The grid blocks that represent high-permeable fault property have relatively higher transmissibility multipliers than surrounding reservoir blocks (TRANSF = 100 for $IDIR-, JDIR-$ and $KDIR+/-$).

Figure 5.119: Gas Saturation Profile for inclined conductive fault 1 year later. $k_v/k_h = 0.01$. The yellow dot-line represents the fault geometry.
Figure 5.120: Gas Saturation Profile for residual gas trapping and leakage 20 years later

Figure 5.121: Gas Saturation Profile for residual gas trapping and leakage 45 years later
Figure 5.122: Gas Saturation Profile for residual gas trapping ($S_{gr}= 0.2$) and inclined conductive fault 100 years later. $k_v/k_h= 0.01$. The red arrows represent the direction of gas propagation (one is through the conductive fault; while, another represents CO$_2$ plume not affected by the fault), and the white arrows indicate the CO$_2$ migration from new sources along the fault by “channeling effect.”

Figure 5.123: Gas Saturation Profile for residual gas trapping and leakage 200 years later
Figure 5.124: Gas Saturation Profile for residual gas trapping and leakage 300 years later

Figure 5.125: Gas Saturation Profile for residual gas trapping and leakage 400 years later

Figure 5.126: Gas Saturation Profile for residual gas trapping and leakage 500 years later
From both Figure 5.122 and 5.123, we can discover the newly-appeared preferential CO₂ flow through the conductive fault, and the CO₂ migration approaches the top of the formation quite quickly. In addition, Figure 5.121 to 5.125 show that the conductive fault zone creates additional virtual sources of CO₂ along the fault. The major behavior of CO₂ flow is controlled by overall reservoir property (dipping). As shown in the above Figure 5.127, this appropriate
combination between the dipping of the reservoir and the conductive fault geometry allows more residual CO₂ trapping by enlarging the contact area of the migration even though the fault zone acts as a conduit that often results in unexpected gas seepage. Anisotropy results in dominantly parallel movement of CO₂, which also increases the area where CO₂ invades. Thus, residual saturation trapping can take an advantage by the interaction between dipping and anisotropy.

5.6 Analysis of CO₂ Plume Behavior with Flow Vectors

As I have investigated, the dynamics of CO₂ plumes is too complicated to analyze only with saturation profiles, which are based on the change of saturation value (scalar) in each grid block. Even though the distribution of gas saturation can show rough trend of CO₂ migration, we cannot see what happens inside of the plume. Furthermore, the saturation profile cannot provide enough information which may explain unexpected CO₂ behavior. Thus, we used the distribution of flow vectors for gas and water phases to analyze the dynamics of CO₂ plumes because vector analysis allows us to measure directly physical quantities (magnitude and direction) of the flow.

5.6.1 Vector Analysis of Declined Fault

The previous simulations assume a dip angle = 5°; thus, the buoyancy plays a significant role in CO₂ migration both vertically and laterally. The simulation
outputs show how dipping condition combined with geologic discontinuity influences the fluid flow tendency. Especially, the effect of the sealing fault (acting as a barrier) is clearly observed in the previous figures as what I expected before the simulation work; thus, it becomes solid that the sealing fault can divide the domain into two sections: fault-dependent and fault-independent.

Figure 5.129: Gas Saturation Profile with Gas Flux Vectors for dipping formation involving a declined sealing fault and anisotropy ($k_v/k_h = 0.01$)

The above Figure 5.129 represents the behavior of CO$_2$ plumes after hitting a sealing fault. Initially, CO$_2$ tend to migrate parallel to the bedding plane due to anisotropy, but the sealing fault prevents CO$_2$ propagation. Thus, CO$_2$ accumulates until reaching endpoint gas saturation of 0.9 (orange colored grid blocks), and then moves upward along the fault. The gas flux vectors explicitly
show the dynamics of CO₂ plumes. On the contrary, the following Figure 5.130 shows the effect of water phase on the gas phase dynamics. The counter current flows of water phase surround the external boundaries of CO₂ plumes, and they fill the inside of plume as well. Therefore, we can predict that CO₂ trapping take an advantage from the counter current flows due to the declined sealing fault.

Figure 5.130: Gas Saturation Profile with Water Flux Vectors for dipping formation involving a declined sealing fault and anisotropy ($k_v/k_h= 0.01$). The white arrows represent the counter current flow of water phase.

On the other hand, in the case of a conductive fault (acting as a conduit), gas flows (purple colored blocks) on the opposite side along the fault are observed. This accumulation indicates that the gas does not build up because on that side of the fault, CO₂ is able to continue migrating in the direction determined
by dip and anisotropy. The following zoomed-in Figure 5.131, which shows a dipping reservoir containing a highly declined conductive fault, shows the gas saturation profile with gas flux arrows. The grid blocks representing fault properties have transmissibility multiplier value = 100, which means that the fault zone can transfer fluids one hundred times more than the non-faulted zone can.

Figure 5.131: Gas Saturation Profile with Gas Flux Vectors for dipping formations involving a declined conductive fault and anisotropy ($k_v/k_h = 0.01$), 300 years later

As the above illustration shows, some flux arrows, surrounded by a yellow circle, moves upward through the fault-assigned grid blocks (purple). These explain the large CO$_2$ saturation (yellow) in the grid blocks along the opposite side of the fault. It is because initial CO$_2$ plume tends to migrate corresponding to the reservoir conditions (anisotropy and dipping). After the plume meets a
conductive fault it passes through fault-assigned grid blocks swiftly and then accumulates in the ordinary grid blocks next to the fault. On the other hand, the upper region along the fault, the area represented by a red circle, also contains CO₂. The conductive fault plays a crucial role in this upward distribution of CO₂ plumes. A large amount of CO₂ migrates through the fault of which transfer capacity is greater than transport rate of the extra domain. However, as gas flow vectors show, the major flow inside the plume is also affected by anisotropy and dipping. Therefore, we can conclude that the existence of a fault has a remarkable impact on the behavior of CO₂ plume, but its effect is local-induced, which means that the basic dynamics of CO₂ is based on the whole domain’s properties.

Figure 5.132: Gas Saturation Profile with Gas Flux Vectors for non-dipping formations involving a declined conductive fault and anisotropy (k_v/k_h= 0.01), 300 years later
The above simulation model (Figure 5.132) assumes the same properties as the previous case (Figure 5.131) except non-dipping condition. The upper contact area of initial CO₂ tends to migrate upward, while the right side of CO₂ shows parallel movement due to water phase’s invasion. In this case we cannot discover such a large CO₂ saturation along the fault as the previous dipping case has shown. Instead, most CO₂ moves upward because CO₂ plumes have dominantly upward movement due to un-tilted condition as flow vectors explain. Thus, we can conclude that the interaction between reservoir conditions and a fault play a significant role in altering the major flow tendency of CO₂.

5.6.2 Vector Analysis of Vertical Conductive Fault

It is also worthwhile to investigate how the geometric property of a fault affects the CO₂ migration. The first case is a vertical fault, in which the fluid flow is aligned with the gravity direction. Gas saturation profile shows that CO₂ passes through the high-permeability fault rapidly, and accumulates under the top surface boundary of the reservoir, instead of buildup along the fault. The simulation model contains the same reservoir properties \( \frac{k_v}{k_h} = 0.01 \), dip angle \( 5° \) and fault’s petrophysical properties \( TRANSF = 100 \), \( IDIR- \), \( JDIR- \) and \( KDIR+/− \) except the fault’s geometry (vertical fault).

The following Figure 5.133 (year 2055) illustrates both the swift CO₂ migration through the fault, resulting in small gas saturation value in fault blocks,
and the formation of CO\textsubscript{2} buildup at the top surface. In addition, there is small flow from the fault into the formation in the up dip direction. Similar to the declined conductive fault case, the invasion of water phase into the bottom of initial CO\textsubscript{2} causes gas to migrate toward the fault.

Figure 5.133: Gas Saturation Profile with Gas Flux Vectors for dipping anisotropic formation \((k_v/k_h= 0.01)\) involving a vertical conductive fault, 75 years later. The yellow line represents the fault, and the part surrounded by red circle shows gas build-up under the top seal.

In the case of non-dipping condition, the frontal portion of CO\textsubscript{2} plumes migrates toward the fault due to the displacement by water phase, similar to the above case (Figure 5.133). However, no horizontal fluid flow occurs while CO\textsubscript{2} rises through the fault as shown the following Figure 5.134. This result can be easily
understood in the way of idea that more fluids tend to flow toward less resistant pathway. That is to say, fluids in the fault must be affected much more by the fault transmissibility, which is larger than other surrounding grid blocks, rather than by anisotropy. Additionally, we can recognize that the CO₂ buildup shows a symmetric formation, which confirms the theoretical fact that under non-dipping condition the displacement between two phases will not be affected by any other driving forces except the effect of gravity.

Figure 5.134: Gas Saturation Profile with Gas Flux Vectors for non-dipping anisotropic formation (kᵣ/kₜ= 0.01) involving a vertical conductive fault, 75 years later
5.6.3 Vector Analysis of Inclined Conductive Fault

In the case of a tilted reservoir, inclined faults with high-permeability enable injected CO₂ to leak towards the top of the aquifer more easily because the dipping condition allows the buoyancy force to be non-zero in the direction of the bedding plane. Therefore, the inclined geometry amplifies CO₂ leakage along the fault by interacting with the high-permeability property of the fault zone. The following Figure 5.135 (year 2180) illustrates the gas saturation profile on which the gas flux vectors are overlapped. The simulation model involves the same reservoir properties (kᵣ/kₜ = 0.01, dip angle = 5°) and fault’s petrophysical properties (TRANSF= 100, IDIR-, JDIR- and KDIR+/−) except the fault’s geometry (inclined fault).

In the case of a dipping aquifer, the major gas flux occurs inside the conductive inclined fault because the combination of dip and high-permeability of the fault increases CO₂ migration through the fault zone (so-called "channeling effect"). Therefore, buoyancy force due to a dip and density difference between two phases allow gas phase move upward with remarkable flow rate (yellow arrow for gas flux in Figure 5.135). Meanwhile, water phase must be displaced by gas phase as CO₂ migrates toward the surface.
Figure 5.135: Gas Saturation Profile with Gas Flux Vectors for dipping anisotropic formation (k_v/k_h = 0.01) involving an inclined conductive fault, 200 years later. The yellow arrow indicates the major behavior of CO₂, and the portion indicated by red circle shows the parallel migration of CO₂ plumes due to dipping condition.

The following Figure 5.136 (year 2180), which shows gas saturation profile with water flux vectors, explains how water phase distributes compared with gas phase.
Figure 5.136: Gas Saturation Profile with Water Flux Vectors for dipping anisotropic formations \((k_v/k_h = 0.01)\) involving an inclined conductive fault, 200 years later. The blue, white and yellow arrows represent the flow tendency of the water phase.

The above illustration represents that water flux vectors rarely appear inside the high-permeability fault blocks; and, the water phase on the left side of the fault moves down due to the gravitational displacement as expressed with blue arrows. In addition, we can discover counter current flows of the water phase inside the CO\(_2\) plumes as well as at the external boundaries (presented with white arrows) except the head part (presented with yellow arrow). Therefore, we can expect that the CO\(_2\) migration can take an advantage of trapping and lateral behavior by counter current flows.
In the case of non-dipping reservoir as shown below (Figure 5.137), the gas phase flux appears remarkably higher through the conductive fault than dipping. The build-up under the top seal creates a symmetric CO$_2$ distribution, which implies there is no driving force for CO$_2$ dynamics except the density difference of phases. Thus, we can expect that it may be important to integrate geologic and petrophysical properties for reducing uncertainty of comprehensive analysis.

Figure 5.137: Gas Saturation Profile with Gas Flux Vectors for non-dipping anisotropic formation ($k_v/k_h=0.01$) involving an inclined conductive fault, 200 years later. The part surrounded by red circle shows the vertical migration of gravity-driven CO$_2$ flow.
In addition, the difference compared with the dipping condition that is the vertical distribution of CO₂ along the fault. The lateral migration of CO₂ results from the combination between anisotropy and dipping. For non-dipping case the buoyancy-driven force mainly controls the CO₂ behavior. Thus, even if the conductive fault has the higher capacity of transfer, the vertical displacement (marked by red circle in Figure 5.137) along the fault is dominant because the domain does not involve a dip largely related to the parallel displacement, which can occur in the case of dipping reservoir (marked by red circle in Figure 5.135).

5.7 Leakage through a Sealing Fault

When it comes to performing the CO₂ sequestration, the most sensitive issue is the CO₂ leakage. Most leakage routes in a depleted reservoir are related to the abandoned wells. This study focuses only on natural pathways to evaluate the potential risk of CO₂ leakage.

High-permeability faults (conduits) are typical natural routes of leakage. They are oriented for shear failure in the existing stress field; thus, if we develop the dynamic relationship between faults' geometry and current state of pressure, the potential leakage path can be predicted. On the other hand, low-permeability faults (barriers) involve seal integrity, which can trap CO₂ with impermeable boundaries. However, the geologic imperfections can happen in this sealing zone mainly due to the local variation of pressure and injection rate as well as tectonic
effects. The regional change of petrophysical properties results in the occurrence of fractures. At a large scale, the overall alteration of geomechanical properties by tectonic processes causes structural transform (transform faults) or addition of geologic discontinuities.

In this simulation work, the focus is made on the impact of geologic imperfection in the sealing fault zone. This will illustrate how the geometric heterogeneity affects the CO$_2$ distribution. The reason why we do not consider the conductive fault is that they are initially assumed to be large-scale leakage pathways.

### 5.7.1 Leakage through Defeat in a Declined Sealing Fault

First, the reservoir model containing a declined sealing fault was revised so that a portion of the fault was assigned conductive petrophysical properties. The leakage characterization is by using a higher transmissibility multiplier value (using "1", $TRANSF= 1$ for $IDIR+/-$, $JDIR+/-$ and $KDIR+/-$) in that region, and zero ($TRANSF= 0$) in the sealing fault zone. The modified grid block is (1, 106, 22). Also, the model contains the same reservoir properties ($k_v/k_h= 0.01$, dip angle$= 5^\circ$ and $S_{gr}= 0.2$). The following Figures show leakage phenomenon:
Figure 5.138: Leakage Analysis: Gas Saturation Profile for a declined sealing fault in the anisotropic reservoir ($k_v/k_h = 0.01$), 300 years later. The yellow line represents the fault structure.

Figure 5.139: Leakage Analysis: Gas Saturation Profile for a declined sealing fault, 400 years later. The red circle indicates the leakage point.
Figure 5.140: Leakage Analysis: Gas Saturation Profile for declined sealing fault, 600 years later

Figure 5.141: Leakage Analysis: Gas Saturation Profile for declined sealing fault 800 years later

Figure 5.142: Leakage Analysis: Gas Saturation Profile for declined sealing fault 1000 years later
As the above flow simulation results have shown, most CO$_2$ rises toward the surface along the fault, but the small amount of CO$_2$ passes through the fault zone involving relatively higher transmissibility and shows a similar propagation corresponding to Buckley-Leverett theory. It means that the seepage creates another gas migration; and it can move independently. In addition, the amount of rising CO$_2$ along the sealing fault changes abruptly at the horizontal level of the
leakage origination; thus, we can estimate that the seepage level represents the level of area from which less residual gas saturation traps happen.

5.7.2 Leakage through Defeat in a Inclined Sealing Fault

In the inclined fault model, we put the leakage properties ($TRANSF= 1$ for $IDIR+/-$, $JDIR+/-$ and $KDIR+/-$) on the grid blocks, (1, 95, 25) and (1, 96, 25). Also, the model contains the same reservoir properties ($k_v/k_h= 0.01$, dip angle=$5^\circ$ and $S_{gr}= 0.2$). The following figures show the effect of imperfection of the seal integrity combined with permeability anisotropy, dipping and inclined fault geometry.

Figure 5.145: Leakage Analysis: Gas Saturation Profile for inclined sealing fault, 200 years later. The yellow line represents the fault.
Figure 5.146: Leakage Analysis: Gas Saturation Profile for inclined sealing fault 300 years later. The red circle points out the leak spot.

Figure 5.147: Leakage Analysis: Gas Saturation Profile for inclined sealing fault 400 years later. The area surrounded by the yellow circle shows unexpected behavior of CO₂ plumes. This dynamics will be discussed with flow vectors.

In the Figure 5.147, we can discover unexpected dynamics of CO₂ plumes (yellow circle). As we have investigated before, the fault has a remarkable effect on the local distribution of CO₂. For this case, the fault contains a leak spot that causes similar CO₂ behavior in the conductive fault case. At first, CO₂ plumes migrate
upward along the sealing fault. After they meet the leak point, two explicit behaviors occur: upward migration along the sealing fault and seepage through the leak. However, the leak region has small capacity of transfer so that CO₂ cannot pass through it enough and then accumulate (so-called "bottleneck state"). The flow vectors in the following Figure 5.148 show clearly the dynamics inside CO₂ plumes:

Figure 5.148: Leakage Analysis with Gas Flux Vectors: Gas Saturation Profile for inclined sealing fault in the anisotropic \( (k_v/k_h=0.01) \) and dipping (dip angle=5°) condition, 600 years later. The area pointed out by yellow circle shows gas phase vectors are dominantly parallel to the bedding plane due to the existence of the leak spot.
Figure 5.149: Leakage Analysis: Gas Saturation Profile for inclined sealing fault 600 years later

Figure 5.150: Leakage Analysis: Gas Saturation Profile for inclined sealing fault 800 years later

Figure 5.151: Leakage Analysis: Gas Saturation Profile for inclined sealing fault 1000 years later
From the above outputs, we can discover the similar CO₂ distribution with the declined fault model. This simulation model shows gas migration along the fault, gas buildup at the top seal of the aquifer, gas seepage with independent flow and divided residual gas saturation traps at the leakage level. The most critical difference is that the CO₂ migration consists of two parts: frontal and behind portion, which are initially divided by the existing sealing fault. As shown the above, the frontal portion may not be affected by the CO₂ leakage (compared with no-leakage model); therefore, we can conclude that the leakage impact will take place locally so that we need to specify each regional variation of properties from the main fault system.
Chapter 6: CONCLUSIONS AND RECOMMENDATIONS

6.1 Summary and Conclusions

The CO₂ injection and storage in underground geologic formations is an important option for reducing CO₂ emissions into the atmosphere. This technology is based on the idea that CO₂ is captured and separated before it is emitted into the air, and injected deep into the earth where it will remain permanently (over 10,000 years). Therefore, trapping CO₂ at depth for enough time, the formation requires a sufficiently impermeable cap rock layer. However, naturally cap rock layers may contain geologic imperfections, such as faults or fractures, which can be the preferential pathway for leakage of CO₂ from depth to the near surface.

The primary aim of this study was to investigate the effects of faults on the stored CO₂ migration after injection ends. Faults play a major role in the distribution and buoyancy-driven flow of CO₂. Simulation results reveal how the fault properties, especially high or low transmissibility of fault blocks, combine with reservoir's anisotropy to affect the CO₂ migration. Numerical analysis and investigation of CO₂ migration has resulted in the following conclusions:

1. Numerical analysis has been carried out to estimate the distance and direction of buoyancy-driven CO₂ flow in homogeneous and in anisotropic reservoirs. The interaction between gas (CO₂) and water (brine) phases was based on the Buckley-Leverett theory. This numerical method allows us to estimate
directly CO₂ advances (distance and angle) associated with rock properties. However, the presence of a fault results in the numerical analysis not to be applicable, and this fact indicates that locally-induced reservoir conditions strongly affect the phase behavior.

2. Immiscible displacement of two phases within a closed domain is driven by gravitational force and the density difference of two phases. Under the dipping condition the driving force component in the direction of the bedding plane has non-zero value. Accordingly, fluid flows should be considered the vector sum of each force component in the tilted reservoir. Analytical solutions provide reasonable estimates of simulated plumes.

3. Dip and anisotropy ($k_v/k_h < 1$) in the reservoir cause the preferential flow to be predominantly aligned with the bedding plane. The smaller $k_v$ prevents CO₂ from flowing upward, instead urging it to move laterally; furthermore, dipping condition forces CO₂ migration more strongly in the direction of bedding plane due to non-zero component of buoyancy driving force in that direction.

4. The property of rocks, which compose the reservoir, has another impact on the distribution of CO₂. The residual gas saturation and the endpoint gas saturation are the main factors for the residual-saturation trapping mechanism. As CO₂ migrates, the flux of CO₂ decreases by the amount left behind as the residual gas saturation. After arriving at no-flow boundaries CO₂ accumulates until CO₂
gas saturation reaches the endpoint value represented on the relative permeability curve.

5. The effect of a fault on the buoyancy-driven flow varies with its geometry, structure and petrophysical properties. In this work, declined versus inclined faults and the high-permeability versus low-permeability faults are the main categories that we focus on.

5a. A sealing fault (low-permeability) blocks further CO₂ migration. For the declined case the gas accumulation along the fault happens first, and then CO₂ moves toward the top surface of the aquifer. The remarkable phenomenon is that counter current flows between gas and water phases occur during the accumulation period; therefore, the Buckley-Leverett theory cannot apply to the flow analysis any more. On the other hand, for the inclined case CO₂ migrates along the fault due to the partial alignment between the main flow trend and the fault direction. CO₂ then forms a build-up near the top surface boundary.

5b. The conductive (high-permeable) fault acts as a conduit in the CO₂ migration, which means that the fault create another pathway for the fluid flow. In the case of a declined fault, CO₂ crosses the fault zone swift and accumulates along the fault until the CO₂ source depletes. The accumulated gas then propagates into the formation up-dip of the fault. Meanwhile, for the inclined fault, typically CO₂ reaches the surface first through the fault, and accumulate the upper part of the reservoir. During upward migration through the fault, CO₂
creates another virtual source along the fault for migration, which allows the larger area in which CO₂ invades. Therefore, we can expect that residual saturation trapping takes an advantage from the interaction between the conductive fault and reservoir conditions.

6. The distribution of fluid phases (CO₂ and brine) in the closed-boundary is controlled mainly by reservoir properties. Even if the appearance of geologically discontinuous structures, mainly faults, has a remarkable influence on the dynamics of CO₂ plumes, its effect must be locally induced. Accordingly, the density difference between two phases, buoyancy due to the dipping condition and anisotropic permeability play a crucial and basic role in the control of the fluids' movement.

6.2 Recommendations

Throughout this simulation study, the reservoir conditions are based on several critical assumptions: homogeneity of permeability, non-fractured system, static and faults. Even if we focus on the faults' effect on the CO₂ migration with the simplified and idealized model, the in-situ reservoir conditions involve numerous factors that we cannot predict in advance. To reduce this ambiguity, future the upcoming simulation study must consider the following factors:
1. The heterogeneity of the rock properties may cause less preferential flow of fluids, which tend to migrate along less resistant paths. Especially, immiscible displacement between two phases, gas and brine, will show more complicated phenomena because brine, representing higher density, will move downward while CO₂, involving lower density, rise upward. Accordingly, the communication between fluids' nature and aquifer's heterogeneity may cause quite different flow trend comparing with homogeneous environment.

2. Capillary pressure can act as a barrier on buoyant flows because fluids can pass through a rock only when pressure overcomes capillary entry. If CO₂ migration encounters a layer whose capillary pressure exceeds the entering pressure of CO₂, the gas phase cannot advance further (so-called "capillary trapping"). This capillary entry pressure is largely correlated to rock permeability; thus, we can predict that the influence of capillary pressure may show quite similar consequence of the anisotropy effect.

3. Naturally, all types of rocks contain fractures, which provide the main path for fluid flows combined with rocks' reservoir properties. A fracture, which is another occurrence of geometric discontinuity in a porous rock, has a strong impact on fluid flow due to its complex distribution. The upcoming simulation model requires characterizing fracture properties to identify the interplay between both geologic imperfections; thus, it may help to minimize structural uncertainty resulted from the structural heterogeneity.
4. The static condition of a fault is one of the most important assumptions in this simulation work. However, generally faults involve dynamic properties, which mean that the earth's tectonic activities and change of reservoir properties cause variation of parameters associated with a fault change. Due to such heterogeneity of boundary conditions simplified numerical analysis of fluid distribution in this study may not be reasonable to explain in-situ condition. Therefore, the most adjustable simulation should be four-dimensional (4-D) scale (so-called "history-matching"), and the dynamic modeling process for upcoming studies needs to use time-dependent function to interpret dynamic behavior of faults.

5. To analyze the dynamic fault change in the CO₂ sequestration procedure it is necessary to couple between fluid flow and geomechanical deformation. It means that we need to separate the non-linear variation of reservoir properties with time-step as well as to localize heterogeneity of faults' effect; and then, we can derive the cumulative effects of dynamic changes in each geologic location. In this coupling process, the dynamic change involves both structural deformation and diverse petrophysical parameters' alteration. Thus, we need to determine the reasonable range of considering elements (rate of deformation, conductivity of fault zone, relative permeability curve for rocks, etc.) In addition, the time-step should be applicable to represent every designated time intervals (periodic, episodic, asymptotic), instead of oversimplified or too fine time-step.
Appendix A: GEM Input File for Base Case

Following codes are from the GEM input data file to simulate the base case, which is assumed as an isotropic, homogeneous and unfaulted reservoir.

```
*TITLE1 'CO2 Gas Storage Model'
*TITLE2 '2D Model : No Faults'
*CASEID 'Tilted Reservoir with no Residual Gas Saturation'
*DIM *MDIMPL 50
*DIM *MDICLU 20000000
*DIM *MDLU 20000000
*OUTPRN *RES *ALL
*OUTPRN *GRID DENG DENO DENW KRG KRO KRW PCG PCW PRES RHOG RHOO
SG SO SW VISG VISO VELOCRC DROP SATP
*OUTSRF *WELL *PSPLIT
*OUTSRF *WELL *TOIP *TGIP *TWIP *RECO *RECG
*OUTSRF GRID DENG DENO DENW KRG KRO KRW PCG PCW PRES RHOG RHOO
SG SO SW VISG VISO VELOCRC
*OUTSRF *RES *ALL
*WSRF *WELL *TIME
*WSRF *GRID *TIME
*INUNIT *FIELD
*WRST 0
*RESULTS XOFFSET 0.0000
*RESULTS YOFFSET 0.0000
*RESULTS ROTATION 0.0000 **Degrees

** Definition of fundamental cartesian grid **
*GRID CART 1 200 50 **Cartesian Grid System (1×200×50 Grid Blocks)
*KDIR DOWN
*DI CON 2 **Grid Block Size, ft
*DJ CON 2
*DK CON 2
*DEPTH 1 100 1 5300 **Standard Point and Depth, ft
*DIP 0 5 **Dip Angle
*NULL MATRIX CON 1
*TRANSI MATRIX CON 1 **Transmissibility Values
*TRANSJ MATRIX CON 1
*TRANSK MATRIX CON 1
*POR MATRIX CON 0.15 **Porosity
*PERMI MATRIX CON 1 **Permeability, md
```
*PERMJ  MATRIX CON 1
*PERMK  MATRIX CON 1
** Property: Pinchout Array Max: 1 Min: 1
** 0 = pinched block, 1 = active block
*PINCHOUTARRAY CON 1
*CPOR  MATRIX 3.0E-6 **Rock Compressibility
*PRPOR  MATRIX 14.7

**---------------------------------------- FLUID COMPONENT DATA ----------
*MODEL   *PR **Peng-Robinson EOS
*NC 2 2
*COMPNAME 'CO2' 'H2O' **Component Indication
**SOLUBILITY *IDEAL
*HCFLAG 0 0
*VISCOR *PEDERSEN
*VISCOEFF 0.291
  1.4
  0.0005747
  4.265
  1.0579
*MIXVC 1
*TRES 140.
*PCRIT 72.809000 217.754600
*TCRIT 304.12780 647.094400
*AC 0.223940 0.344000
*VCRIT 0.094000 0.056000
*MW 44.01000 18.015000
*PCHOR 78.00000 52.00000
*SG 0.818000 1.000000
*TB -109.21000 212.00000
*ZCRIT 0.274139 0.229409
*VISVC 0.094000 0.056000
*VSHIFT 0.024668 0.234867
*OMEGA 457235530 457235530
*OMEGB 077796074 077796074
*BIN -0.0576003
*PHASEID DEN **Phase Identification Criteria

**---------------------------------------------ROCKFLUID DATA----------------------------
*ROCKFLUID
RPT 1 SCALING-OLD
*SGT **Gas-Oil Relative Permeability Values
**Gas Saturation
  0 0 1
  0.1 0.00308642 0.790123457 **Relative Permeability of Gas Phase
  0.15 0.008505173 0.694444444 **Relative Permeability of Oil Phase
  0.2 0.017459427 0.604938272 **Oil phase is regarded as Water Phase
  0.25 0.030500363 0.521604938
  0.3 0.048112522 0.444444444
  0.35 0.070733492 0.37345679
  0.4 0.098765432 0.308641975
**INITIAL DATA**

*INITIAL
*USER_INPUT

**Global (Overall) Compositions**

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**NUMERICAL CONTROL**

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*NORM *PRESS 100.
*NORM *SATUR 0.15
*NORM *GMOLAR 0.15
*ITERMAX 200
*NORTH 20
*CONVERGE *PRESS 0.514884

**Well DATA**

*RUN
*TIME 0
*DTMIN 0.0001
*TIME 10
*TIME 30
*TIME 60
**Max Time Step Size Increased**

**10,000-year-Simulation**

**Terminate Simulation**

******************************************************************************
Appendix B: GEM Input File for Complex Case

The following Input data file is to simulate the effect of geologic discontinuity (structural gas trapping by faults) and residual gas saturation (residual gas trapping) in the tilted reservoir. Especially, the file includes a declined geometry and low-permeability (sealing fault) and anisotropic permeability of the reservoir.

******************************************************************
RESULTS SIMULATOR GEM 200500
FILENAME OUTPUT SRFOUT RESTARTOUT INDEXOUT MAINRESULTSOUT
*TITLE1 'CO2 Storage Model'
*TITLE2 '2D Model : Declined Fault'
*CASEID 'Tilted Reservoir with Residual Gas Saturation'
*DIM *MDIMPL 50
*DIM *MDICLU 20000000
*DIM *MDLU 20000000
*OUTPRN *RES *ALL
*OUTPRN *GRID DENG DENO DENW KRG KRO KRW PCG PCW PRES RHOG RHOO SG SO SW VISG VISO VELOCRC DROP SATP
*OUTSRF *WELL *PSPLIT
*OUTSRF *WELL *TOIP *TGIP *TWIP *RECO *RECG
*OUTSRF GRID DENG DENO DENW KRG KRO KRW PCG PCW PRES RHOG RHOO SG SO SW VISG VISO VELOCRC
*OUTSRF *RES *ALL
*WSRF *WELL *TIME
*WSRF *GRID *TIME
*INUNIT *FIELD
*WRST 0
**Distance units: ft
RESULTS XOFFSET 0.0000
RESULTS YOFFSET 0.0000
RESULTS ROTATION 0.0000 **Degrees
*****************************************************************************
** Definition of fundamental cartesian grid
*****************************************************************************
*GRID CART 1 200 50
*KDIR DOWN
*DI CON 2
*DJ CON 2
*DK CON 2
*DEPTH 1 100 1 5300
*DIP 0 5

*NULL MATRIX CON 1

*FAULT 0 1:1 1:200 **Fault Zone
*FAULTARRAY CON 0 **Connection Type between Grid Blocks
**(Standard Connection)

*TRANSI MATRIX CON 1
*TRANSJ MATRIX CON 1
*TRANSK MATRIX CON 1

*TRANSF 'Fault' 0.00 **Transmissibility Multipliers in the Fault Zone
*1 85 1 IDIR+ **("0" means "sealing" fault)
*1 86 2 IDIR+
*1 87 3 IDIR+
*1 88 4 IDIR+
*1 89 5 IDIR+
*1 90 6 IDIR+
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*TRANSF  'Fault'  0.0

**Applied Grid Blocks in I-direction**

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**Applied Grid Blocks in J-direction
**Applied Grid Blocks in J-direction**

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**Applied Grid Blocks in K-direction
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**Applied Grid Blocks in K-direction
**$ Property: Porosity   Max: 0.15   Min: 0.15
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*PERMI MATRIX CON 1
*PERMJ MATRIX CON 1
*PERMK MATRIX CON 0.01

**Property: Pinchout Array   Max: 1   Min: 1
***0 = pinched block, 1 = active block
*PINCHOUTARRAY CON 1

*CPOR MATRIX 3.0E-6
*PRPOR MATRIX 14.7

**---------------------------------------- FLUID COMPONENT DATA ----------
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*COMPNNAME 'CO2' 'H2O'
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*VISCOR PEDERSEN
*VISCOEFF 0.291
1.4
0.0005747
4.265
*MIXVC 1
*TRES 140.
*PCRIT 72.809000 217.754600
*TCRIT 304.12780 647.09440
*AC 0.223940 0.344000
*VCRIT 0.094000 0.056000
*MW 44.01000 18.01500
*PCHOR 78.00000 52.00000
*SG 0.818000 1.000000
*TB -109.21000 212.00000
*ZCRIT 0.274139 0.229409
*VISVC 0.094000 0.056000
*VSHIFT 0.024668 0.234867
*OMEGA 0.457235530 0.457235530
*OMEGB 0.077796074 0.077796074
*BIN -0.0576003
*PHASEID DEN

**-----------------------------------------------------ROCKFLUID DATA---------------------
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*RPT 1 SCALING-OLD
*SGT 0 0 1 *Oil- Gas Relative Permeability Data

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*HYSKRG 0.2

**-------------------------------------------------------------------------INITIAL DATA-------------------

*INITIAL

*USER_INPUT

*SW MATRIX CON 0

*PRES MATRIX CON 2295.

*ZGLOBALC 'CO2' MATRIX *IJK 1 1:100 41:50 1.0

*ZGLOBALC 'H2O' MATRIX *IJK 1 101:200 41:50 1.0

*ZGLOBALC 'H2O' MATRIX *IJK 1 1:200 1:40 1.0
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*NORM *PRESS   1000
*NORM *SATUR  0.25
*NORM *GMOLAR  0.15
*ITERMAX    200
*NORTH    20
*CONVERGE *PRESS  0.514884
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*TIME 0
*DTMIN 0.0001
*TIME 10
*TIME 30
*TIME 60
*TIME 91
*TIME 121
*TIME 182
*TIME 273
*DTMAX 10.
*TIME 365
*TIME 577
*TIME 730
*DTMAX 25.
*TIME 1095
*TIME 1825
*TIME 3652
*TIME 5478
*TIME 7305
*TIME 9131
*TIME 10957
*TIME 12783
*TIME 14610
*TIME 16436
*TIME 18262
*TIME 21915
*TIME 23741
*TIME 27393
*DTMAX 100.
*TIME 36525
*TIME 73050
*TIME 109575
*TIME 146100
*DTMAX 1000.
*TIME 182625
*TIME 219150
*TIME 255675
*TIME 292200
*TIME 328725

*TIME 365250
*TIME 730500
*TIME 1095750
*TIME 1461000
*TIME 1826250
*TIME 2191500
*TIME 2556750
*TIME 2922000
*TIME 3287250
*TIME 3652500

*STOP

******************************************************************
NOMENCLATURE

English Symbols

A : grid block face area
D : depth
D : fault displacement
d : distance of fluid migration
k : permeability
k_r : relative permeability
L : grid block length
M : mobility
MW : molecular weight
N_i : moles of component i per unit of grid block volume
N_{n_r+1} : moles of water per unit of grid block volume
P_c : critical pressure
p_c : capillary pressure
q : flow rate
q_i : molar injection / production rate of component i
R : ideal gas constant (8.31451 J/mol · K)
S_m : saturation of phase m
T : transmissibility multiplier
$T_c$ : critical temperature

$T_m$ : molar transmissibility of phase $m$

$t$ : time

$t$ : thickness

$\Delta t$ : time step

$\Delta x$ : grid block length

$u$ : velocity

$V$ : grid block volume

$V_{clay}$ : volume of clay

$V_m$ : molar volume, the volume of 1 mole of gas or liquid

$v$ : interstitial velocity

$y_{im}$ : mole fraction of component $i$ in phase $m$

$\Delta z$ : bed thickness

Greek Symbols

$\alpha$ : dip angle

$\alpha$ : rotating coupling coefficient

$\theta$ : direction of fluid migration

$\gamma_m$ : gradient of phase $m$

$\mu$ : viscosity
ϕ : porosity

ρₘ : molar density of phase \( m \)

ρᵣ : reduced density of the reference substance

τ : fault throw

ω : acentric factor

ψᵢ : material-balance or volume-consistency function

Subscript

\( f \) : fault

\( i \) : component

\( h \) : horizontal face

\( m \) : phase, ‘g’ for gas, ‘o’ for oil and ‘w’ for water

mix : mixture property

\( n \) : mole fraction

\( n_c \) : number of components

\( o \) : reference substance property

og : oil and gas phases

\( v \) : vertical face

wo : water and oil phases

\( w \) : weight fraction
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