

**MODELING GEOCHEMICAL AND GEOMECHANICAL
EFFECTS OF CO₂ REACTIVE TRANSPORT IN DEEP
SALINE LIMESTONE AQUIFER**

BY

HAIDAR AHMED ALMAJED

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DEANSHIP OF GRADUATE STUDIES

This thesis, written by **HAIDAR AHMED ALMAJED** under the direction of his thesis advisor and approved by his thesis committee, has been presented and accepted by the Dean of Graduate Studies, in partial fulfillment of the requirements for the degree of **MASTER OF SCIENCE IN PETROLEUM ENGINEERING**.



Dr. Murtada Al Jawad
(Advisor)



Dr. Dhafer Al Shelhi
Department Chairman



Dr. Mustafa AL Ramadhan
(Member)



Dr. Talal Al Shafloot
(Member)



Dr. Suliman Al-Homidan
Dean of Graduate Studies

Date: Aug 2024



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2024

DEDICATION

To my beloved family, whose unwavering support, encouragement, and endless patience have been the backbone of my academic journey. Your love and sacrifices have given me the strength to persevere through every challenge. This thesis is as much a testament to your belief in me as it is to my hard work. I am forever grateful for the inspiration, guidance, and understanding you have provided every step of the way.

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LIST OF ABBREVIATIONS

CCS	Carbon capture and storage
CT	Computed Tomography
DNN	Deep Neural Network
FEA	Finite Element Analysis
FEM	Finite Element Methods
GHGs	Greenhouse gases
Gt	Giga tonnes
ICSU	International Council of Scientific Unions
IEA	International Energy Agency
IPCC	Intergovernmental Panel on Climate Change
LNG	Liquefied Natural Gas
MMV	Monitoring, Measurements and Verification
UNEP	United Nations Environment Programme

ABSTRACT

Full Name : Haidar Ahmed Almajed
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This thesis assesses the effectiveness of carbon capture and storage (CCS) in deep saline aquifers as a key method for mitigating greenhouse gas (GHG) emissions. Through extensive numerical modeling, the study assesses the long-term storage and trapping mechanisms of CO₂ sequestration. It combines diffusivity equations for two-phase CO₂-water flow with the Peng-Robinson equation of state for assessing thermodynamic behavior. Residual trapping is explored through hysteresis in capillary pressure-saturation relationships, while geomechanical stability is examined using the Mohr-Coulomb criterion. Geochemical reactions, specifically calcite dissolution and precipitation induced by CO₂ interaction in limestone aquifers, are analyzed for their impact on aquifer porosity and permeability. The study also assesses how these geochemical changes influence the mechanical properties of the aquifer, providing insights into potential structural and volumetric modifications. The research models an 11.2 km² aquifer with varied porosity and permeability, focusing on scenarios with different injection rates, temperatures, and salinity levels to optimize sequestration strategies. This work aims to enhance operational strategies, risk assessments, and monitoring for secure, long-term CO₂ storage, while also understanding the geochemical and geomechanical implications on the aquifer's properties.

ملخص الرسالة

الاسم الكامل: حيدر أحمد الماجد

عنوان الرسالة: نموذج لتأثيرات الجيوكيميائية والجيوميكانكية لنقل ثاني أكسيد الكربون التفاعلي في طبقات المياه الجوفية الجيرية المالحة العميقة

التخصص: هندسة البترول

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تقيّم هذه الأطروحة فعالية تقنيات الحيازة على الكربون وتخزينه في الخزانات الملحية العميقة، وهي استراتيجية حاسمة لتقليل انبعاثات غازات الاحتباس الحراري. من خلال النمذجة العددية المكثفة، تقوم الدراسة بتقييم آليات التخزين طويل الأمد والاحتجاز لعزل ثاني أكسيد الكربون. تجمع بين معادلات الانتشارية لتدفق ثاني أكسيد الكربون والماء ثنائي الطور مع معادلة بنغ-روبينسون لتقييم السلوك الديناميكي الحراري. يتم استكشاف الاحتجاز المتبقي من خلال التآرجح في علاقات الضغط الشعري بالتشبع، بينما يتم فحص الاستقرار الجيوميكانيكي باستخدام معيار مور-كولومب. تُحلل التفاعلات الجيوكيميائية، وتحديدًا ذوبان وترسيب الكالسيت الناتج عن تفاعل ثاني أكسيد الكربون في الخزانات الجيرية، لتقييم تأثيرها على مسامية ونفاذية الخزان. تقيّم الدراسة أيضًا كيفية تأثير هذه التغييرات الجيوكيميائية على الخصائص الميكانيكية للخزان، مما يوفر رؤى حول التعديلات الهيكلية والحجمية المحتملة. تتمذج الأبحاث خزانًا بمساحة 11.2 كم² مع مسامية ونفاذية متنوعة، مع التركيز على سيناريوهات بمعدلات حقن مختلفة ودرجات حرارة ومستويات ملوحة لتحسين استراتيجيات العزل. تهدف هذه الأعمال إلى تحسين الاستراتيجيات التشغيلية، وتقييم المخاطر، والرصد لتأمين التخزين طويل الأمد لثاني أكسيد الكربون، مع فهم التداعيات الجيوكيميائية والجيوميكانكية على خصائص الخزان.

CHAPTER 1

INTRODUCTION

1.1 Background

Climate change is a defining challenge of the 21st century, driven primarily by the increasing concentration of greenhouse gases (GHGs) in the Earth's atmosphere [1]. The combustion of fossil fuels for energy generation, transportation, and industrial processes, as well as land-use changes such as deforestation, have led to a substantial rise in the atmospheric levels of carbon dioxide (CO₂), methane, and other GHGs. In light of the data available, it is evident that global temperatures have experienced an approximate 1.1°C increase since the late 19th century, with the previous decade standing out as the period with the highest recorded temperatures [2]. **Figure 1** shows the global surface temperature change from 1850-1900 to 2020. It clearly illustrates the significant warming trend, with the last decade (2011-2020) being the hottest on record, further emphasizing the severity of the climate change challenge.

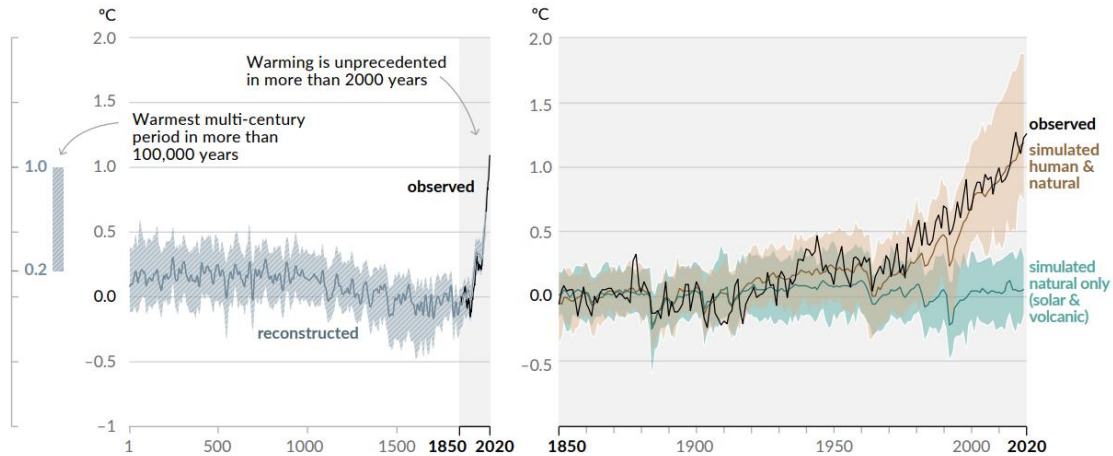


Figure 1: Variations in global surface temperature [2]

The impacts of climate change are serious and wide-ranging, affecting many parts of our planet and the lives of people all over the world.

1. **Sea level rise:** As the Earth's temperature increases, the acceleration of glacier and ice sheet melting is causing a significant increase in sea levels [3]. This poses a grave threat to coastal communities, causing increased flooding, erosion, and saltwater intrusion into freshwater sources [4]. The increasing sea level presents a notable danger to small island countries and heavily populated coastal urban areas, which could lead to the large-scale relocation of millions of people [5]. **Figure 2** illustrates the projected global sea level rise under different emissions scenarios, highlighting the potential severity of this consequence of climate change. In the most optimistic scenario (RCP 2.6), wherein CO₂ emissions are completely phased out by the year 2100, an approximate rise of 0.5 meters in sea levels is anticipated. Conversely, under the high-emissions scenario (RCP 8.5), it is projected that sea levels could ascend by over 1 meter by 2100, with a sustained increase in the ensuing centuries [6].

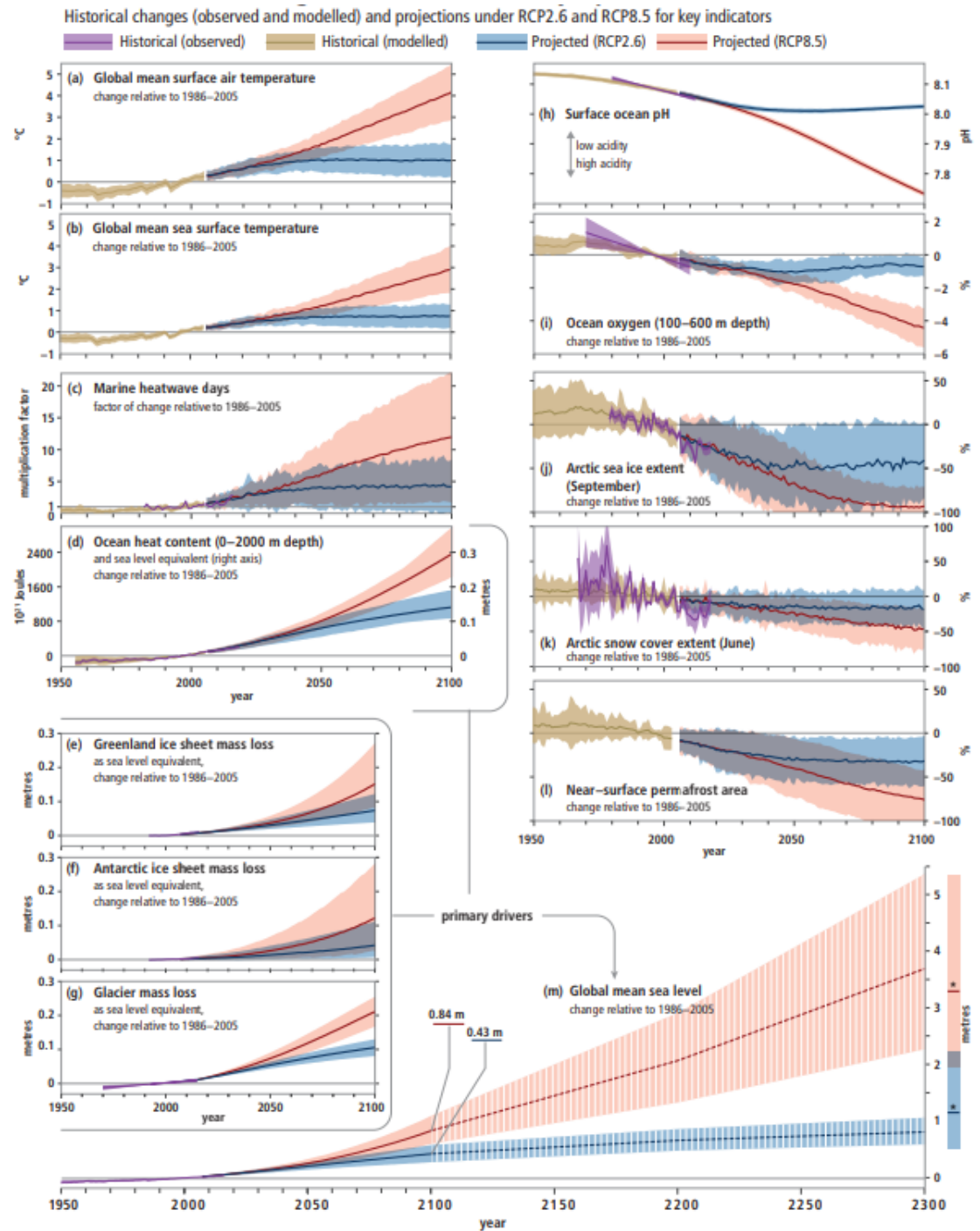


Figure 2: The analysis encompasses historical and projected changes in the ocean and cryosphere from 1950 onwards, comprising observed data and model simulations. Future changes are delineated with respect to both low (RCP2.6) and high (RCP8.5) greenhouse gas emissions scenarios [6]

2. **Ocean acidification:** The world's oceans are essential in ameliorating the impact of human activities on the environment by absorbing a substantial amount of the excess CO_2 released into the atmosphere. Consequently, the chemical composition of the oceans is undergoing changes, leading to increased acidity [7], as illustrated in **Figure 3**. The phenomenon known as ocean acidification yields significant repercussions for marine ecosystems, particularly impacting organisms with calcium carbonate shells or skeletons, such as corals and certain plankton species. The disruption of these foundational species can have cascading effects throughout the entire marine food web [8].

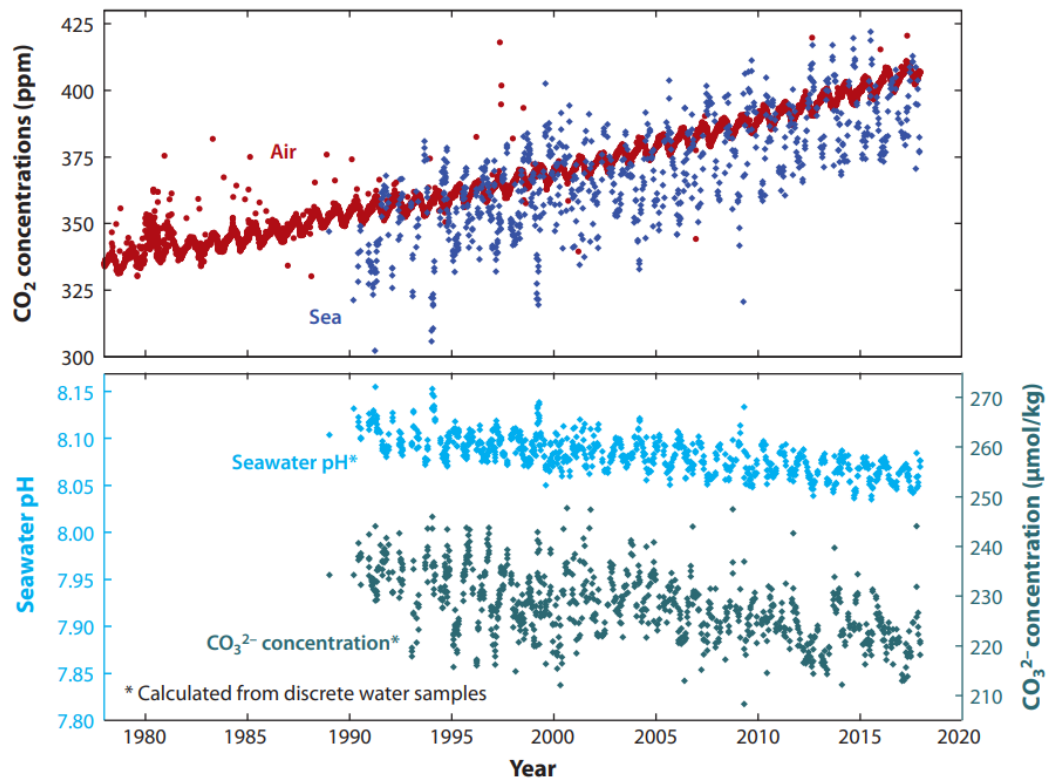


Figure 3: Trends in CO_2 Concentrations in Air and Sea and Corresponding Seawater pH and CO_3^{2-} Concentration Over Time [7]

3. **Melting glaciers and ice sheets:** The phenomenon of climate change is contributing to the rapid deterioration of glaciers and ice sheets in polar and mountainous regions [9], [9]. This not only contributes to a rise in sea levels but also impacts the availability of freshwater resources for communities that rely on glacial meltwater for irrigation, drinking water, and hydroelectric power. The rapid melting of glaciers and icebergs in the Arctic provides clear evidence of the significant changes occurring in Earth's cryosphere due to climate change [10].
4. **Extreme weather events:** As global temperatures rise; the Earth's atmosphere has the capacity to retain a greater amount of moisture. This phenomenon is a contributing factor to the heightened frequency and increased severity of extreme weather events, including hurricanes, heatwaves, droughts, and floods [11]. These events can have devastating impacts on agricultural productivity, infrastructure, and human health, particularly in developing countries with limited adaptive capacity [12].
5. **Exacerbation of inequalities:** Climate change has a disproportionate impact on vulnerable and marginalized communities, particularly those residing in developing countries, low-income populations, and indigenous areas [12], [13] , illustrated in **Figure 4**. Limited resources are often available to these groups to adjust to the effects of climate change, and they rely more on sectors sensitive to climate such as agriculture and fisheries [12], [14]. As a result, existing inequalities can be worsened by climate change and can obstruct endeavors to alleviate poverty and advance sustainable development [15]. Climate change has the potential to worsen current inequalities and impede initiatives to alleviate poverty and advance sustainable

development. High-income countries, which represent only 15.4% of the global population, are responsible for 34.4% of CO₂ emissions. In contrast, low-income countries, which comprise 8.8% of the world's population, contribute just 0.6% to global emissions [16].

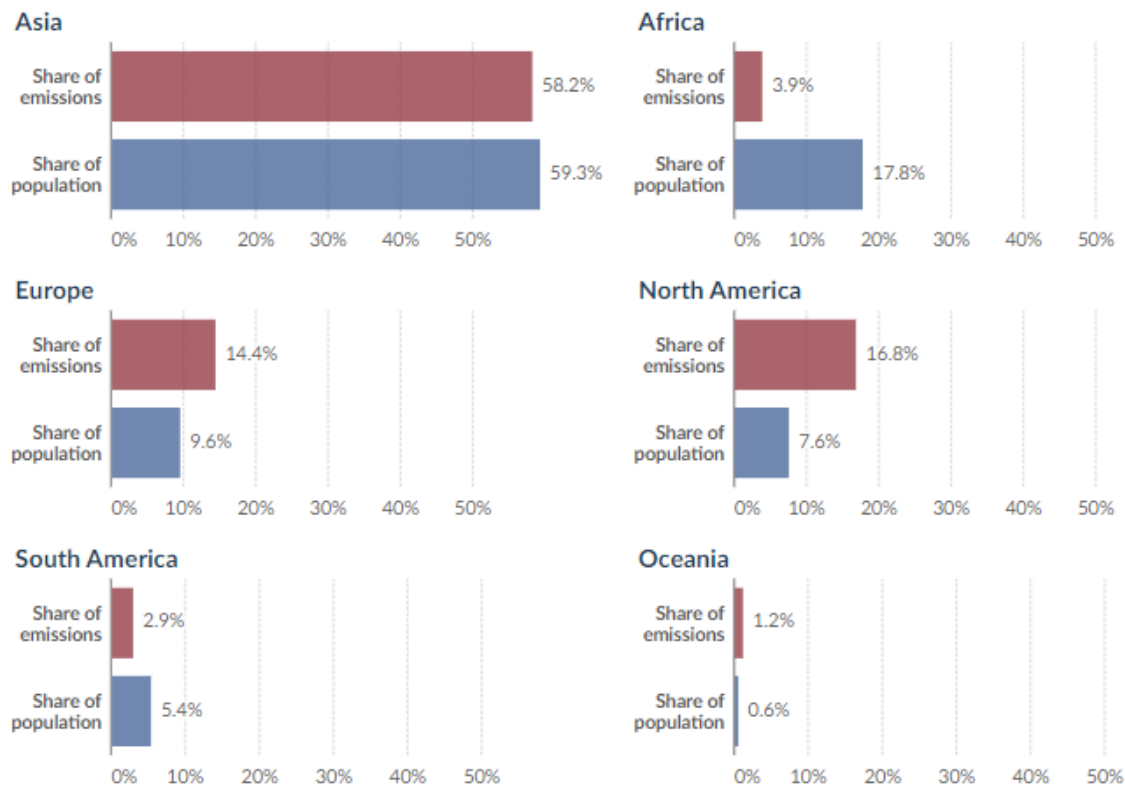


Figure 4: Regional Comparison of Share of CO₂ Emissions and Population [16]

The visual representations in Figures 2-4 help to illustrate the severity and disparate impacts of climate change across various dimensions, from sea level rise projections to the unequal distribution of CO₂ emissions and population by income level. The pictures highlight the pressing need to prioritize the most vulnerable communities worldwide when addressing climate change through mitigation and adaptation efforts.

In response to the global climate crisis, CCS technologies have surfaced as an essential component within the spectrum of solutions required for mitigating the effects of climate change [17]. CCS encompasses the process of capturing, transporting, and securely storing CO₂ in geological formations to prevent its release into the atmosphere. The pressing need for CCS is emphasized by the staggering global CO₂ emissions of 36.3 billion tonnes in 2019. This data unequivocally indicates that the world is failing to align with the primary goal of the Paris Agreement, which aims to limit the increase in global temperature to well below 2°C above pre-industrial levels [18].

One notable approach within the realm of CCS involves the sequestration of CO₂ in saline water aquifers. Through this method, CO₂ is deliberately injected and securely stored, thereby offering a promising avenue for long-term carbon mitigation and environmental impact reduction. Saline aquifers are widespread, have large storage capacities, and are often located near major CO₂ emission sources. The injection of CO₂ occurs within aquifers at depths typically exceeding 800 meters, thus maintaining a supercritical state facilitated by high pressure and temperature conditions. Subsequently, the introduced CO₂ undergoes dissolution within the formation water, interacts with the host rock, and becomes sequestered due to diverse physical and chemical mechanisms [19], illustrated in **Figure 5**.

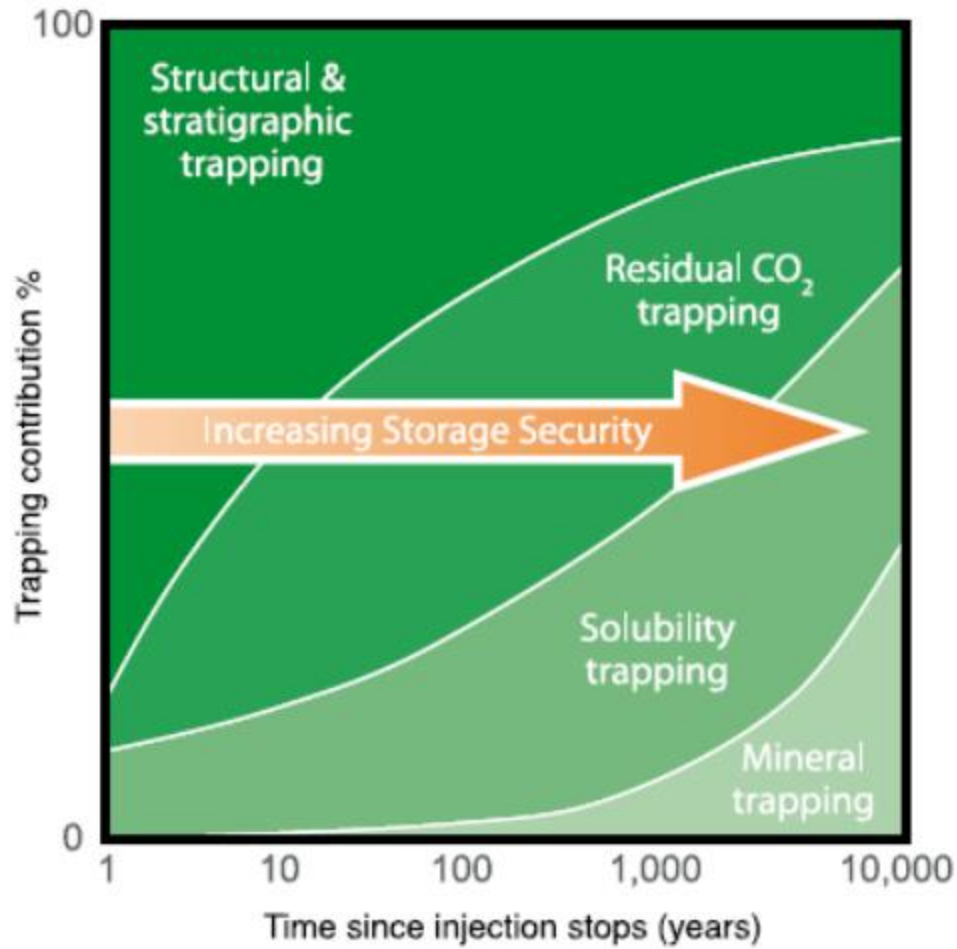


Figure 5: Contributions of Different CO₂ Trapping Mechanisms Over Time to Increasing Storage Security [20]

The estimated storage capacity of saline aquifers worldwide for CO₂ ranges between 1,000 and 10,000 gigatonnes (Gt CO₂). This capacity is adequate for storing the CO₂ emissions generated globally for several centuries at current levels [21]. To date, several successful large-scale CCS projects in saline aquifers have been implemented worldwide, such as the Sleipner project in Norway [22], the Quest project in Canada [23], and the Illinois Basin-Decatur project in the United States [24].

Similar to the estimate of storage resources, it is important to categorize the scope and level of detail of regional resource evaluations. The set of classifications used to establish the depth and comprehensiveness of evaluations in various countries are based on the CSLF pyramid, as shown in **Figure 6**. The criteria for classification are as follows [25]:

- **Full:** Full evaluations, encompassing published Atlases, that encompass the majority or entirety of potential storage basins along with corresponding accurate resource estimations.
- **Moderate:** National surveys or atlases do not include thorough resource calculations, but there is fragmented coverage through state, provincial, or basin-scale atlases, or detailed assessments.
- **Limited:** Additional investigation limited to specific basins or locations.
- **Very limited:** There is little to no existing research on the storage potential.

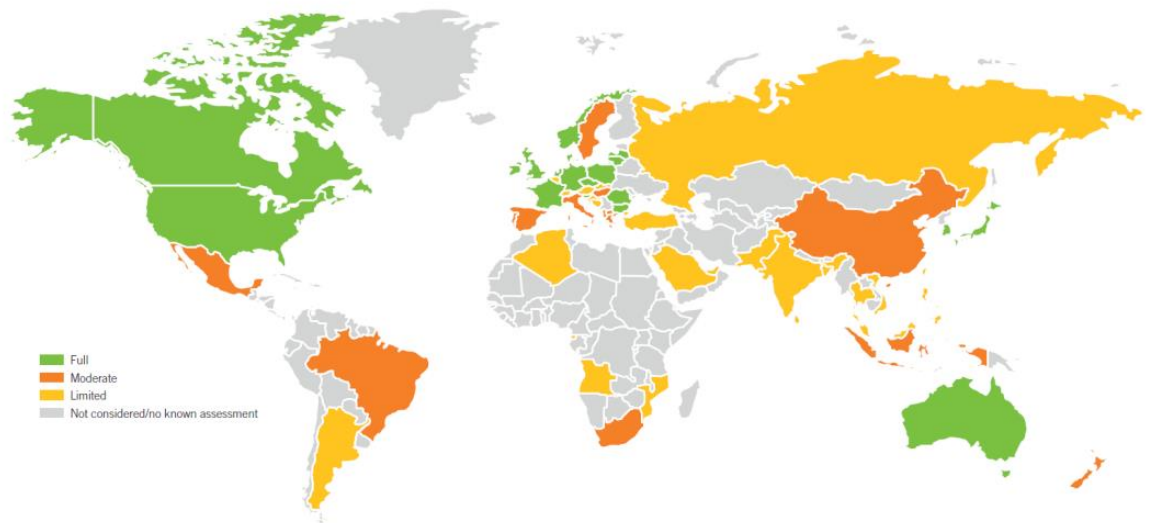


Figure 6: Global Assessment of CCS Storage Potential in Saline Aquifers [25]

Regardless of the potential of CCS in saline aquifers, several challenges remain, such as high costs, limited infrastructure, and public acceptance [26]. Additionally, it is crucial to persist in researching and monitoring the enduring impacts and environmental ramifications of CO₂ injection in order to attain a more comprehensive comprehension of its implications [27]. However, CCS in aquifers is viewed as a critical and practical approach for making substantial cuts in worldwide CO₂ emissions and lessening the effects of climate change [25].

1.2 Motivation

Saudi Arabia has established an ambitious objective to shift towards achieving zero carbon emissions by the year 2060. As a significant producer of oil, attaining this goal will necessitate the adoption of diverse approaches, such as CCS technologies [28]. Storing CO₂ in deep saline water aquifers is a potentially effective method, as these aquifers have significant storage capacity. The effective application of this method relies on a thorough comprehension of the factors affecting the storativity of these formations and the geomechanical alterations that may take place during and following the injection [25]. This thesis aims to assess the storativity changes in saline water aquifers resulting from varying parameters. This research aims to contribute to the advancement of secure and efficient CO₂ storage methods, ultimately supporting Saudi Arabia's efforts to achieve its zero-carbon target by 2060 by addressing these essential factors.

1.3 Objectives

This study seeks to improve our comprehension of changes in storativity and the geomechanical impacts related to the injection of CO₂ into limestone saline aquifers. The main goals of the research are:

1. Examine how aquifer salinity, injection temperature, and injection rates affect the storativity of limestone saline aquifers during the process of CO₂ sequestration.
2. Assess the geomechanical consequences of CO₂ injection to guarantee the secure and effective containment of the stored CO₂.

This research seeks to offer important findings and suggestions to ensure the secure and effective execution of CO₂ sequestration projects in limestone saline aquifers. These efforts contribute to the larger aim of reducing GHG emissions and attaining carbon neutrality.

CHAPTER 2

LITERATURE REVIEW

2.1 The Early History of CCS and the Growing Recognition of Climate Change

In 1977, Cesare Marchetti, an Italian physicist, published a seminal paper titled "On Geoengineering and the CO₂ Problem" [29]. This publication is widely recognized as one of the initial suggestions for the capture and storage of CO₂ in geological structures to prevent its release into the atmosphere. Marchetti put forward his forward-thinking idea before the widespread acknowledgment of climate change as a worldwide concern and the creation of groups such as the Intergovernmental Panel on Climate Change (IPCC) [30].

Marchetti's paper was a response to the growing concerns about the potential impacts of rising CO₂ levels on the Earth's climate. At the time, the concept of anthropogenic climate change was gaining traction in scientific circles, and there was a need to explore viable solutions. Marchetti recognized the significant contribution of burning fossil fuels to the increase in atmospheric CO₂ levels. He suggested capturing CO₂ from primary sources like power plants and injecting it into deep geological formations, including deep saline aquifers and depleted oil and gas reservoirs [29].

Marchetti's proposal, while lacking detailed technical analysis, served as the cornerstone for considering CCS as a viable climate change mitigation strategy. His pioneering work has since spurred further research and development in this domain.

During the late 1970s and early 1980s, there was an increasing body of scientific evidence supporting the idea of human-caused climate change. Additionally, the initial World Climate Conference took place in Geneva in 1979. In the 1970s, the World Meteorological Organization (WMO) began to focus on the potential impacts of human activities on the climate system. This was followed by the emergence of several significant scientific reports and studies in the 1980s that further brought attention to climate change, including the U.S. National Academy of Sciences' 1983 report "Changing Climate"[30].

During this period, the Villach Conference in 1985 stands out as a crucial event. It was convened by the United Nations Environment Programme (UNEP), WMO, and the International Council of Scientific Unions (ICSU). The conference brought together prominent researchers and policymakers to deliberate on the existing knowledge about climate change and its potential impacts. The resulting "Villach Statement" underscored the urgent need to address climate change and advocated for international cooperation in formulating policies and response strategies [31].

In 1988, the Toronto Conference on the Changing Atmosphere, convened by the Canadian government, marked a significant milestone in addressing climate change. The conference called for a 20% reduction in worldwide carbon dioxide emissions by 2005 and stressed the urgent need for immediate action to tackle formations [32].

Recently, The Paris Agreement represents a landmark in global climate policy by establishing ambitious targets to restrict the global temperature increase to well below 2°C above pre-industrial levels, with efforts to limit the increase to 1.5°C [32]. This agreement holds substantial implications for CCS technology and its role in mitigating climate change.

2.2 Experimental Work

In 1993, Gunter et al. conducted a pioneering experimental study to explore the possibility of CO₂ storage in geological formations [32]. This study, released during the 1990s, investigated the geochemical and hydrological elements of storing CO₂ in deep saline aquifers and oil and gas reservoirs.

In their experiments, Gunter et al. (1993) exposed core samples from various sedimentary formations to supercritical CO₂ under simulated reservoir conditions. They analyzed the interactions between CO₂, brine, and rock samples, focusing on geochemical reactions, mineral dissolution and precipitation, and the potential for CO₂ trapping through various mechanisms [32].

One of the key findings from these experiments was the identification of different trapping mechanisms that contribute to the secure storage of CO₂ in geological formations. Gunter et al.

Three years later, in another study, Gunter et al. (1997) emphasized the significance of structural and stratigraphic trapping. They highlighted that injected CO₂ is physically confined by impermeable cap rocks or geological formations [33]. Furthermore, they noticed that some of the injected CO₂ can get trapped in the rock formation as disconnected

bubbles or clusters within the pore spaces. This trapping process can greatly increase the storage capacity of a reservoir.

In 2004, Rochelle and colleagues carried out a set of studies to explore the chemical reactions between CO₂, brine, and rock specimens obtained from the Utsira Formation [34]. This formation is a significant saline reservoir in the North Sea utilized for extensive CO₂ storage. The Utsira Formation, known for its high permeability as a sandstone formation, has been identified as a promising location for CO₂ sequestration due to its favorable geological features.

The experiments conducted by Rochelle and colleagues in 2004 involved subjecting rock samples from the Utsira Formation to brine that was saturated with CO₂ under simulated reservoir conditions. They monitored the changes in the rock samples and brine composition over time to study the geochemical reactions occurring. The findings from the experiments revealed that the injection of CO₂ into the brine resulted in a decrease in pH, leading to the dissolution of minerals like calcite and feldspar found in the rock samples. This dissolution caused the release of ions such as calcium, magnesium, and silica into the brine solution. During the duration of the experiments, Rochelle et al. observed the formation of secondary carbonate minerals, specifically calcite and dolomite, due to the interaction among the released ions, as illustrated in **Figure 7**. The emergence of these secondary minerals played a crucial role in regulating the pH and geochemistry of the CO₂-brine system. The precipitation of carbonate minerals is a significant aspect of CO₂ sequestration as it can contribute to the long-term immobilization of CO₂ through mineral trapping. Mineral trapping involves the reaction of dissolved CO₂ with the rock matrix to form stable carbonate minerals, effectively securing the CO₂ in solid form.

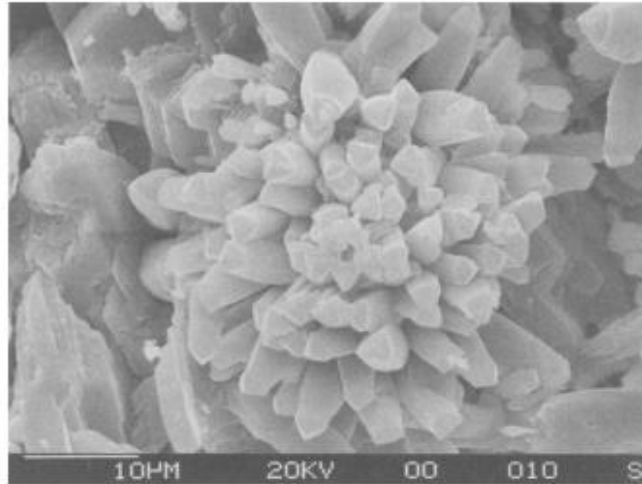


Figure 7: Formation of Calcite Needles on Corroded Anhydrite: An SEM Analysis [34]

Additionally, They highlighted that the extent and rate of mineral dissolution and precipitation reactions were influenced by factors such as the composition of the rock samples, as well as the temperature and pressure conditions. Their findings highlighted the importance of understanding the site-specific geochemical conditions when assessing the potential for CO₂ storage in a particular geological formation.

Kharaka et al. (2006) conducted experiments to study how CO₂, brine, and rock samples from the Frio Formation, a sandstone aquifer in the Texas Gulf Coast Basin, interacted chemically [35]. The Frio Formation has been considered as a potential target for CO₂ sequestration due to its favorable geological characteristics, including high permeability and porosity.

They conducted experiments in which they introduced CO₂ into brine solutions containing rock samples from the Frio Formation under simulated reservoir conditions. The chemical composition of the brine and rock samples was analyzed over time to comprehend the

geochemical reactions taking place. The experiments showed that injecting CO₂ into the brine solution led to a quick decrease in pH, causing the breakdown of carbonate and silicate minerals present in the rock samples. The decomposition process resulted in the release of several ions, such as calcium, magnesium, iron, and silica, into the brine solution. Over time, the researchers observed the emergence of secondary carbonate minerals, predominantly calcite and iron-rich carbonates, due to the interaction between the dissolved ions and the CO₂ in the brine. The creation of these secondary minerals occurred relatively rapidly, suggesting that mineral trapping could play a significant role in the long-term storage of CO₂ in the Frio Formation. The formation of secondary carbonate minerals is crucial for CO₂ sequestration, as it can help permanently immobilize CO₂ through mineral trapping, which is considered one of the most secure methods of CO₂ storage. It was emphasized that the speed and extent of mineral dissolution and precipitation reactions were influenced by various factors, including the original mineral composition of the rock samples, the chemical composition of the brine, and the prevailing pressure and temperature. The researchers underscored the importance of understanding the specific geochemical conditions at the site when evaluating the feasibility of carbon dioxide sequestration in a particular geological formation.

Izgec et al. (2008) carried out a series of studies to explore the impact of injecting CO₂ on the wettability and relative permeability of reservoir rocks [36]. These properties play a part in governing fluid flow and storage capacity in geological formations. Wettability refers to a solid surface's tendency to prefer contact with one fluid phase over another, while relative permeability defines each fluid phase's ability to flow through a porous medium in the presence of other phases. The researchers utilized core samples sourced

from a carbonate reservoir in Turkey to conduct CO₂ injection experiments under reservoir conditions. They assessed changes in wettability and relative permeability of the rock samples before and after CO₂ injection using a variety of methods, including contact angle measurements, core flooding, and X-ray computed tomography (CT) scanning.

The tests showed that introducing CO₂ into the carbonate reservoir rocks caused a significant change in their wettability. Initially, the rock samples displayed mixed-wet or oil-wet properties, indicating a preference for oil over water on their surfaces. However, following CO₂ injection, the wettability of the rock samples shifted towards a more water-wet state. This change was linked to the CO₂ dissolving in the brine and altering the rock surface chemistry. The transition to a more water-wet state has important implications for CO₂ storage and enhanced oil recovery (EOR) processes. In a water-wet system, the injected CO₂ tends to occupy the center of the pore spaces, while the brine forms a thin film on the rock surfaces. This fluid distribution can enhance CO₂ storage efficiency by helping trap the CO₂ in the pore spaces instead of allowing it to rise due to buoyancy forces. They observed changes in the rock specimens' relative permeability after injecting CO₂. Specifically, the relative permeability of the brine phase increased, while that of the oil phase decreased. This was associated with a shift in wettability towards a more water-wet state and alterations in pore-scale fluid distribution.

In a study conducted by Al-Ameri et al. (2016), a series of experiments utilized core samples from a sandstone reservoir in the United Arab Emirates [37]. The rock samples underwent exposure to CO₂-saturated brine under simulated reservoir conditions for various durations, spanning from 1 to 12 months. The researchers assessed the mechanical properties of the rock samples, including their elastic moduli, compressive strength, and

tensile strength, before and after CO₂ exposure using methods such as ultrasonic velocity measurements and uniaxial compression tests.

The experiments revealed that prolonged exposure to CO₂-saturated brine caused significant changes in the mechanical properties of the sandstone specimens. Over a period of 12 months, the elastic moduli, comprising Young's modulus and shear modulus, experienced reductions of up to 30%. Furthermore, the compressive strength and tensile strength of the rock samples also decreased by 20-30% during the same timeframe. These alterations in mechanical properties were attributed to the geochemical interactions between CO₂, brine, and the rock matrix. The presence of CO₂ in the brine created an acidic environment, which accelerated the dissolution of minerals, such as feldspars and carbonates, present in the sandstone samples. This mineral dissolution caused the weakening of the rock structure and the modification of its pore arrangement, ultimately resulting in reduced mechanical strength and stiffness.

The results of Al-Ameri et al. (2016) hold considerable importance for the future integrity and safety of CO₂ storage reservoirs. The degradation of rock mechanical properties due to prolonged CO₂ exposure could potentially compromise the stability of the reservoir and increase the risk of CO₂ leakage or induced seismicity, as illustrated in **Figure 8**. The authors suggested that these effects should be carefully considered in the site selection, design, and monitoring of CO₂ sequestration projects to ensure their long-term success and safety.

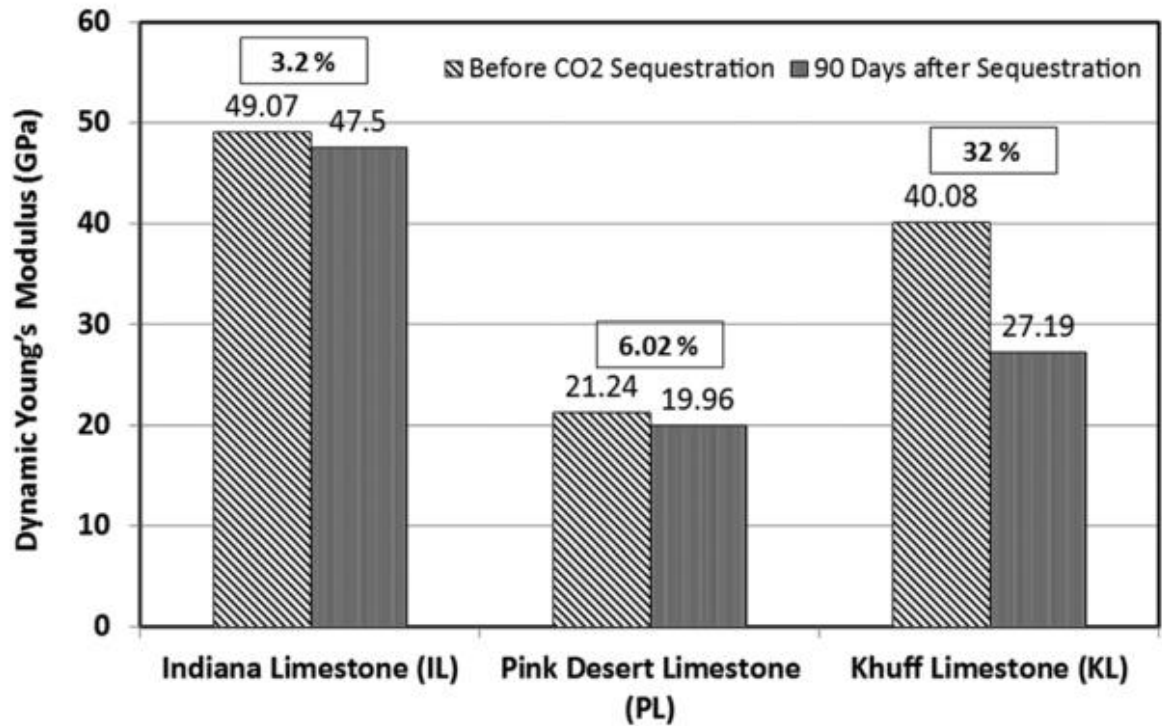


Figure 8: Impact of CO₂ Sequestration on the Dynamic Young's Modulus of Various Limestone Types [35]

In a 2020 study by Zhang et al., the researchers investigated the effects of CO₂ flooding on the mechanical properties of carbonate reservoir rocks [38]. These rocks play a critical role in CO₂ sequestration and EOR due to their high porosity and permeability. The study involved CO₂ flooding experiments on core samples from a carbonate reservoir in China under reservoir conditions. Through various techniques such as ultrasonic velocity measurements, triaxial compression tests, and Brazilian tests, the researchers observed changes in the mechanical properties of the rock samples, including their elastic moduli, compressive strength, and tensile strength before and after exposure to CO₂. The findings revealed a significant impact of CO₂ flooding on the mechanical properties of the carbonate rock samples, showing a decrease of 10-20% in elastic moduli, including Young's modulus

and shear modulus, following CO₂ exposure. Additionally, the compressive strength and tensile strength of the rock samples decreased by 15-25% after CO₂ injection.

They determined that the alterations in the mechanical properties resulted from the interaction among CO₂, brine, and carbonate minerals. This process involved CO₂ dissolving in the brine, leading to an acidic environment that facilitated the dissolution of calcite and dolomite, the primary minerals found in the carbonate samples. This dissolution created new pore spaces and altered the rock structure, ultimately causing a reduction in mechanical strength and stiffness. The researchers also noted that the degree of mechanical degradation depended on the duration of CO₂ exposure, as well as the original porosity and permeability of the rock samples. Samples with higher initial porosity and permeability experienced more pronounced decreases in mechanical properties following CO₂ flooding, underscoring the significant role of CO₂ flow and transport in the pore network in the geochemical and geomechanical processes.

In a 2023 study, Al-Dhafeeri et al. examined how the temperature of CO₂-saturated brine affects the creation of wormholes and changes in rock properties when CO₂ is injected into carbonate reservoirs [39]. They wanted to understand how temperature impacts the formation of highly conductive flow channels, or wormholes, which result from the dissolution of carbonate minerals during CO₂ injection. This research is valuable as it sheds light on how temperature may affect CO₂ sequestration.

They investigated the effects of temperature on the creation of wormholes and changes in rock properties during the injection of CO₂ into core samples from a carbonate reservoir in Saudi Arabia. The experiments involved injecting CO₂-saturated brine at different temperatures (50°C, 70°C, and 90°C) under reservoir conditions and using X-ray computed

tomography (CT) scanning to monitor the development of wormholes. The findings revealed that higher temperatures (70°C and 90°C) led to more rapid and extensive formation of wormholes compared to lower temperatures (50°C), mainly due to the increased reactivity of CO₂ and faster carbonate mineral dissolution kinetics at elevated temperatures. As a result of the wormhole formation, the porosity and permeability of the carbonate samples notably increased, particularly at higher temperatures. However, the mechanical strength of the rock samples declined after CO₂ injection, with more significant reductions observed at higher temperatures, which was attributed to the dissolution of carbonate minerals and the formation of wormholes, as illustrated in **Figure 9**.

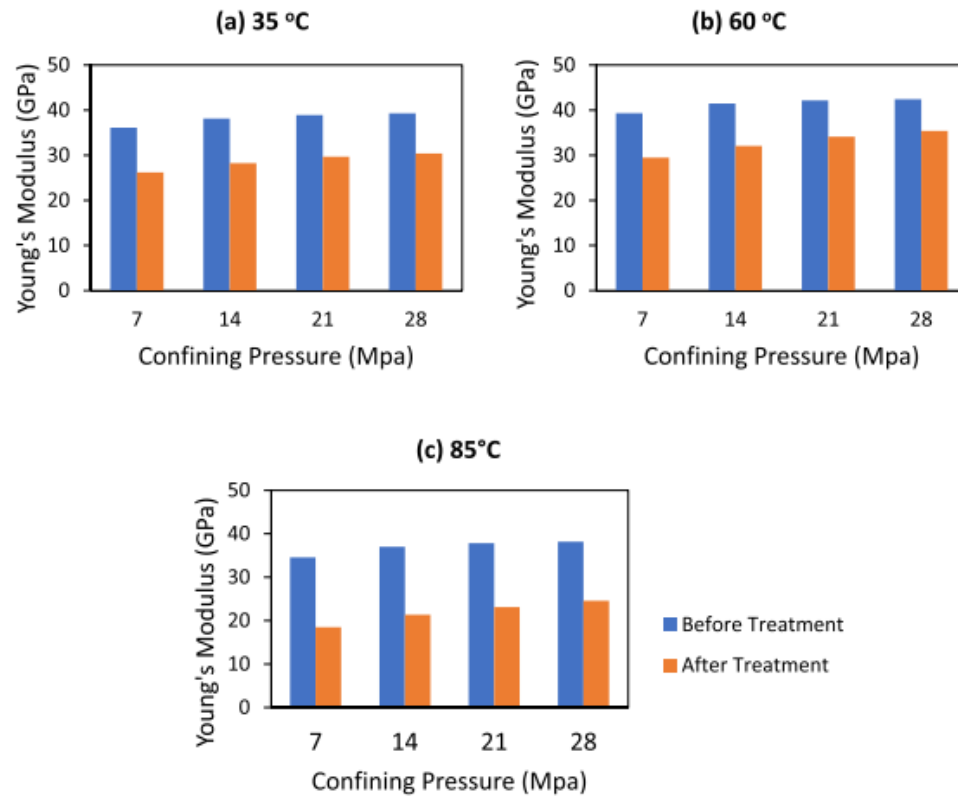


Figure 9: Variation of Young's Modulus Before and After CO₂ Treatment at Different Temperatures [39]

In their 2024 study, Al-Dhafeeri et al. conducted research on the effects of brine salinity saturated with CO₂ on the formation of wormholes and changes in rock properties. The main objective of the study was to investigate how brine salinity influences the creation of wormholes and modifies rock properties during the injection of CO₂ into carbonate reservoirs. Brine salinity was found to play a critical role in CO₂ sequestration processes, as it can impact the solubility of CO₂ in the brine and the interaction of CO₂ with carbonate minerals [55].

In 2024, Al-Dhafeeri and his team conducted a series of experiments in which they injected CO₂ into core samples from a carbonate reservoir in Saudi Arabia. Their primary objective was to explore the correlation between brine salinity and the formation of wormholes, as well as the alteration of rock properties. The researchers introduced CO₂-saturated brine with different salinity levels (50,000 ppm, 100,000 ppm, and 200,000 ppm) under reservoir conditions. They utilized X-ray CT scanning to monitor the development of wormholes and conducted measurements of rock properties such as porosity, permeability, and mechanical strength before and after the CO₂ injection.

The results of the experiments revealed a significant impact of brine salinity on both the generation of wormholes and the transformation of rock properties during CO₂ injection. Notably, at lower salinity levels (50,000 ppm), the formation of wormholes was more extensive and rapid in comparison to higher salinity levels (100,000 ppm and 200,000 ppm). This was attributed to the heightened solubility of CO₂ in lower salinity brine, which led to increased reactivity with carbonate minerals and faster dissolution. The creation of wormholes was found to increase the porosity by up to 20% and permeability by several fold, particularly at lower salinity levels. However, the mechanical strength of the rock

samples declined post-CO₂ injection, with more pronounced reductions observed at lower salinity levels. The weakening of the rock fabric and reduction in load-bearing capacity were attributed to the dissolution of carbonate minerals and the formation of wormholes. Additionally, the researchers observed variations in the pattern and morphology of the wormholes based on brine salinity. Lower salinity levels resulted in more branched and interconnected wormholes, while higher salinity levels led to more localized and discrete formations. These differences in wormhole morphology could have implications for CO₂ flow and transport within the reservoir, as well as the efficiency of CO₂ storage and enhanced oil recovery operations.

These experimental studies have yielded valuable insights into the feasibility, efficiency, and safety of carbon dioxide (CO₂) sequestration in various geological formations. They highlight the significance of taking into account the specific geochemical conditions at each site, the interrelated influences of geochemical reactions and fluid-rock interactions, and the possible implications of CO₂ injection on reservoir integrity and storage capacity.

However, experimental studies alone cannot fully capture the complexity and scale of CO₂ sequestration in real-world geological formations. Numerical modeling has emerged as a powerful tool to complement experimental work and provide a more comprehensive understanding of the processes involved in CO₂ sequestration.

2.3 Numerical Work

Experimental research has provided important knowledge about the processes involved in CO₂ sequestration. However, the use of numerical modeling has become increasingly crucial for anticipating the long-term behavior and destiny of injected CO₂ in geological formations. Numerical models have the capability to replicate the intricate interplay between fluid movement, geochemical reactions, and geomechanical processes at different spatial and temporal levels. This enables a more extensive evaluation of CO₂ storage capacity, injectivity, and containment.

In 1996, Weir et al. developed a mathematical model to simulate the injection of CO₂ into depleted oil and gas reservoirs [40]. The model considered the flow of CO₂ and brine in porous media, as well as the dissolution of CO₂ in the formation water. The main objective was to investigate the potential storage capacity of depleted reservoirs and how reservoir properties affect CO₂ injection and migration.

The model utilized mass conservation equations for CO₂ and brine, as well as Darcy's law for fluid flow in porous media. It also accounted for the compressibility of CO₂ and brine, as well as the pressure and temperature dependence of CO₂ solubility in brine. The authors employed numerical methods, such as finite difference schemes, to solve the governing equations and simulate CO₂ injection and migration in a hypothetical depleted reservoir. The study analyzed the impact of various reservoir parameters, such as permeability, porosity, and reservoir thickness, on the storage capacity and migration of injected CO₂. The results suggested that the storage capacity of depleted reservoirs was primarily influenced by the reservoir volume and the solubility of CO₂ in brine. Additionally, the

authors observed that the migration of CO₂ was affected by reservoir heterogeneity, with higher permeability zones facilitating faster CO₂ migration.

Around the same time, Law and Bachu utilized numerical modeling to investigate how reservoir heterogeneity impacts the injection and storage of CO₂ [41]. Their work aimed to demonstrate the influence of heterogeneity on the migration and distribution of injected CO₂, emphasizing the need for detailed reservoir characterization in the planning of CO₂ storage initiatives.

The researchers created a numerical model in two dimensions to incorporate the differences in reservoir characteristics, including porosity and permeability. This model relied on the principles of mass conservation for CO₂ and brine, alongside Darcy's law for fluid flow in porous media. The investigation focused on a potential reservoir with varying levels of heterogeneity, encompassing both homogeneous and highly heterogeneous scenarios.

The outcomes appeared that reservoir heterogeneity had an impact on the migration and distribution of injected CO₂. In homogeneous reservoirs, the CO₂ plume migrated uniformly, while in heterogeneous reservoirs, the CO₂ preferentially migrated through high-permeability zones, leading to a more complex and irregular plume shape. The study also found that heterogeneity affected the storage capacity of the reservoir, with highly heterogeneous reservoirs having a lower effective storage capacity compared to homogeneous reservoirs.

In the study conducted by Lindeberg (1997), the potential long-term consequences of injecting CO₂ into deep saline aquifers were investigated using a computer model [42]. The focus was on assessing the capacity of saline aquifers to store CO₂ and the importance of

solubility trapping in this process. Lindeberg's numerical model was based on the conservation of mass for CO₂ and brine, along with Darcy's law for fluid flow driven by density in porous media. The model also took into account the effects of pressure and temperature on CO₂ solubility in brine, as well as the diffusion of dissolved CO₂ within the aquifer. To solve the governing equations and simulate the migration and dissolution of CO₂, an FEM was applied. The research examined the influence of factors such as aquifer thickness, permeability, and CO₂ injection rate on the storage capacity and containment of the saline aquifer. The results highlighted the significance of solubility trapping in the long-term storage of CO₂, as a substantial portion of the injected CO₂ was found to dissolve in the brine over time. The study concluded that the storage capacity of the aquifer depended largely on the volume of brine available for CO₂ dissolution and the rate of CO₂ diffusion within the aquifer, as illustrated in **Figure 10**.

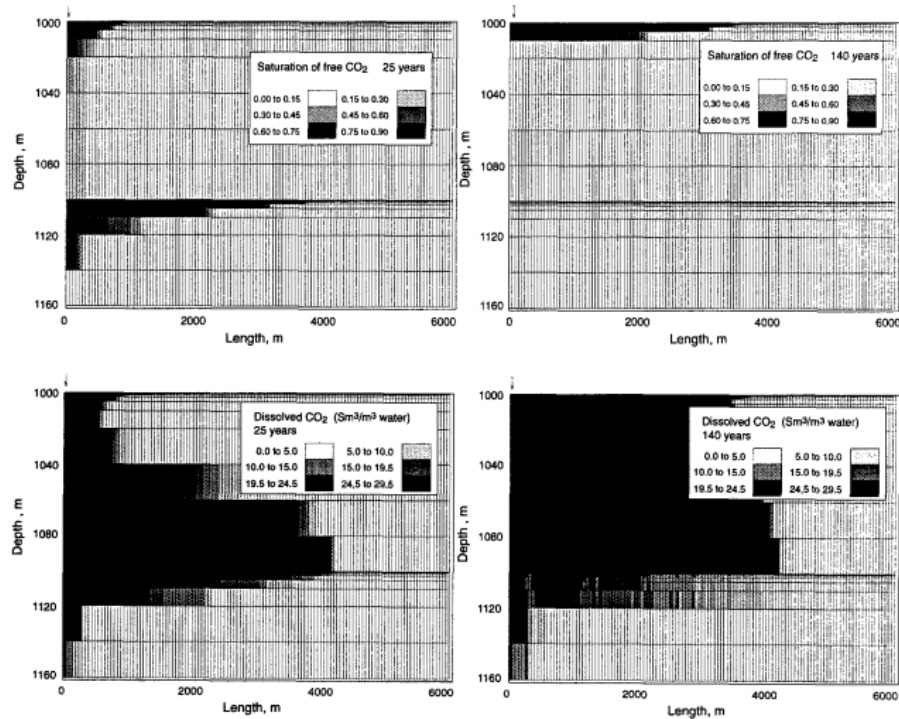


Figure 10: Temporal and Spatial Distribution of Free and Dissolved CO₂ in an Aquifer [42]

The research conducted by Lindeberg in 1997 offered valuable perspectives on the extended-term destiny of CO₂ that is injected into saline aquifers and the significance of solubility trapping in CO₂ storage. The study showcased the potential of using numerical modeling to evaluate the capacity and confinement of saline aquifers for CO₂ storage. Furthermore, it emphasized the importance of accurately representing density-driven flow and CO₂ dissolution in the modeling of CO₂ sequestration initiatives.

In 2003, Pruess et al. presented the TOUGH2 simulator, an extensively employed numerical model specifically developed to simulate the movement and transportation of various phases and components in porous media [43]. This model is widely utilized for various purposes related to the sequestration of CO₂.

The TOUGH2 simulator is a highly flexible numerical software designed to replicate a variety of underground flow and transport phenomena, including fluid flow, heat transfer, and chemical reactions. It utilizes the integral finite difference method, which enables customizable partitioning of the computational area and accurate representation of intricate geological shapes. This simulator is capable of managing multiple fluid stages (e.g., gas, liquid, and supercritical) and different chemical components (e.g., CO₂, water, and dissolved solids), and it incorporates equation-of-state modules to characterize the thermodynamic properties of fluids and their interactions with porous media.

They demonstrated the effectiveness of the TOUGH2 simulator in modeling CO₂ injection into saline aquifers and depleted oil and gas reservoirs for CO₂ sequestration purposes. Their case studies showcased the simulator's capability to simulate complex processes

related to CO₂ storage, such as multiphase flow, CO₂ dissolution, and geochemical reactions. The TOUGH2 simulator has significantly influenced CO₂ sequestration modeling and has been widely adopted in both academic and industrial settings to investigate diverse CO₂ storage scenarios.

In 2004, Xu and colleagues performed a numerical modeling investigation to explore the geochemical reactions and transport mechanisms associated with the storage of CO₂ in deep saline aquifers [44]. In their study, researchers aimed to improve our understanding of the long-term fate of CO₂ injected into geological formations and the potential for mineral entrapment in diverse rock structures. Xu et al. developed a reactive transport model in 2004 to incorporate multiphase fluid flow, heat transfer, and geochemical reactions. The model was tailored to simulate the introduction of supercritical CO₂ into an imaginary saline aquifer with a varied mineral composition typical of Gulf Coast Sediments, as illustrated in **Figure 11**. The researchers examined how CO₂ moves and spreads within the underground water storage, along with the chemical interactions between CO₂, salty water, and the rock formation.

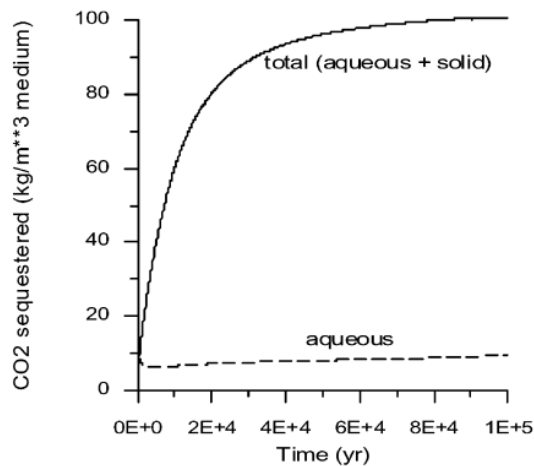


Figure 11: Long-Term CO₂ Sequestration Trends in Gulf Coast Sediments [44]

They conducted numerical simulations to demonstrate the potential efficacy of mineral trapping as a long-term method for storing CO₂. This method entails the dissolution of CO₂ in formation brine, which causes carbonate minerals such as calcite, dolomite, and siderite to precipitate due to geochemical reactions with the rock matrix, resulting in changes in porosity, as illustrated in **Figure 12**.

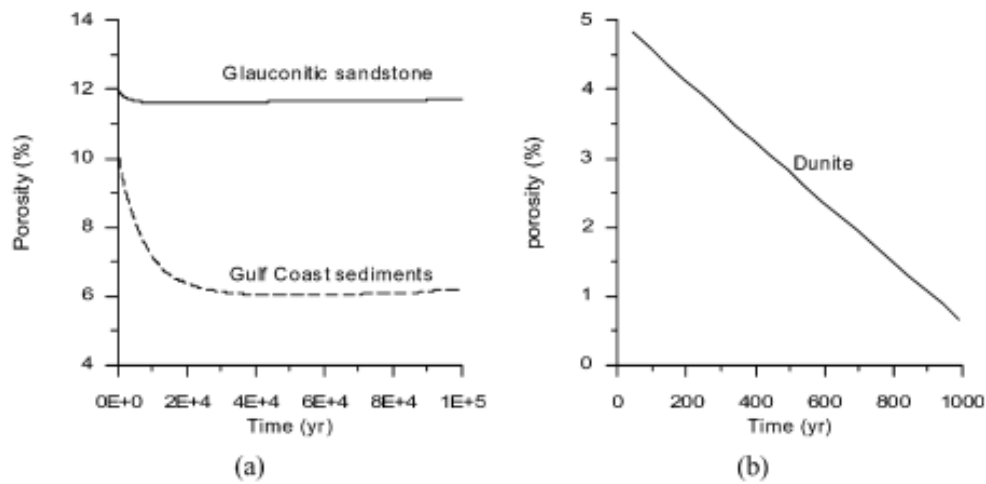


Figure 12: Porosity Changes Over Time in Different Rock Types Due to CO₂ Injection [44]

Xu et al. and his team observed that the diversity and speed of mineral entrapment in the saline aquifer were affected by its geochemical heterogeneity. The presence of active minerals, such as feldspar and chlorite, encouraged the formation of carbonate minerals and the storage of CO₂. Conversely, the existence of less reactive minerals, such as quartz, constrained the degree of mineral entrapment. The simulations also indicated that the dispersion and destiny of injected CO₂ were significantly shaped by the geochemical heterogeneity of the aquifer. The CO₂ plume moved predominantly through areas with high

permeability, while geochemical reactions and mineral entrapment occurred more extensively in regions with favorable mineral compositions.

Krevor et al. (2012) integrated numerical modeling with machine learning techniques to optimize CO₂ injection strategies and maximize storage efficiency in heterogeneous reservoirs [45].

The research aimed to create a framework for optimizing CO₂ storage projects, considering complex interactions between reservoir heterogeneity, multiphase flow, and geochemical reactions. Using a numerical reservoir simulator, the researchers simulated CO₂ injection into diverse saline aquifers. The model accounted for varying reservoir characteristics, multiphase flow, and geochemical reactions such as mineral dissolution and precipitation. To enhance the CO₂ injection approach, the researchers utilized machine learning methods, particularly genetic algorithms, to determine the best injection parameters. By combining the genetic algorithm with the reservoir simulator, they were able to assess different injection scenarios and identify the most effective strategy for maximizing storage efficiency and minimizing CO₂ leakage risk. The study demonstrated that integrating numerical modeling and machine learning techniques can significantly improve the effectiveness and safety of CO₂ storage projects. Furthermore, it indicated that the optimized injection strategy could increase storage capacity and reduce the risk of CO₂ leakage compared to conventional methods.

Additionally, Victor Vilarrasa and Roman Makhnenko, along with Sohrab Gheibi (2016), conducted an in-depth geomechanical analysis to understand the impact of CO₂ injection sites on fault stability [46].

The study delves into the effects and geological challenges of storing carbon dioxide in deep saline formations. It primarily examines the variations in stress levels along faults when carbon dioxide is injected into either the hanging wall or the foot wall. According to the research, injecting carbon dioxide leads to overpressure, which significantly diminishes fault stability, irrespective of the injection location. The unequal distribution of fluid pressure resulting from the fault's low permeability causes uneven changes in total stress around the fault, ultimately rendering it unstable. Nonetheless, the researchers highlight that the stability of the caprock near the injection wells is not compromised, thereby lowering the risk of carbon dioxide leakage, as illustrated in **Figure 13**.

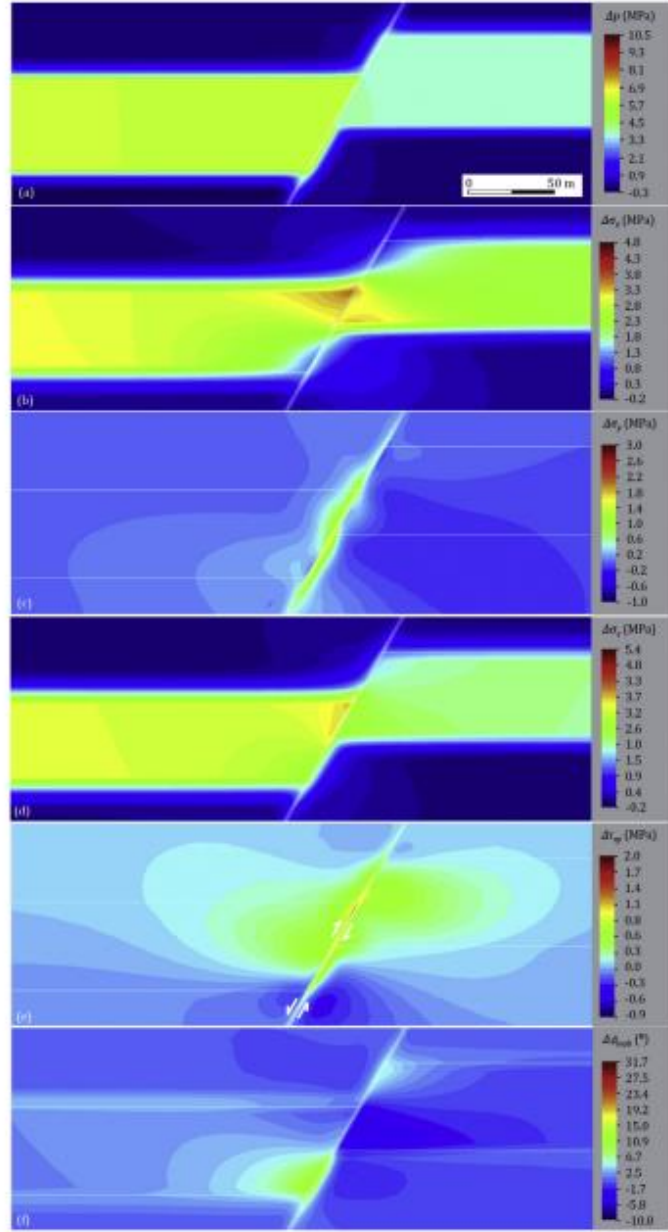


Figure 13: Variations in Fluid Pressure and Stress Distribution Due to CO₂ Injection Near a Fault [46]

Moreover, the study explores how the fault core permeability impacts fault stability, noting that higher permeable faults are less affected by injection pressures. Their findings underline the necessity of precise pressure management to store large CO₂ volumes without triggering fault reactivation or inducing seismicity. The research concludes that while fault

reactivation is a risk, proper site selection, monitoring, and management can maintain overall site integrity, ensuring the long-term success of geologic carbon sequestration efforts.

Michal et al. (2022) developed a machine learning-based surrogate model to optimize the placement of injection wells in a CO₂ storage project [47]. The research aimed to tackle the computational difficulties involved in optimizing well placement in large-scale CO₂ storage projects. Traditional numerical simulation-based optimization methods can be both time-consuming and computationally expensive for this purpose. To address this, the researchers employed a deep neural network (DNN) to construct a surrogate model that can predict the performance of CO₂ injection scenarios based on well locations and injection rates. The DNN was trained using a large dataset of numerical simulation results generated by a high-fidelity reservoir simulator. After training the DNN surrogate model, it was employed alongside a genetic algorithm to optimize the positioning of injection wells and injection rates for a specific CO₂ storage initiative. The results showed that the surrogate model, which was based on machine learning, could reliably forecast the performance of CO₂ injection strategies. This led to a substantial decrease in computational time when compared to conventional optimization methods based on numerical simulations. The authors exhibited that implementing the surrogate model for optimization in extensive CO₂ storage projects led to an augmented CO₂ storage capacity and minimized the risk of CO₂ leakage in comparison to scenarios that were not optimized.

2.4 CCS Projects

As we move forward from the progress made in numerical modeling of CO₂ sequestration, it is crucial to investigate how these methods can be practically applied in real-life CO₂ storage initiatives. Over the last few decades, there have been numerous CO₂ sequestration projects carried out globally, including small-scale test runs and large-scale commercial endeavors. These projects have offered valuable insights into the practicality, performance, and difficulties associated with storing CO₂ in various geological formations, such as saline aquifers, depleted oil and gas reservoirs, and unmineable coal seams [48].

2.3.1 The Sleipner CO₂ storage project

The Sleipner CO₂ storage project, located in the North Sea off the coast of Norway, as illustrated in **Figure 14**, is a pioneering venture in CCS and has been in operation since 1996. This project is operated by Equinor, a Norwegian multinational energy company formerly known as Statoil. The Sleipner project is widely recognized as one of the most successful and longest-running CO₂ storage projects in the world, having stored over 20 million tonnes of CO₂ to date [49].

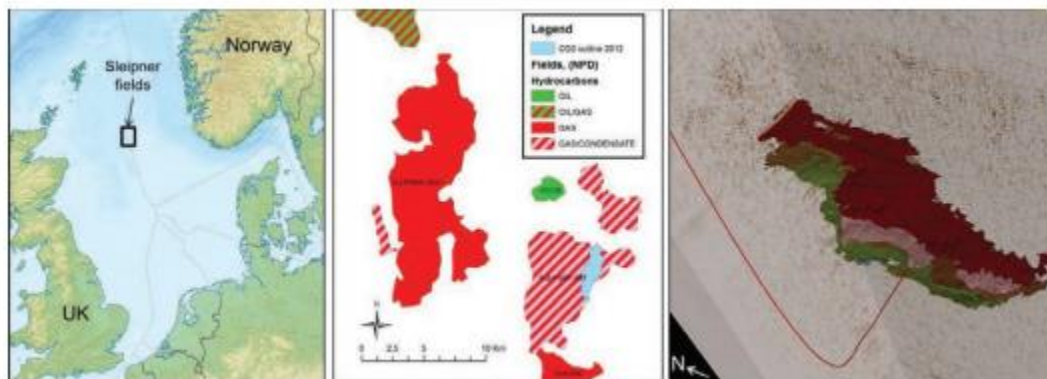


Figure 14: Sleipner CO₂ Plume Maps and Seismic Data [49]

The Sleipner project is designed to capture CO₂ from the Sleipner West gas field, which contains approximately 9% CO₂ in its natural gas. Rather than releasing this separated CO₂ into the atmosphere, Equinor chose to store it in a deep saline aquifer using a CCS project. The CO₂ is separated from the natural gas using an amine-based absorption process, then compressed and transported through a pipeline to an offshore injection site located around 250 kilometers away. At this site, the CO₂ is injected 800-1,000 meters below the seabed into the Utsira sandstone formation, which is an extensive and permeable storage site with a thickness of 200-300 meters and covers an area of about 26,000 square kilometers in the North Sea. To ensure the secure and efficient storage of CO₂, the project is subject to thorough monitoring through methods such as seismic surveys, gravity measurements, and wellbore monitoring. The success of the Sleipner project has not only demonstrated the viability of CO₂ storage in deep saline aquifers but has also provided valuable operational experience and data for future CCS projects globally. As a result, the Sleipner project has been recognized as a significant achievement in the advancement of CCS technology and has received numerous accolades for its contribution to climate change mitigation.

2.3.2 The Illinois Basin Decatur Project

The Illinois Basin Decatur Project (IBDP) is an initiative located in Decatur, Illinois, USA, aimed at storing CO₂ on a pilot scale. Managed by the Illinois State Geological Survey (ISGS) and the Midwest Geological Sequestration Consortium (MGSC), this collaborative effort involves state geological surveys, universities, and private companies. The main objective of the IBDP is to demonstrate the feasibility and safety of CO₂ storage in the

Illinois Basin, a large sedimentary basin covering most of Illinois, as well as parts of Indiana and Kentucky [50].

Since 2011, the Illinois Basin Decatur Project (IBDP) has been actively involved in injecting CO₂ into the Mt. Simon Sandstone, a deep saline aquifer found at depths ranging from 1,800 to 2,200 meters below the surface. The Mt. Simon Sandstone is characterized by its substantial thickness, porosity, and permeability. It's important to note that the injected CO₂ is contained by the Eau Claire Shale, which overlies the sandstone and acts as a cap rock. This containment prevents the upward migration of the injected CO₂. The source of the injected CO₂ is an ethanol production facility operated by Archer Daniels Midland (ADM) in Decatur, which produces around 1 million tonnes of CO₂ annually as a byproduct of ethanol production. The captured CO₂ is compressed and then transported to the injection site through a short pipeline situated near the ADM facility.

At the injection site, which is adjacent to the ADM facility, the CO₂ is injected into the Mt. Simon Sandstone through a single injection well at a depth of approximately 2,100 meters below the surface. This injection well is equipped with various monitoring instruments, including pressure and temperature sensors, to oversee the injection process and ensure the safe and efficient storage of the CO₂. Since its inception in 2011, the IBDP has successfully injected and stored over 1 million tonnes of CO₂ in the Mt. Simon Sandstone, as depicted in **Figure 15**. The project has demonstrated that it is possible to securely and efficiently store CO₂ in deep saline aquifers located in the Illinois Basin. This discovery holds promise for potential large-scale storage endeavors in the future. With an estimated CO₂ storage capacity of approximately 20 to 80 billion tonnes, the Illinois Basin emerges as one of the most favorable areas for CCS initiatives in the United States.

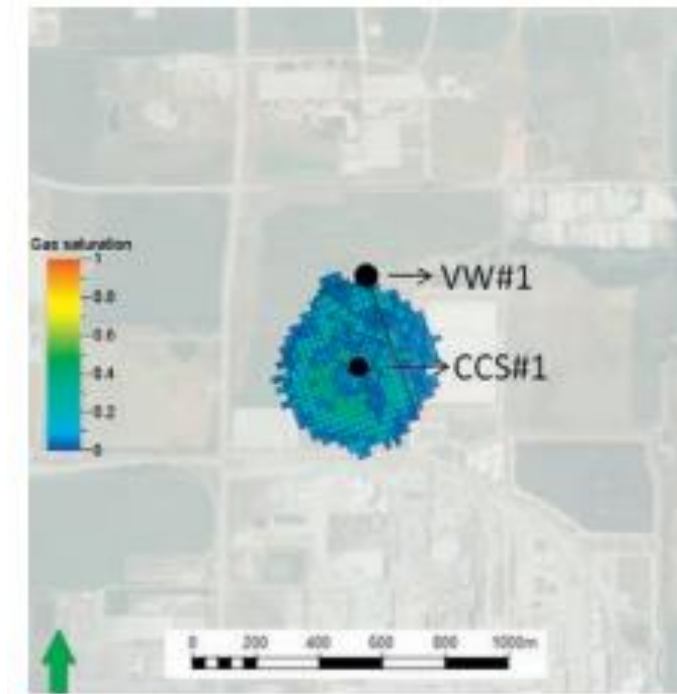


Figure 15: Simulated distribution of CO₂ in the reservoir as of March 2012 [50]

The IBDP has established a comprehensive monitoring program to track the flow and destiny of the injected CO₂ underground. This program involves seismic surveys, geophysical logging, pressure and temperature monitoring, and groundwater sampling. The data gathered from this monitoring program has provided valuable knowledge about the behavior of CO₂ in the Mt. Simon Sandstone and has contributed to refining numerical models for CO₂ storage in the Illinois Basin.

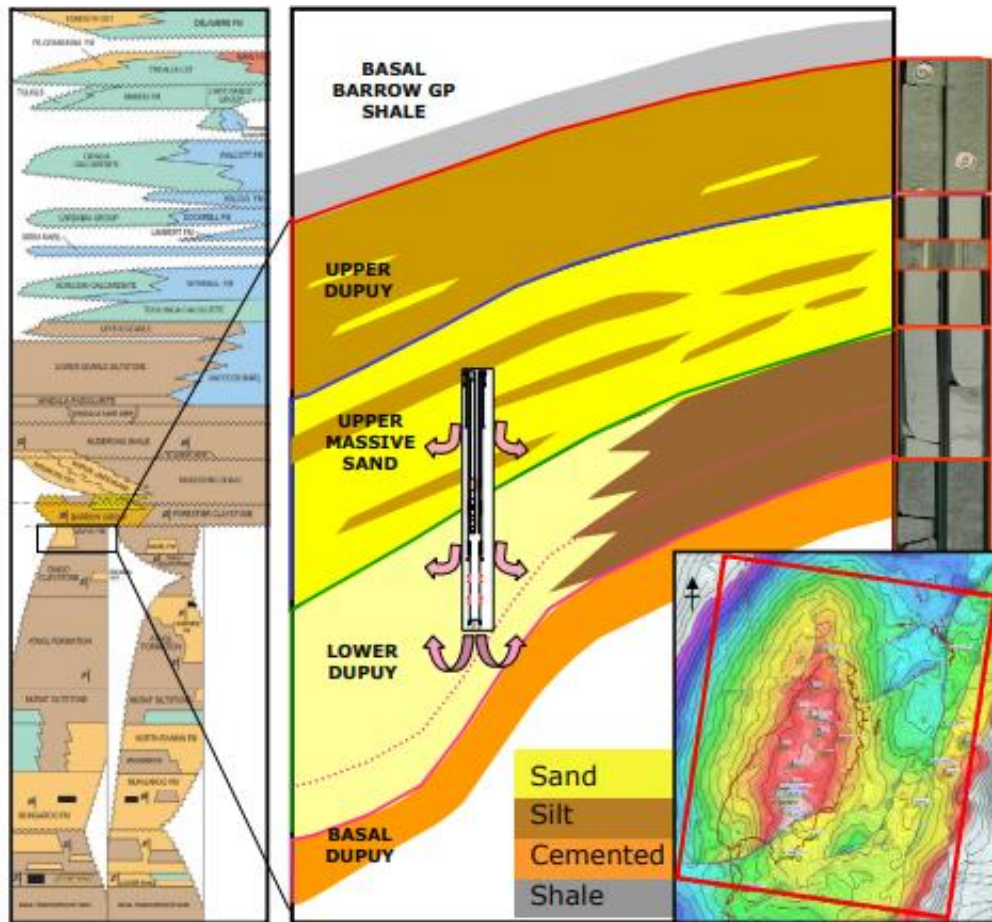
The achievements of the IBDP have paved the way for the implementation of more extensive CCS initiatives in the Illinois Basin. In 2017, the U.S. Department of Energy declared its backing for the Illinois Storage Corridor Project, which seeks to create a local CO₂ storage center in the Illinois Basin. This project will utilize the insights and information gained from the IBDP to construct a large-scale CO₂ storage framework, enabling the adoption of CCS technology in the region.

2.3.3 The Gorgon Carbon Dioxide Injection Project

The Gorgon LNG project is centered around extracting natural gas from the Gorgon and Jansz-IO gas fields off the coast of Western Australia and transporting it to a processing facility on Barrow Island to be cooled and liquefied for export [51].

The gas extracted contains a high concentration of CO₂, which needs to be removed to meet LNG product specifications and reduce GHG emissions. The separated CO₂ is then compressed and injected into the Dupuy Formation, a deep saline aquifer located about 2,300 meters below Barrow Island. Managed by Chevron Australia, the Gorgon Carbon Dioxide Injection Project is a significant initiative aimed at the sequestration of CO₂, integral to the overall Gorgon LNG development. The project represents a collaborative effort with Chevron owning 47.3%, ExxonMobil and Shell each owning 25%, while Osaka Gas, Tokyo Gas, and JERA own 1.25%, 1%, and 0.417% respectively., as illustrated in **Figure 16**.

The Dupuy Formation, located beneath Barrow Island and the surrounding offshore area, is a significant sandstone formation covering approximately 500 square kilometers. It consists of porous and permeable sandstone and is sealed by a thick layer of shale, which prevents the upward migration of injected CO₂. CO₂ injection at the Gorgon project began in August 2019 after the establishment of CO₂ injection facilities and the drilling of nine injection wells. The project aims to capture and store up to 4 million tonnes of CO₂ annually, which represents about 40% of the total CO₂ emissions from the Gorgon LNG facility. Over its lifetime, the project is expected to store more than 100 million tonnes of CO₂, making it one of the world's leading CO₂ sequestration initiatives



2.3.4 The Quest CCS project

Some important CCS projects to mention are the Quest CCS project in Alberta, Canada, which is managed by Shell Canada [52]. This initiative aims to capture and store approximately 1 million tons of CO₂ annually from the Scotford upgrader, a bitumen upgrading facility situated near Edmonton, Alberta, as depicted in **Figure 17**. The Quest project stands as one of the initial large-scale CCS projects globally and has been active since 2015.

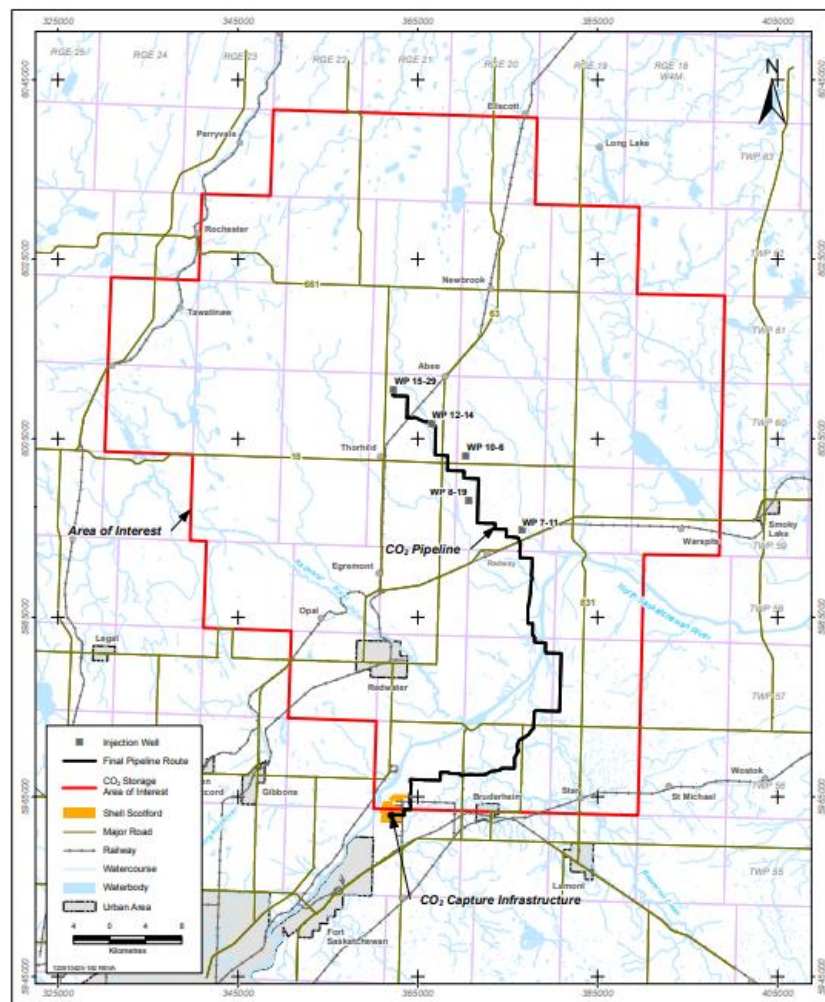


Figure 17: Map of Project Components and Area of Interest for Quest CCS Project [52]

The Scotford Upgrader is a key component of Shell's Athabasca Oil Sands Project, which focuses on the extraction and upgrading of bitumen from the Athabasca oil sands deposit in northern Alberta. A significant part of this initiative is the Quest project, which aims to capture and store about one-third of the CO₂ emissions from the Scotford Upgrader in a deep saline aquifer. This effort marks a substantial step towards reducing GHG emissions.

The Quest project is notable for its capacity to store up to 1 million tonnes of CO₂ per year, which accounts for approximately 35% of the Scotford Upgrader's total CO₂ emissions. Over its lifespan, the project is expected to store more than 27 million tonnes of CO₂, equivalent to the annual emissions from around 250,000 homes. To achieve this, the project employs extensive monitoring and verification measures, including seismic surveys, pressure monitoring, and geochemical sampling. These techniques are used to track the migration and behavior of CO₂ in the subsurface, ensuring its secure and permanent storage.

One of the standout features of the Quest project is its comprehensive environmental Monitoring, Measurements, and Verification (MMV) program, which exceeds current regulatory requirements. This program includes a network of monitoring wells and sensors that provide real-time data on the pressure, temperature, and geochemical composition of the injected CO₂ in the surrounding formations. The collected data is crucial for calibrating and validating numerical models that predict the long-term behavior of the CO₂, ensuring that the storage site performs as anticipated.

Additionally, the Quest project emphasizes community engagement and public communication. Shell works closely with local communities, stakeholders, and Indigenous groups to address concerns and share information about the project. The initiative also features a visitor center and public viewing area, allowing the public to learn about the project and see the facilities firsthand.

The Quest project has gained widespread recognition for its significant impact on advancing CCS technology, earning multiple awards. The monitoring program, which employs cutting-edge technologies such as seismic surveys, geophysical logging, and pressure monitoring, ensures the safe and effective storage of CO₂.

These projects demonstrate the practical applications and benefits of CCS technology, providing valuable data and experience for future developments in CO₂ sequestration.

CHAPTER 3

METHODOLOGY

3.1 Computational Modeling

When modeling CO₂ sequestration in saline aquifers, the GEM simulator from Computer Modeling Group (CMG) is a highly effective tool. This simulator excels due to its robust capabilities in simulating multiphase fluid flow, geochemical interactions, and thermal dynamics, which are crucial for understanding and predicting the behavior of CO₂ once injected into geological formations.

In our study, the focus was on accurately capturing the dynamics of two-phase flow involving water and CO₂. This was achieved by integrating diffusivity equations with the Peng-Robinson equation of state—a well-regarded model for predicting the properties of gases and liquids under varying pressures and temperatures. The Peng-Robinson equation is particularly useful for handling the complex behaviors of the CO₂ and water mixture in the subsurface environment.

The GEM simulator plays a crucial role in accurately modeling the injection process and the movement of the CO₂ plume within the aquifer. This is due to its advanced capability to handle variations in composition and phase behavior. It effectively simulates the complex interactions between the injected CO₂ and the resident brine, including important geochemical reactions with the rock matrix, like mineral dissolution or precipitation. These interactions can have a significant impact on the porosity and permeability of the rock,

ultimately influencing the migration path of the CO₂ plume and the storage capacity of the aquifer.

It is essential for the simulator to account for thermal effects, as changes in temperature within the aquifer can influence the density of CO₂ in brine, as well as its viscosity attributes and the rate of geochemical reactions. These factors are critical for predicting the long-term destiny of stored CO₂, evaluating the geological storage's integrity, and confirming the efficiency of the sequestration process.

3.1.1 Governing Equations of Fluids

3.1.1.1 Diffusivity Equations

Diffusivity equations were employed to model the two-phase flow of CO₂ and water within the saline aquifer. These equations are fundamental in describing the pressure and saturation distribution in porous media. The water phase equation is given by:

The water phase equation is:

$$\frac{\partial}{\partial t} (\phi S_w \rho_w) = \nabla \cdot \left(\frac{k k_{rw}}{\mu_w} (\nabla p_w - \rho_w g) \right) + q_w \quad (3.1)$$

And the CO₂ phase equation is :

$$\frac{\partial}{\partial t} (\phi S_g \rho_g) = \nabla \cdot \left(\frac{k k_{rg}}{\mu_g} (\nabla p_g - \rho_g g) \right) + q_g \quad (3.2)$$

Where:

- ϕ is the porosity
- S_w and S_g are the saturations of water and gas, respectively
- ρ_w and ρ_g are the densities of water and gas, respectively
- k is the absolute permeability
- kr_w and kr_g are the relative permeabilities of water and gas, respectively
- μ_w and μ_g are the viscosities of water and gas, respectively
- p_w and p_g are the pressures of water and gas, respectively
- g is the gravitational acceleration
- q_w and q_g are the source/sink terms for water and gas, respectively

3.1.1.2 Energy Conservation Equation

In this study, the GEM simulator was used to model the thermal interactions between CO₂ and water in the reservoir. The energy conservation equation, coupled with the mass conservation equations for both phases, forms the basis of the thermal simulation. The governing energy conservation equation is expressed as:

For water:

$$\frac{\partial}{\partial t}(\phi \rho_w c_{p,w} T) + \nabla \cdot (\rho_w c_{p,w} u_w T) = \nabla \cdot (k_r \nabla T) + q_T \quad (3.3)$$

For CO₂:

$$\frac{\partial}{\partial t}(\phi \rho_g c_{p,g} T) + \nabla \cdot (\rho_g c_{p,g} u_g T) = \nabla \cdot (k_r \nabla T) + q_T \quad (3.4)$$

Where:

- $\rho_w c_{p,w}$ and $\rho_g c_{p,g}$ are the products of density and specific heat capacity for water and gas, respectively
- T is the temperature
- u_w and u_g are the velocity vectors for water and gas, respectively
- k_r is the thermal conductivity
- q_T is the source/sink term for heat

3.1.1.3 Peng-Robinson Equation

The Peng-Robinson equation of state (PR EOS) is a sophisticated model that has been widely utilized in the petroleum and chemical industries to predict the phase behavior and properties of fluids. It is particularly effective in applications involving non-ideal gases and liquids, including scenarios like CO₂ sequestration where the fluid behavior under high pressure and temperature conditions near the critical point is critical.

$$P = \frac{RT}{V_m - b} - \frac{a(T)}{V_m(V_m + b) + b(V_m - b)} \quad (3.5)$$

Where:

- P is the pressure.
- R is the universal gas constant.
- V_m is the molar volume.
- $a(T)$ is a temperature-dependent function.
- b is a constant related to the size of the molecules.

3.1.2 Geomechanics

In the geomechanics module of CMG, I employed the constitutive law, elasto-plasticity, and the Mohr-Coulomb model to accurately depict the mechanical behavior of the reservoir rock under different stress conditions. These models are crucial for comprehending and forecasting the deformation and failure mechanisms in the reservoir, which are vital for maintaining the integrity and effectiveness of CO₂ sequestration.

3.1.2.1 Constitutive Law

The constitutive law outlines how stress and strain are related in materials. In the case of reservoir rocks, this relationship typically begins with linear elasticity and then transitions to elasto-plastic behavior as stress increases. In geomechanics, the constitutive law can generally be represented by:

$$\sigma_{ij} = D_{ijkl}\varepsilon_{kl} \quad (3.6)$$

Where:

- σ_{ij} is the stress tensor.
- D_{ijkl} is the elastic stiffness tensor.
- ε_{kl} is the strain tensor.

3.1.2.2 Elasto-Plasticity

Elasto-plasticity describes the material behavior where elastic deformation occurs up to a yield point, beyond which plastic deformation occurs. Elastic strain is related to stress through Hooke's law:

$$\varepsilon_{ij} = C_{ijkl}^{-1} \sigma_{kl} \quad (3.7)$$

Where:

- C_{ijkl}^{-1} is the inverse of the elastic compliance tensor.

3.1.2.3 Mohr-Coulomb Model

The Mohr-Coulomb model is a fundamental yield criterion commonly used to describe how materials fail under shear stress. It utilizes two key parameters: cohesion (c) and the internal friction angle (ϕ). The Mohr-Coulomb failure criterion can be expressed as:

$$\tau = c + \sigma \tan \phi \quad (6)$$

Where:

- c is the cohesion of the material.
- ϕ is the internal friction angle.

3.1.2.4 Impact of Porosity on the Geomechanical Properties of Rocks

The equations provide insight into how the mechanical properties of rocks change as porosity increases. Specifically, as the porosity increases, Young's modulus decreases, reflecting a reduction in the rock's overall stiffness and load-bearing capacity. This relationship is expressed through a non-linear equation:

The presence of pores within the rock structure leads to these changes by diminishing the material's ability to resist deformation under load. Similarly, the Poisson's ratio also adjusts with changing porosity, indicating a shift in the volumetric strain response due to compressive stress. This adjustment is captured by the following equation, which shows the dependency of Poisson's ratio on porosity in a non-linear fashion [53].

$$E = E_0 * (1 - \phi)^2 \quad (3.8)$$

$$\nu = \nu_0 + (0.5 - \nu_0)(1 - (1 - \phi)^{1.3}) \quad (3.9)$$

Both equations highlight the critical impact of porosity on the geomechanical properties of rocks, underscoring the importance of considering these factors in geotechnical assessments and engineering projects.

3.1.3 Hysteresis

Hysteresis effects are fundamental in CO₂ sequestration projects, especially regarding capillary and residual trapping mechanisms. Hysteresis describes the behavior in which the relationship between capillary pressure and saturation follows different paths during the drainage (injection) and imbibition (post-injection) stages. This phenomenon significantly influences how CO₂ is distributed and immobilized within a saline aquifer [54].

During the injection phase, CO₂ pushes out the resident brine along the drainage capillary pressure curve. Once injection ceases and the system shifts to the post-injection phase, the CO₂ plume repositions itself and is captured by capillary forces on the imbibition capillary pressure curve. Hysteresis causes the imbibition curve to have higher capillary pressures than the drainage curve resulting in a significant amount of CO₂ being residually trapped in the pore spaces, as illustrated in **Figure 18**.

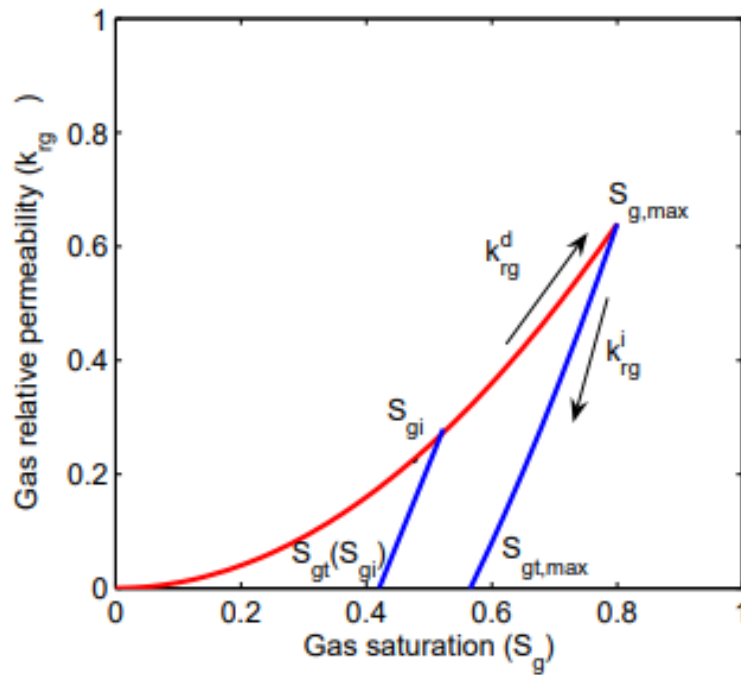


Figure 18: Hysteresis Effects [54]

Residual trapping plays a vital role in securing long-term CO₂ storage by effectively encapsulating a substantial portion of CO₂ within the formation. Overlooking hysteresis effects may result in underestimating the potential for this type of trapping, thereby compromising assessments of the project's long-term storage capacity and security. The relative permeability values used in the CMG model, as shown in **Figure 19**, underscore this point.

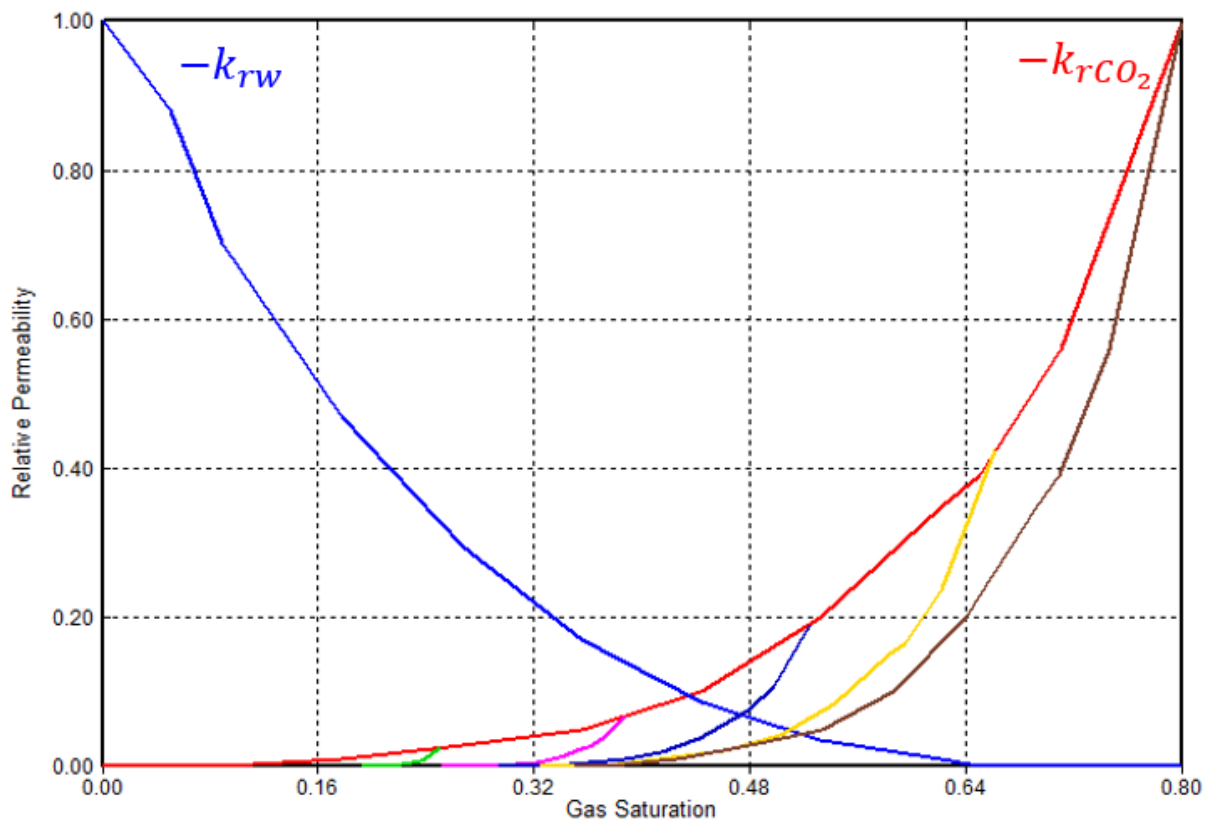


Figure 19: Hysteresis curves (CMG Data set)

3.1.4 Chemical Reactions

The B-dot model is used in CMG for simulating dissolution and precipitation processes, particularly within the context of geochemical reactions in reservoir simulations. This model is effective in accounting for the detailed chemical interactions between injected fluids, reservoir brine, and minerals, thus providing insights into changes in porosity, permeability, and overall reservoir integrity.

$$\log \gamma_i = -\frac{BaIAz_i^2\sqrt{I}}{1 + Ba_i\sqrt{I}} + bI \quad (3.10)$$

$$I = \frac{1}{2} \sum c_j z_j^2 \quad (3.11)$$

where:

- γ_i is the activity coefficient of ion i
- A and B are temperature-dependent constants
- z_i is the charge of ion i
- I is the ionic strength
- a_i is the ion size parameter
- c_j is the concentration of ion j
- b is an empirical parameter that adjusts the model for specific ion interactions or conditions.

- l is a correction factor or a specific interaction parameter that accounts for deviations in the model, such as ion pairing or other specific ion effects.

In the context of geochemical reactions in reservoir simulation, particularly when using the B-dot model, the equilibrium constants often involve activities instead of concentrations.

The activity-based equilibrium constant K_a is given by:

$$K_a = \frac{(aC)^c (aD)^d}{(aA)^a (aB)^b} \quad (3.13)$$

Where:

- a represents the activity of the species in the reaction.
- A, B, C and D are the chemical species involved in the reaction.
- aA, aB, aC and aD represent the activities of the chemical species A, B, C and D , respectively.
- a, b, c and d are the stoichiometric coefficients of the species A, B, C and D in the balanced chemical equation.

During the process of CO₂ sequestration, it is crucial to ensure that the reservoir rock remains stable and intact. The rate of chemical reactions can be used to forecast the dissolution and precipitation of minerals, which in turn impact the porosity and

permeability of the rock. Below is the corrected and detailed version of the equation for the reaction rate:

$$r = V \cdot A \cdot k \left(1 - \frac{Q}{K_a}\right) \quad (3.14)$$

Where:

- r is the reaction rate.
- V is the volume.
- A is the surface area.
- k is the rate constant.
- Q is the ion activity product.
- K_a is the equilibrium constant.

When $Q < K_a$, the term $\left(1 - \frac{Q}{K_a}\right)$ is positive, indicating that the reaction proceeds forward (mineral dissolution).

When $Q > K_a$, the term $\left(1 - \frac{Q}{K_a}\right)$ is negative, indicating that the reaction proceeds in reverse (mineral precipitation).

When $Q = K_a$, the term $\left(1 - \frac{Q}{K_a}\right)$ is zero, indicating that the reaction is at equilibrium and there is no net reaction rate.

The following equation provided encapsulates a fundamental approach to modeling time-dependent reaction rates in chemical systems, which is especially pertinent to the study of CO₂ sequestration dynamics. Here's a breakdown of the key components of this equation and their relevance in the context of CO₂ sequestration:

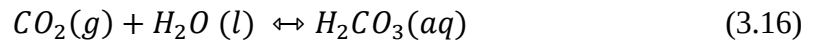
$$\frac{V}{\Delta t} (N_i^{n+1} - N_i^n) = r_i \quad (3.15)$$

Where:

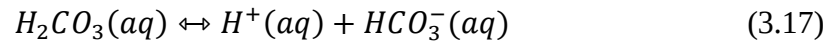
- N_i^n the concentration of substances such as dissolved CO₂ or mineral ions at specific time steps.
- Δt The time step .

The dissolution of calcite ($CaCO_3$) in the presence of carbonic acid (H_2CO_3) involves a series of reactions. These reactions describe the interactions between calcite, carbonic acid, and the resultant species in solution. Here is a comprehensive set of reactions:

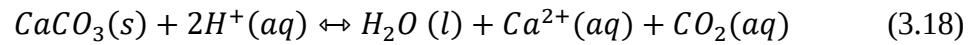
- Formation of Carbonic Acid:



- Dissociation of Carbonic Acid:



- Dissolution of Calcite:



3.2 Model Description

The model domain represents a hypothetical saline aquifer formation suitable for CO₂ sequestration. It spans an area of 11.2 square kilometers, with a thickness of 1,000 feet (approximately 305 meters) and is located at a depth of 2,640 feet, with a temperature of 125°F. A single injection well is strategically positioned at one corner of the model domain to facilitate the injection of CO₂. This well is completed as an open hole in the bottom 150 feet of the formation, as illustrated in **Figure 20**.

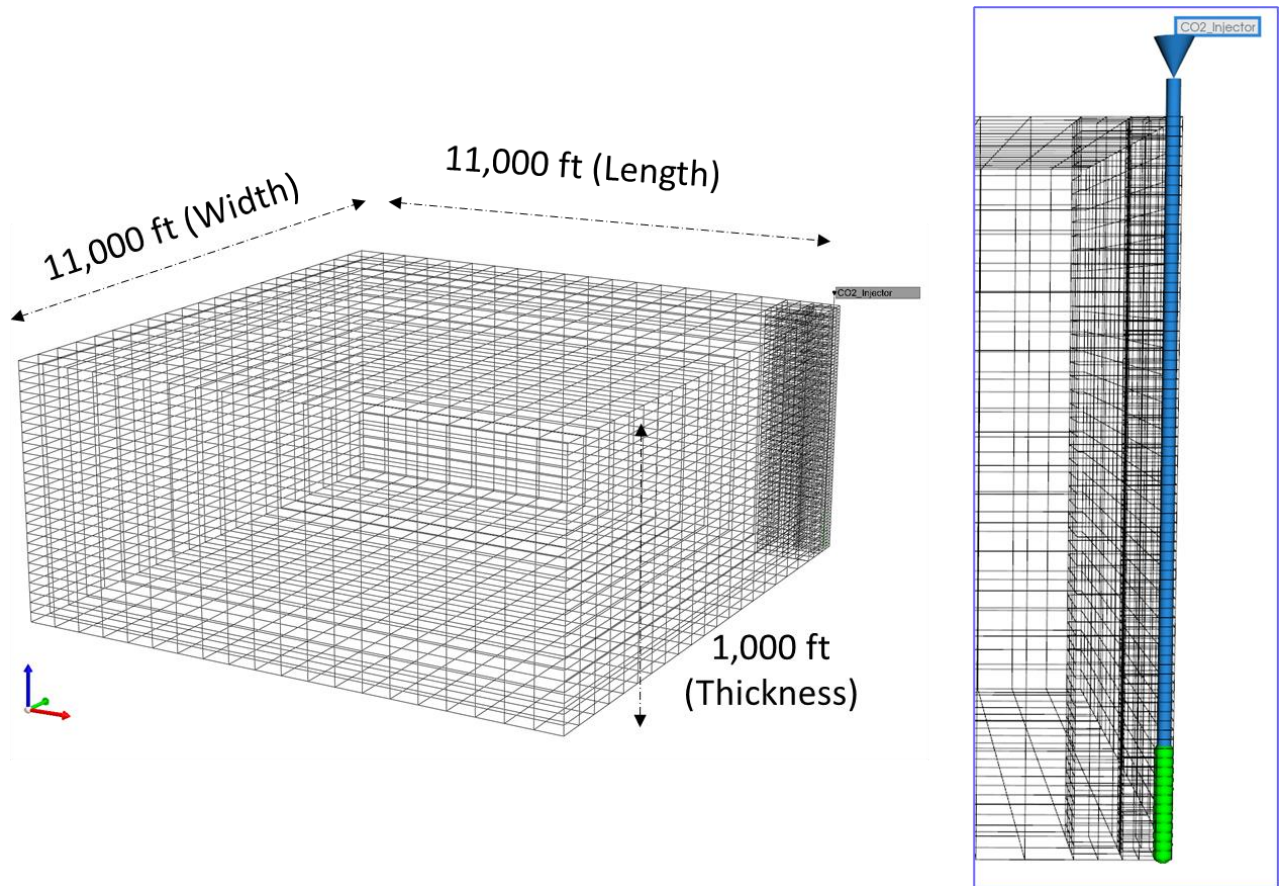


Figure 20: Model overview

3.2.1 Grid refining

The model grid consists of 10,946 cells, with varying grid resolutions ranging from coarse to fine. The grid is designed to capture the necessary spatial details while maintaining computational efficiency. The finer grid cells are strategically placed near the injection well and potential areas of interest, as illustrated in **Figure 21**, such as potential leakage pathways or areas of high-pressure buildup. This grid refinement strategy allows for accurate representation of the CO₂ plume migration and pressure distribution in critical regions. Near the injection well, particularly in the bottom sections where CO₂ is introduced into the formation, the mesh was highly refined. This localized mesh refinement ensures that the critical regions near the wellbore, where high gradients in pressure, saturation, and fluid velocities are anticipated, are accurately captured.

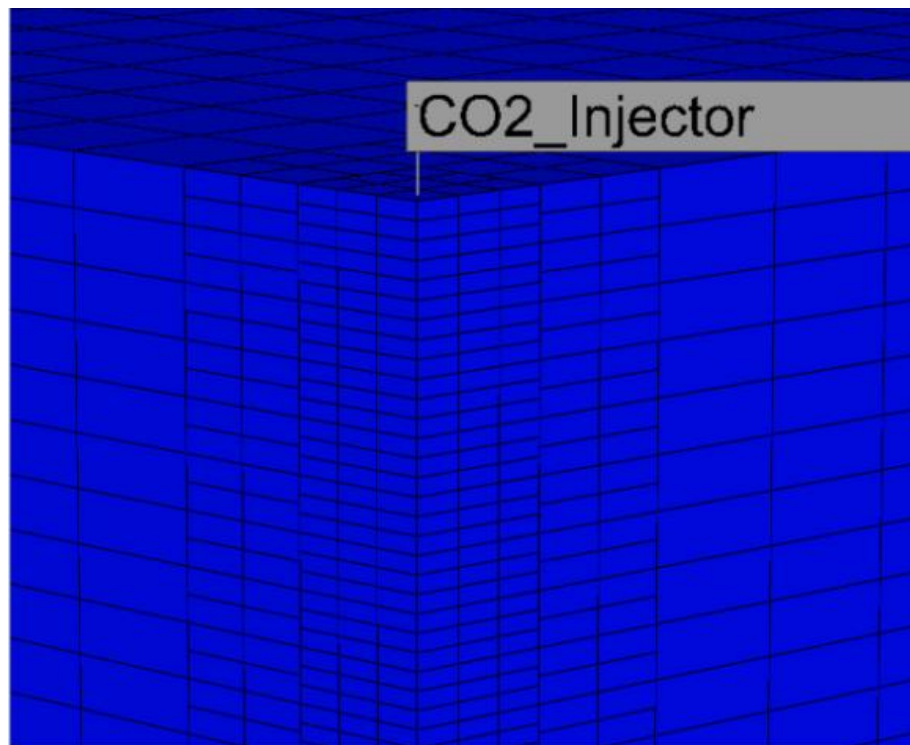


Figure 21: Grid refining

3.2.2 Porosity and Permeability Distribution

The model accurately represents the heterogeneous nature of the saline aquifer formation by incorporating realistic distributions of porosity and permeability values.

3.2.2.1 Porosity

The porosity values assigned to the grid cells range from 0.05 to 0.38, as shown in **Figure 22 (Bottom)**, reflecting the variability in the pore space within the formation. The porosity range provided is derived from well log data, core analyses, and geological interpretations of the depositional environment, as well as the diagenetic processes that have impacted the formation's pore system.

3.2.2.2 Permeability

The model domain contains a significant amount of variation in permeability, demonstrating both heterogeneity and anisotropy, which is common in sedimentary formations.

The horizontal permeability values range from 7 to 314 milliDarcy (mD), as illustrated in **Figure 22 (Top)**, accounting for the variations in pore connectivity and flow paths within the formation.

The vertical permeability values are approximately 10% of the corresponding horizontal permeability values, reflecting the anisotropic behavior commonly observed in layered reservoir systems. This anisotropy results in preferential flow paths and reduced vertical fluid mobility typically seen in such formations. The spatial distribution of porosity was constructed using geostatistical techniques, such as kriging, and permeability was calculated through a power-law relationship with porosity.

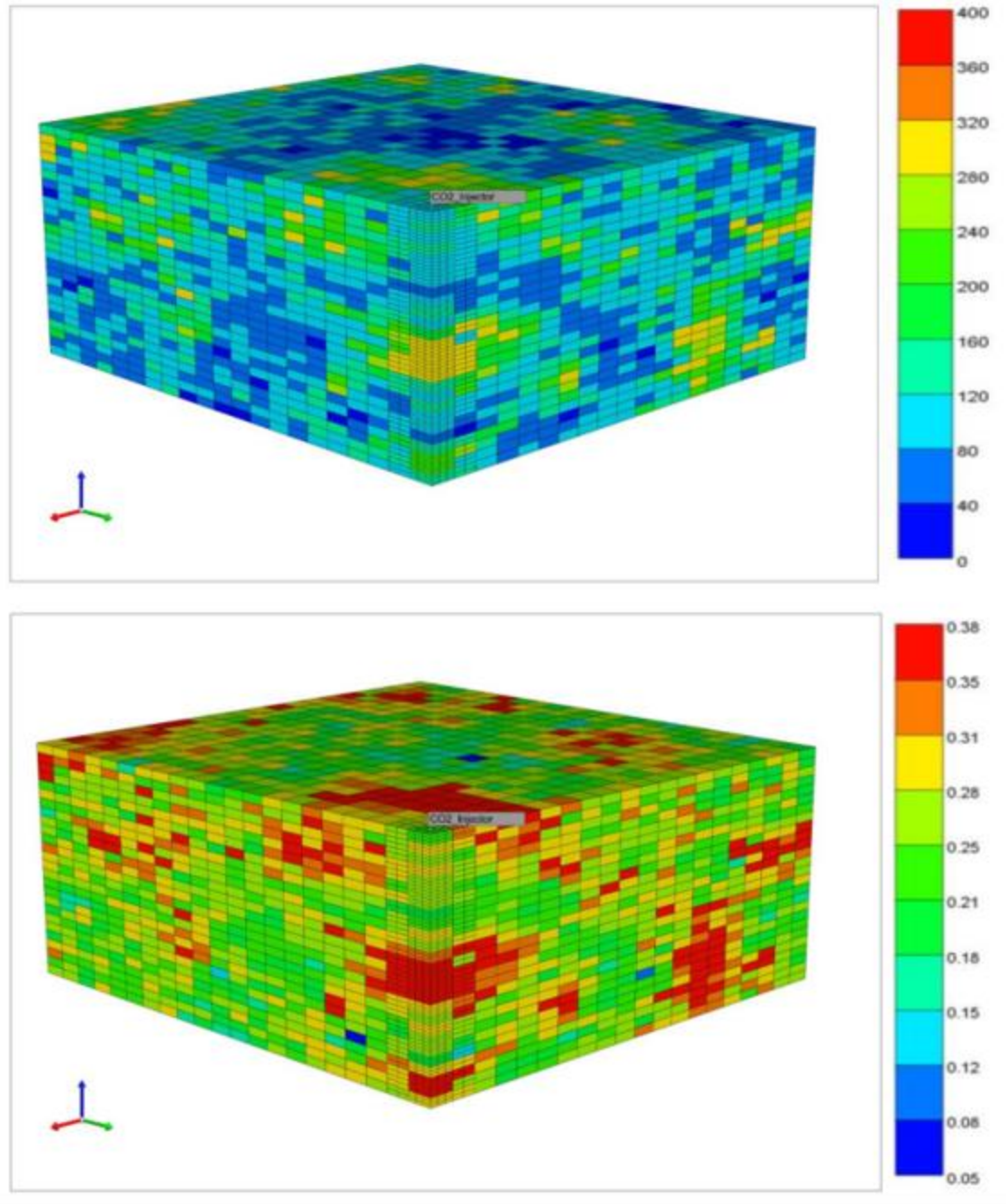


Figure 22: Top Image: Horizontal Permeability Distribution (in milliDarcy) Bottom Image: Porosity Distribution (as a fraction)

The table below presents an overview of the model parameters and their corresponding values used in the CO₂ sequestration study, as seen in **Table 1**.

Table 1: Overview of Model Parameters and Their Values for CO₂ Sequestration Study

Model's parameters	Value
Depth of Top	2,640 ft
Thickness	1,000 ft
Area	11.2 km ²
Number of grids	10,946 cells
Temperature at 2640'	125 °F
Pressure at 2640'	1,126 psi
Lithology	Limestone
Porosity	0.05-0.38, Avg = 0.24
Permeability(h)	7-314 mD, Avg = 92 mD
Permeability(v)	10% * Permeability(h)

3.2.3 Model's Lithology

Figure 23 presents the mechanical properties of three geological layers involved in CO₂ sequestration. Sandstone potentially serves as the top layer to the surface. Shale acts as the caprock, its impermeable nature making it essential for preventing fluid escape and ensuring containment. Limestone, located at the base, functions as the primary aquifer, suitable for water storage and acting as a secondary trapping mechanism due to CO₂ solubility. These layers collectively support the structural integrity and functionality of the sequestration system.

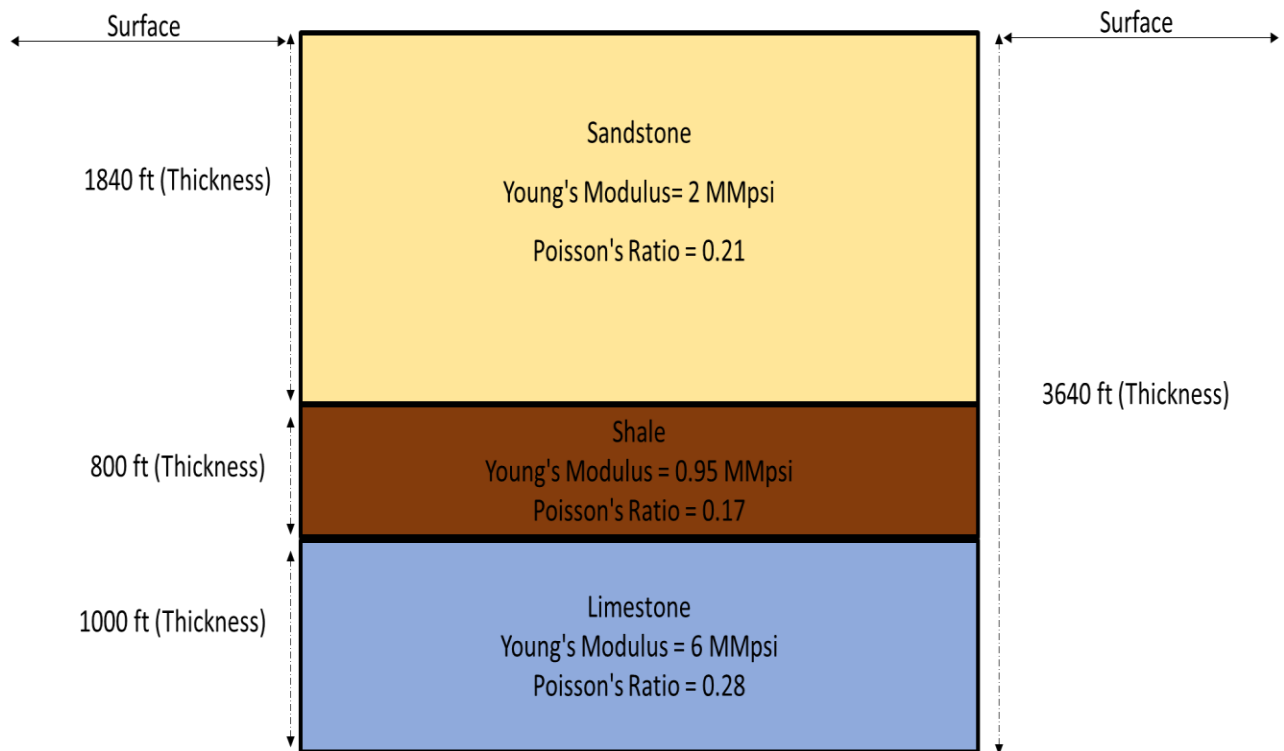


Figure 23: Model's Lithology

3.2.4 Stresses Distribution

Figure 24 shows a 3D model of a geological formation with marked vertical and horizontal stresses. It is designed to mimic real-world conditions under which CO₂ is injected into a subsurface environment.

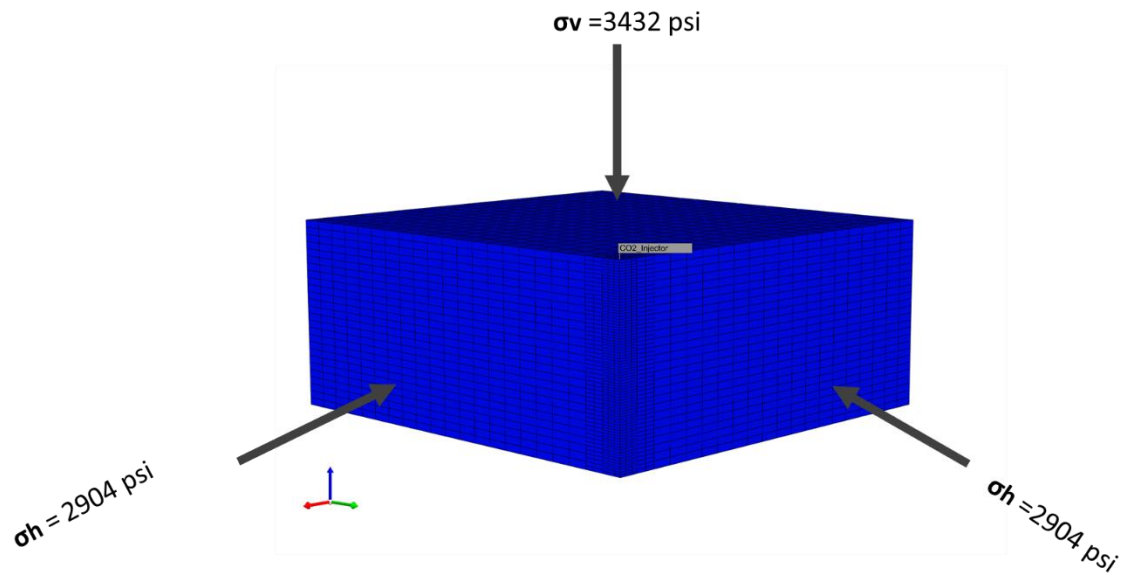


Figure 24: Stresses distribution

3.2.3 Aquifer salinity

The salinity of the saline aquifer formation is a crucial factor in determining the physicochemical properties of the resident brine and its interactions with the injected CO₂. In this model, the composition of the dissolved salts in the aquifer has been carefully characterized and incorporated, based on the study by Al-Dhafeeri et al. (2024) [55], as shown in **Table 2**.

Table 2: Brine composition [55]

Ions	Formation Water (ppm)
Na ⁺	59,491
Ca ²⁺	19,040
Mg ²⁺	2,439
SO ₄ ²⁻	350
Cl ⁻	132,060
HCO ₃ ⁻	354
Total Dissolved Salt (TDS)	213,734

3.3 Modeling Scenarios

To comprehensively evaluate the performance and potential risks associated with CO₂ sequestration in the saline aquifer formation, a series of modeling scenarios were designed, as illustrated in **Table 3, 4** and **5**. These scenarios explore the impact of various operational and formation parameters on the CO₂ plume migration, pressure buildup, and long-term storage performance. The scenarios are categorized based on different injection temperatures, injection rates and durations, and aquifer water salinity levels. The details of these scenarios are summarized in the following tables:

Table 3: CO₂ Injection Temperature

Scenario	Description
A	Gas injection at 90°C
B	Gas injection at 100°C
C	Gas injection at 110°C
D	Isothermal injection

Table 4: CO₂ Injection Rates and Duration

Scenario	Description
A	Injection rate designed for a 30-year injection period
B	Injection rate designed for a 40-year injection period
C	Injection rate designed for a 50-year injection period
D	Injection rate designed for a 60-year injection period

Table 5 : Aquifer Water Salinity

Scenario	Description
A	Salinity of 200,000 ppm
B	Salinity of 150,000 ppm
C	Salinity of 100,000 ppm
D	Salinity of 50,000 ppm

The modeling scenarios for CO₂ sequestration focus on examining the effects of varying injection temperatures, rates, durations, and aquifer water salinity levels to assess the performance and risks associated with CO₂ storage in saline aquifers. These scenarios help understand how different operational parameters like injection temperature influence the thermophysical properties of CO₂ and its interaction with the brine, as well as the potential thermal effects on the aquifer formation.. This comprehensive analysis is crucial for optimizing CO₂ injection strategies, ensuring the security of the stored CO₂, and developing effective monitoring and mitigation plans to support long-term sustainable storage in saline aquifers.

CHAPTER 4

RESULTS AND DISCUSSION

4.1 Description of the CO₂ Plume

The "Description of the CO₂ Plume" offers a comprehensive examination of the CO₂ plume's dynamics and behavior throughout and following the injection process in a saline aquifer. It delves into the alterations in gas saturation under different circumstances and emphasizes the physical mechanisms that impact the spread and durability of the plume.

4.1.1 Gas Saturation

During the ongoing injection of CO₂, as shown in **Figure 25**, the plume initially spreads laterally, covering an area between 150-350 feet near the wellbore. The reason for this specific distribution is the rapid increase in pressure and the varying density between the CO₂ injected and the surrounding aquifer brine. Over time, the CO₂ moves upward due to buoyancy forces and collects beneath the cap rock. The CO₂ gets trapped there because it is less dense than the brine.

However, once the injection stops, an imbibition cycle begins. During this phase, the aquifer brine starts to invade the regions previously occupied by CO₂, as seen in **Figure 26**. This process forces the CO₂ into residual saturation, resulting in a more extensive lateral spread of the CO₂ beneath the cap rock. The invading brine displaces the CO₂, causing it to redistribute and occupy smaller pore spaces in the formation, enhancing the overall trapping efficiency and stability of the CO₂ plume beneath the cap rock.

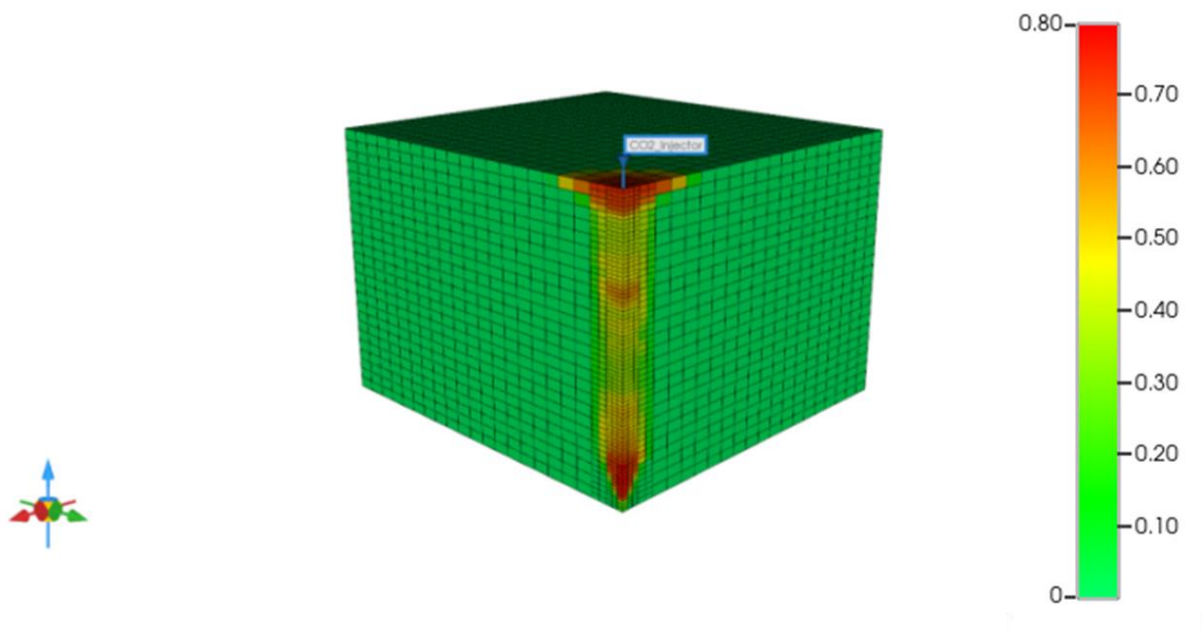


Figure 25: Gas saturation during injection

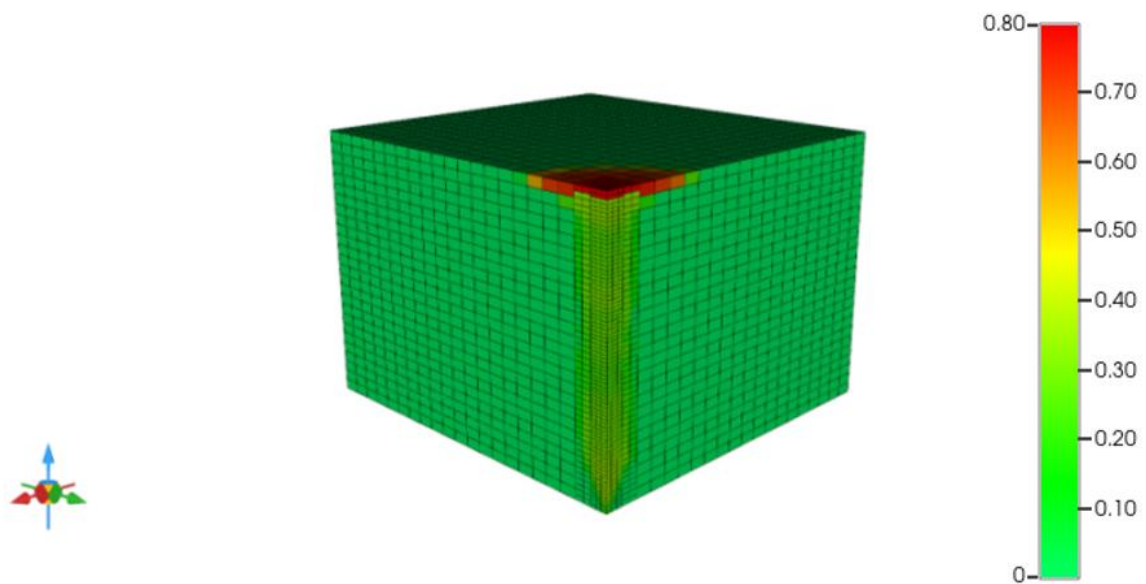


Figure 26: Gas saturation after injection

4.1.2 Dissolution and Precipitation of Calcite

The dissolution and precipitation of calcite significantly influence the geomechanical properties of the aquifer during CO₂ injection. Near the injection well, the acidic nature of CO₂ dissolved in brine promotes the dissolution of calcite, which increases porosity and enhances CO₂ migration and storage capacity. This is evidenced by the increased porosity observed close to the wellbore, as shown in **Figure 27**.

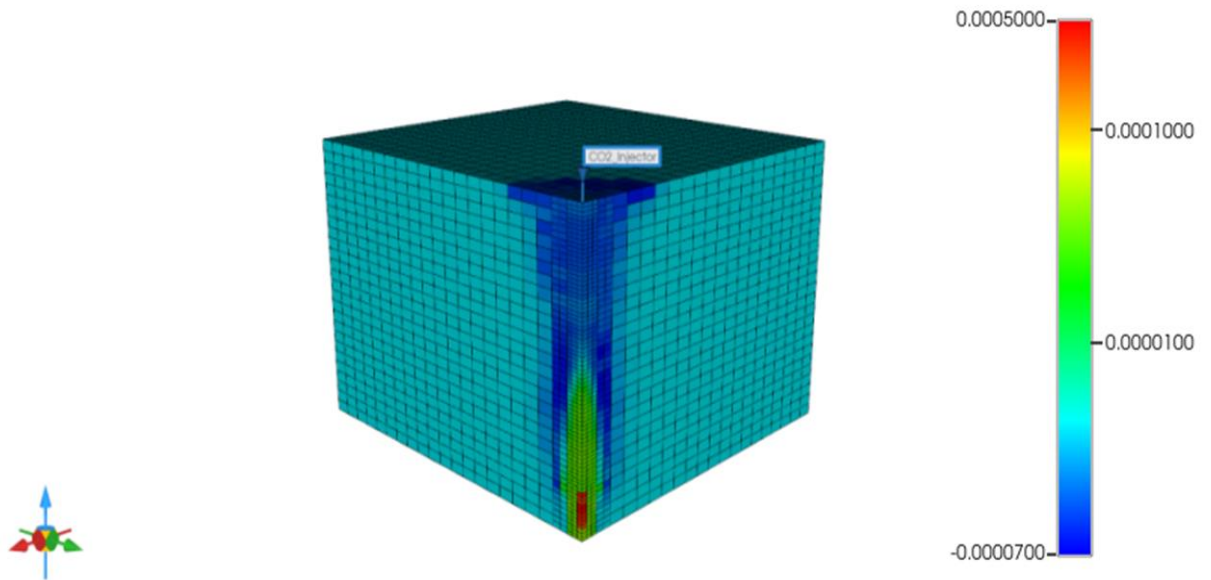


Figure 27: Changes in porosity resulting from the dissolution or precipitation of calcite

As the CO₂ plume moves farther from the injection site, calcite precipitation occurs due to shifts in pH, pressure, and temperature. This results in a reduction of porosity in areas distant from the wellbore, as depicted in **Figure 28**.

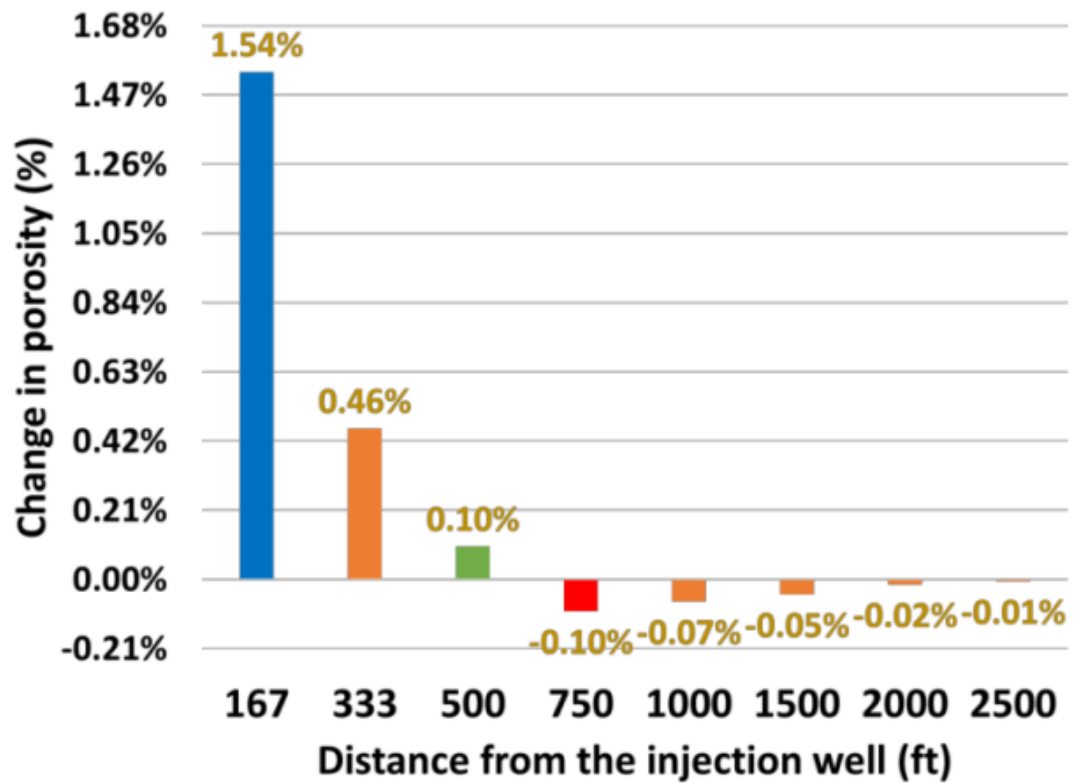


Figure 28: Porosity changes as a function of distance from the injection well

The pH distribution across the formation, illustrated in **Figure 29**, shows a more acidic environment near the wellbore, which facilitates calcite dissolution. Farther from the wellbore, where the pH is less acidic, calcite precipitation dominates, leading to decreased porosity. These processes collectively demonstrate the dynamic geochemical interactions that affect CO₂ sequestration, highlighting the importance of understanding spatial variations in pH and their impact on calcite solubility and the overall stability of the CO₂ plume.

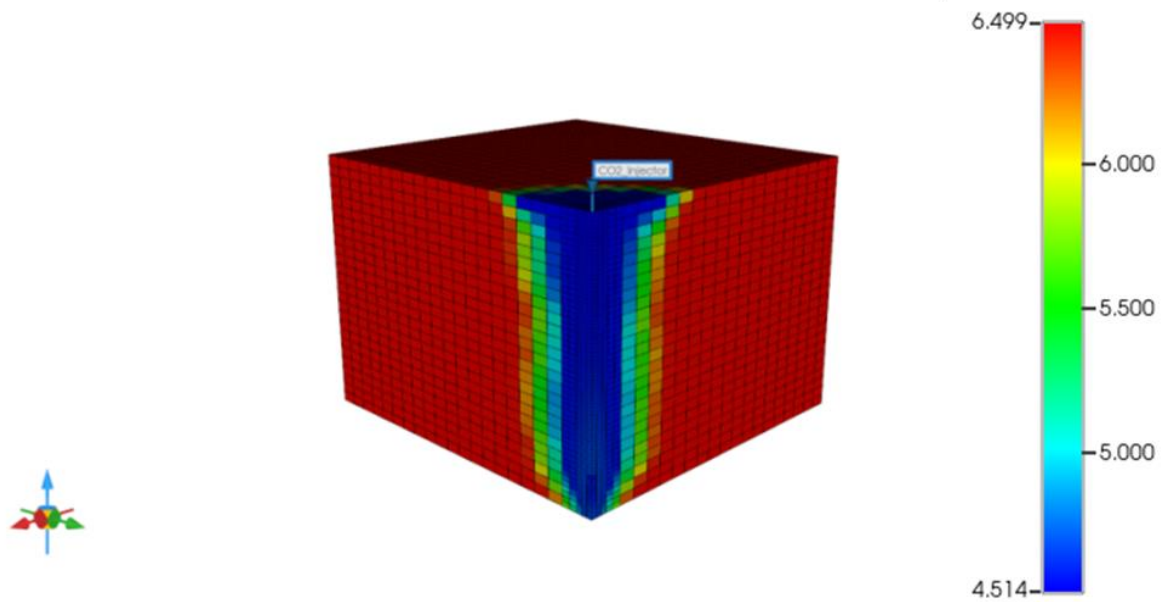


Figure 29: pH distribution

4.2 Trapping mechanisms of CO₂

The evaluation of CO₂ sequestration effectiveness involves a detailed long-term monitoring strategy extending over a 1000 years post-injection. This analysis is vital in understanding the distribution and stabilization of CO₂ within the geological formation. Initially, CO₂ is primarily trapped structurally beneath the caprock in its supercritical phase, distinct from the surrounding brine. As time progresses, this supercritical CO₂ begins to dissolve into the brine, enhancing the solubility trapping mechanism, which increasingly dominates as the monitoring extends.

Immediately after the cessation of CO₂ injection, a notable and rapid increase in residual CO₂ trapping occurs. This surge, as depicted in **Figure 30**, corresponds to the imbibition cycle where brine reoccupies the pore spaces, significantly reducing CO₂ saturation to a residual level influenced by the capillary pressure-saturation hysteresis. This swift increase in residual trapping is crucial for securing long-term immobilization of CO₂ within the formation. Additionally, the dissolved CO₂ continues to increase slowly over time, demonstrating the ongoing solubility trapping process that progressively incorporates CO₂ into the aquifer system.

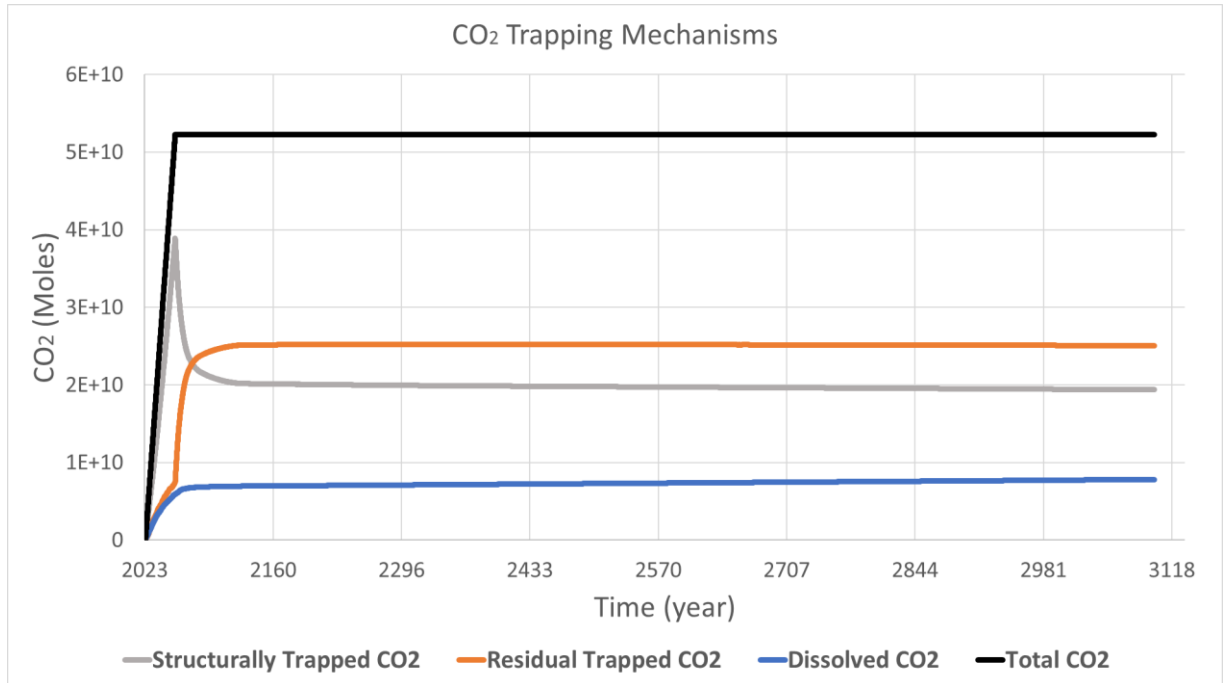


Figure 30: CO₂ trapping mechanism contribution

Throughout the thousand-year timeline, solubility trapping also intensifies, with CO₂ dissolving into the brine to form a carbonic acid solution, which then dissociates into bicarbonate and carbonate ions. This transformation provides a robust barrier against CO₂ leakage, ensuring its stable integration into the aquifer system.

Figure 30 illustrates the various CO₂ trapping mechanisms over time, highlighting the transitions between structural, residual, and dissolved states of CO₂. The graph captures the cumulative effect of these trapping mechanisms, offering insights into their relative contributions to the overall security and efficiency of CO₂ sequestration. This data is essential for developing targeted monitoring and risk management strategies to ensure the integrity and effectiveness of CO₂ storage sites over extended periods.

4.3 Injection Rates and Duration Scenarios

In the examination of injection rate and duration scenarios for CO₂ sequestration, the constraints were set to maintain an injection pressure below 3000 psi to prevent leakage. The dynamics observed suggest that as the injection rate increases, the cumulative CO₂ injected into the formation rises accordingly. This relationship is clearly depicted in **Figures 31 and 32**, where higher injection rates correlate with a larger cumulative amount of CO₂ injected in shorter periods, due to the rapid build-up of pressure that necessitates these shorter durations.

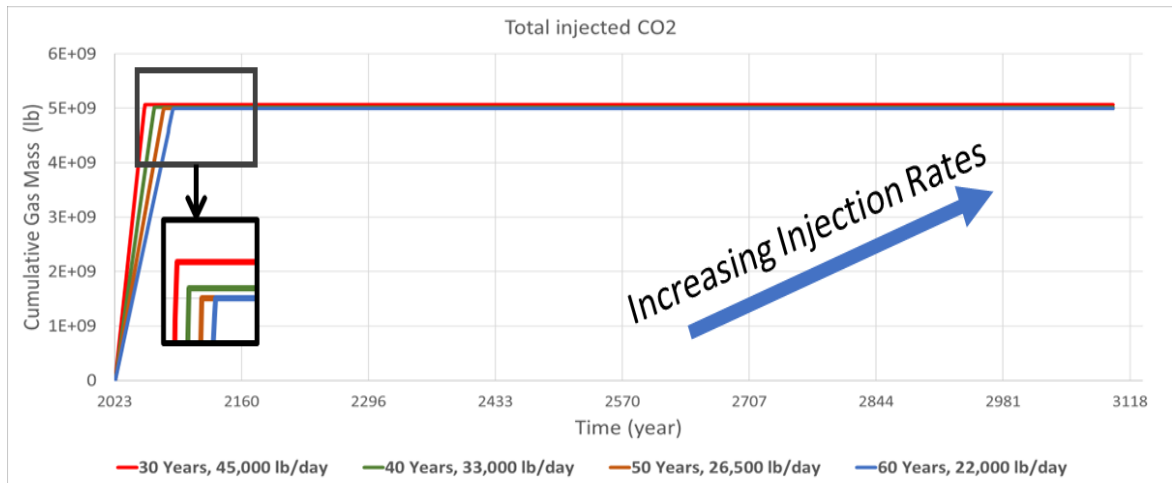


Figure 31: Cumulative CO₂ Injection over Time (Injection Period Scenarios)

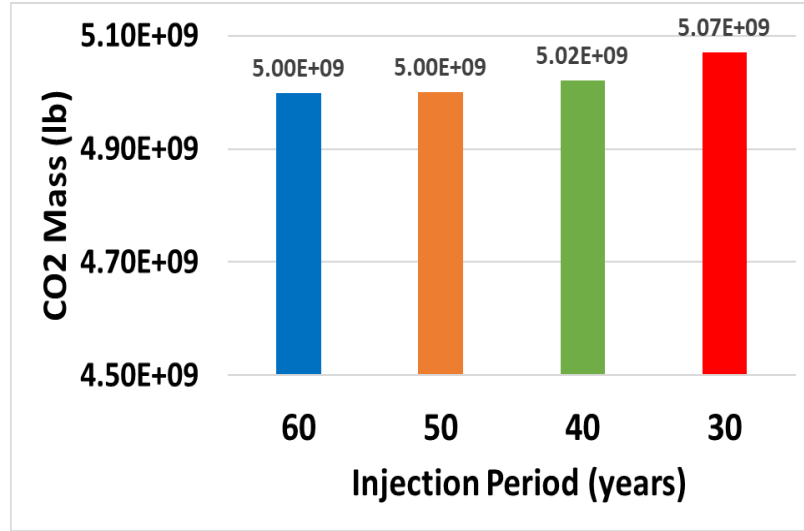


Figure 32: Cumulative CO₂ Injection (Injection Period Scenarios)

On the other hand, lower injection rates enable prolonged injection durations but yield a lesser total volume of CO₂ injected over the same timeframe. This is a critical trade-off, as depicted in **Figure 33**, which shows that lower injection pressures result in reduced CO₂ solubility in water. The intricate balance between injection rate, period, and the total volume of CO₂ injected underscores the need to finely tune operational parameters to optimize storage capacity while ensuring the safety and sustainability of the sequestration project.

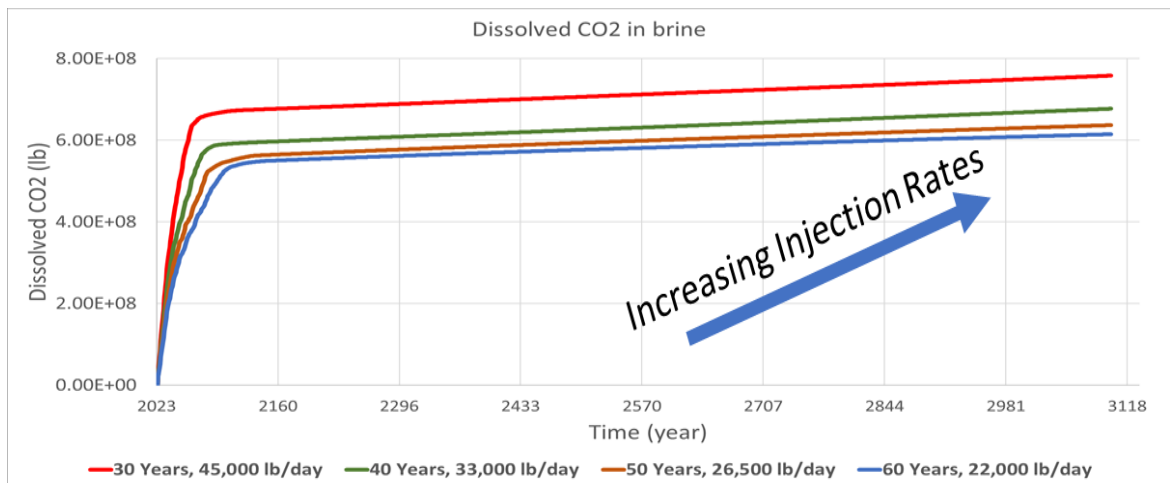


Figure 33: CO₂ Solubility in Water (Injection Period Scenarios)

4.4 Salinity scenarios

The investigation of salinity's impact on CO₂ sequestration revealed distinct trends across varying salinity levels. Lower salinity environments demonstrated superior CO₂ storage capacity, as shown in **Figures 34** and **35**, where the cumulative CO₂ injection over time and across different salinity levels is depicted. This enhanced storativity can be attributed to the reduced ionic strength at lower salinity levels, which promotes CO₂ solubility in water.

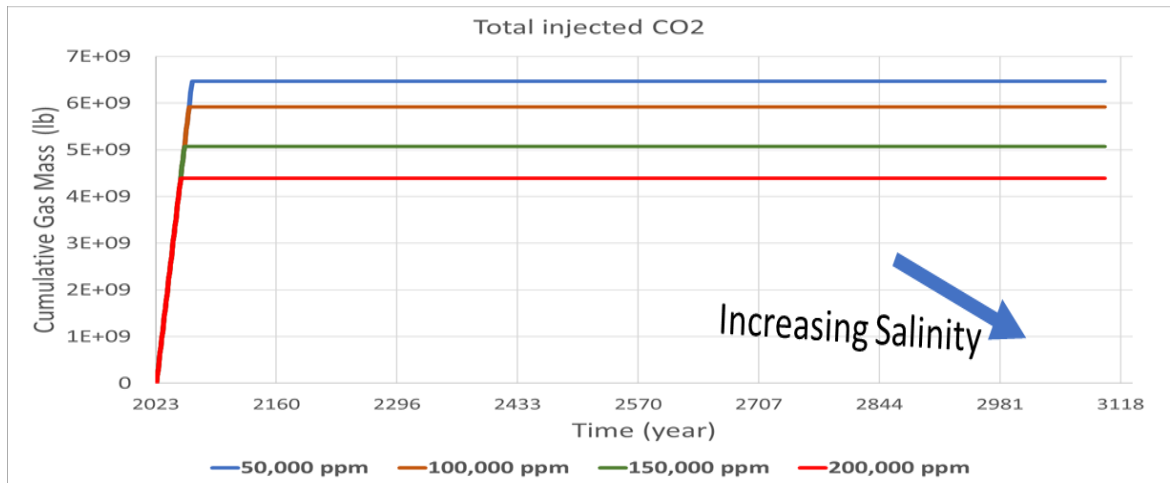


Figure 34: Cumulative CO₂ Injection over Time (Salinity Change Scenarios)

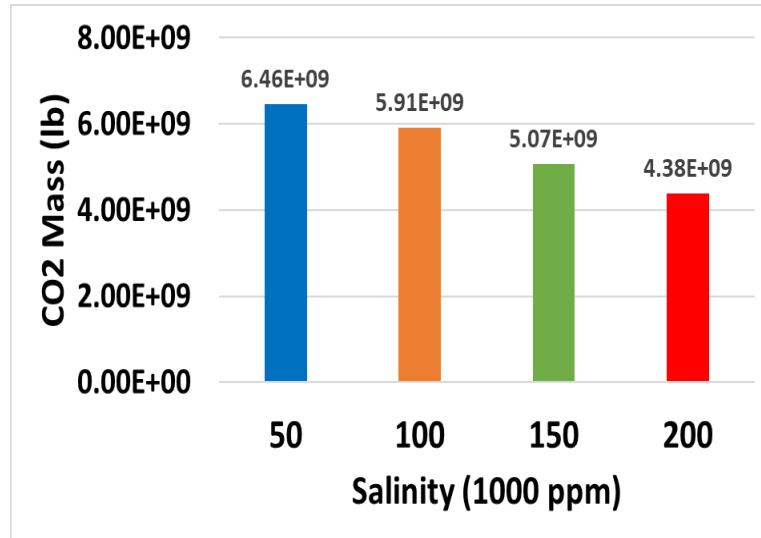


Figure 35: Cumulative CO₂ Injection (Salinity Change Scenarios)

Higher salinity conditions, on the other hand, impede this solubility due to increased ionic strength, leading to diminished CO₂ storage capacity, as observed in **Figure 36**. These insights highlight the critical role of salinity in optimizing CO₂ sequestration strategies, emphasizing the need to tailor operational parameters to the specific salinity characteristics of the target storage formation.

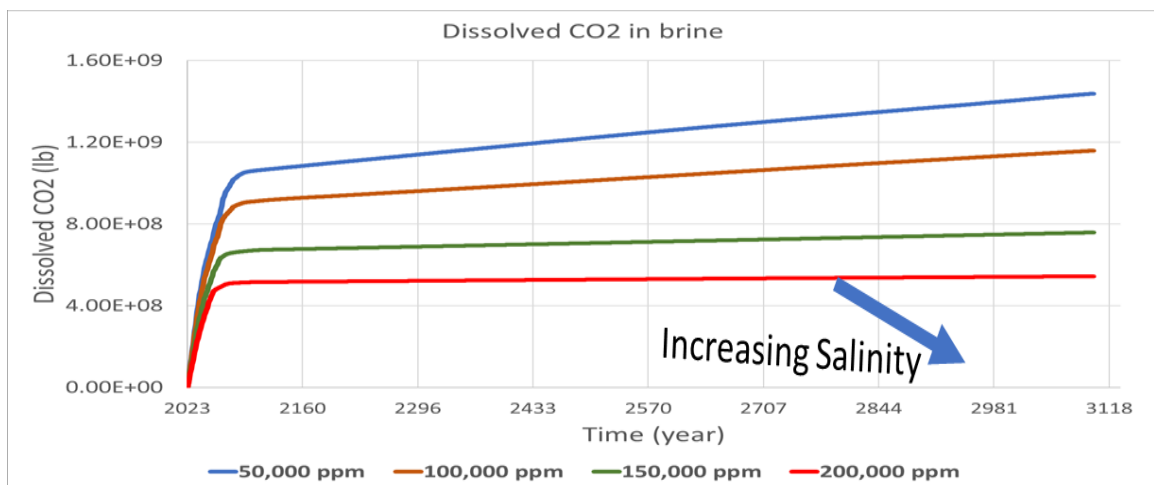


Figure 36: CO₂ Solubility in Water (Salinity Change Scenarios)

4.5 Temperature Scenarios

The impacts of varying injection temperatures on CO₂ sequestration were analyzed, maintaining all temperatures above 88°F to ensure CO₂ remained in a supercritical state. Lower injection temperatures were found to enhance CO₂ storage, as seen in **Figure 37** and **38**, due to the increased solubility of CO₂ in water, which improves its sequestration potential.

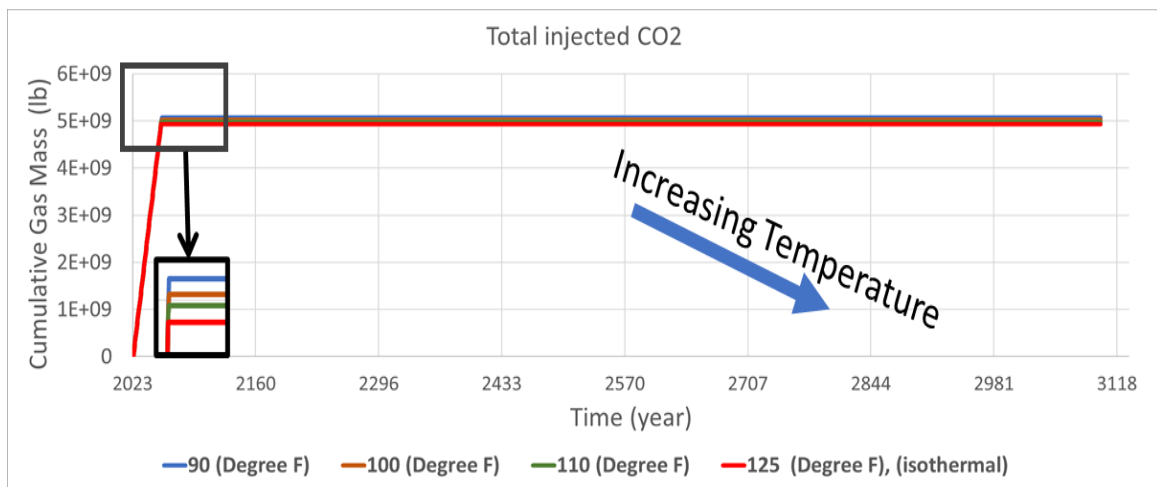


Figure 37: Cumulative CO₂ Injection over Time (Temperature Change Scenarios)

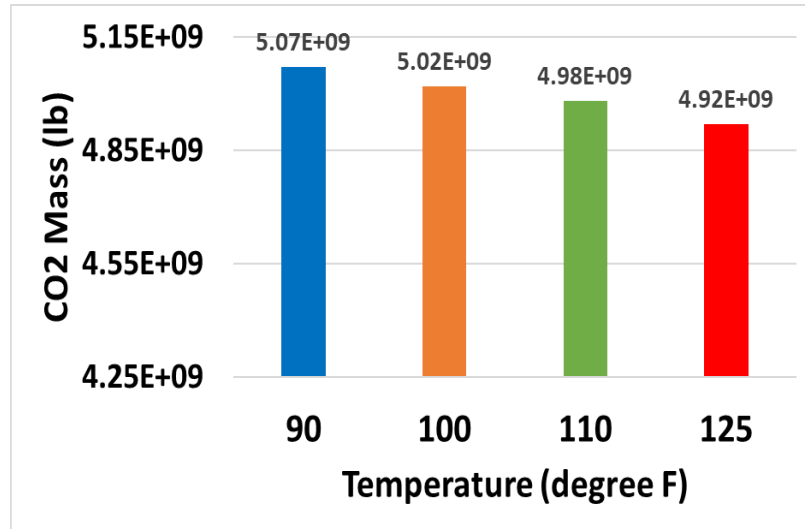


Figure 38: Cumulative CO₂ Injection (Temperature Change Scenarios)

As illustrated in **Figure 39**, the higher solubility at lower temperatures allowed for prolonged injection periods before reaching the designated pressure limits. These findings underscore the critical role of injection temperature in maximizing CO₂ solubility and optimizing storage efficiency in carbon sequestration projects.

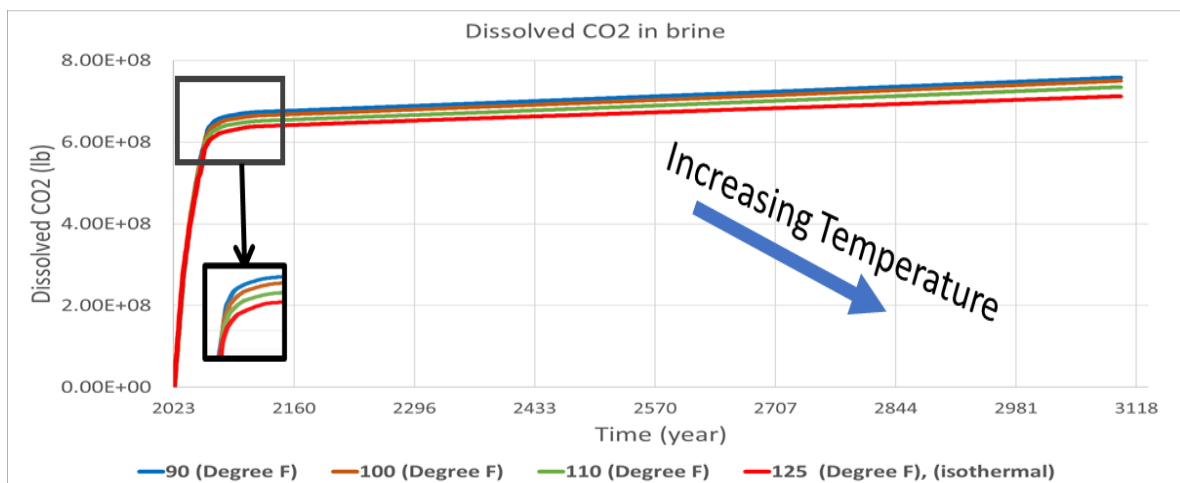


Figure 39: CO₂ Solubility in Water (Temperature Change Scenarios)

4.6 Geomechanical Changes

The study's analysis of geomechanical changes provides essential insights into the effects of CO₂ sequestration on the formation's mechanical properties. Mechanical properties were recalculated based on porosity variations as detailed in **equations 8 and 9**. Although **Figure 28** highlighted porosity changes near the wellbore, with variations ranging between 0.6% and 2%, these alterations had only a minimal impact on the formation's overall mechanical properties. This observation emphasizes the limited influence of localized porosity changes on the broader geomechanical stability of the system. Furthermore, the consistent application of a uniform shut-in pressure of 3000 psi across all scenarios facilitated uniform changes in effective stress, resulting in similar geomechanical responses regardless of the scenario. The consistent vertical displacements observed, ranging from 0.17 to 0.18 feet across all scenarios, are indicative of the formation's response to injected CO₂ and related pressure changes. These minor and uniform displacements reassure us that there are no concerns regarding vertical displacement at the surface facility.

This uniformity in geomechanical behavior is pivotal in validating the effectiveness of CO₂ sequestration strategies, particularly in terms of minimizing potential adverse effects like surface deformation or formation destabilization. The findings confirm the geomechanical integrity of the formation under prolonged CO₂ injection pressures, providing a solid foundation for predicting long-term storage capabilities and ensuring environmental safety in large-scale sequestration endeavors.

CHAPTER 5

CONCLUSIONS AND RECOMMENDATIONS

5.1 Conclusions

This research explored the impact of temperature, salinity, and injection rates on CO₂ solubility in brine, within the framework of CCS technologies. The study conclusively found that these factors markedly affect CO₂ solubility, which in turn has significant ramifications for both the efficiency and safety of CCS operations.

Temperature was found to have an inverse relationship with CO₂ solubility in brine. Lower injection temperatures enhanced CO₂ storage capacity due to increased solubility of CO₂ in water. This relationship allowed for prolonged injection periods before reaching designated pressure limits, optimizing storage efficiency in carbon sequestration projects [56].

Salinity showed a negative correlation with CO₂ solubility. Lower salinity environments demonstrated superior CO₂ storage capacity, attributed to reduced ionic strength promoting CO₂ solubility in water. Higher salinity conditions impeded this solubility due to increased ionic strength, leading to diminished CO₂ storage capacity [57].

Injection rates demonstrated a complex relationship with CO₂ solubility and storage capacity. Higher injection rates correlated with larger cumulative amounts of CO₂ injected in shorter periods, due to rapid pressure build-up. Conversely, lower injection rates enabled

prolonged injection durations but yielded lesser total volumes of CO₂ injected over the same timeframe [56].

Refer to **Table 6** below to understand how varying injection periods, temperatures, and salinity levels impact CO₂ storativity and vertical displacement in geological formations during capture and CCS operations.

Table 6: Comparative Effects of Temperature, Salinity, and Injection Periods on CO₂ Storativity

Parameter	Injection Periods (Years)	Temperature (°F)	Salinity (ppm)
Range	30, 40, 50, 60	90, 100, 110, 125	50,000, 100,000, 150,000, 200,000
Total Injected CO ₂ (mT)	Increasing with lower periods	Increasing with lower temperatures	Increasing with lower salinity
Storativity Change (%)	+1.4, +1.38, +0.98, 0	+3.05, +2.02, +1.12, 0	+47.5, +34.9, +15.8, 0

The behavior of the CO₂ plume and its trapping mechanisms involve several key stages. Initially, there is a lateral spread of the CO₂ plume near the wellbore, followed by its upward migration and accumulation beneath the cap rock due to buoyancy forces. After the injection phase, the imbibition cycle leads to a more extensive lateral spread of CO₂ beneath the cap rock, enhancing the trapping efficiency. Over the long term, monitoring reveals a transition from initial structural trapping to increased residual and solubility trapping, which significantly enhances the security of CO₂ storage.

Our analysis of geomechanical changes revealed minimal impact on the formation's overall mechanical properties. Porosity variations near the wellbore ranged between 0.6% and 2%, but these localized changes had limited influence on the broader geomechanical stability of the system. Vertical displacements were consistently small, ranging from 0.17 to 0.18

feet across all scenarios, indicating the robustness of the geological structure under the examined conditions.

The uniform application of a 3000 psi shut-in pressure across all scenarios resulted in similar geomechanical responses regardless of the specific injection parameters. This uniformity in geomechanical behavior validates the effectiveness of our CO₂ sequestration strategies in terms of minimizing potential adverse effects like surface deformation or formation destabilization.

These results underscore the importance of carefully considering and optimizing temperature, salinity, and injection rate parameters in CCS projects. The complex interplay between these factors highlights the need for site-specific optimization to maximize storage capacity while ensuring the safety and sustainability of sequestration efforts. Notably, the amount of CO₂ stored can vary significantly depending on these parameters, with values ranging from 15 to 26 kilograms of CO₂ per cubic meter based on the used model. These findings underscore the necessity of optimizing CCS parameters to enhance storage capabilities and ensure operational safety. The model used aligns with the data from the Sleipner project, as detailed in **Table 7** below, which highlights varied storage capacities across different formation types and projects.

Table 7: CO₂ Storage Capacities in Different Geological Formations: Representative Projects [58], [59]

Formation Type	Example Project	Storage Range (kg CO ₂ /m ³)
Saline Aquifers	Sleipner, Norway	5 - 50 (Avg. 10 - 30)
Coal Beds	San Juan Basin, USA	1 - 40 (Avg. 5 - 15)
Depleted Oil and Gas Reservoirs	Weyburn, Canada	2 - 200 (Avg. 30 - 80)

5.2 Recommendations

Based on the findings and insights garnered from this study, the following recommendations are proposed to refine modeling approaches and enhance the understanding of geomechanical and geochemical behaviors in CO₂ sequestration:

5.2.1 Well Bore Stability:

Focus on studying the effects of CO₂ sequestration on well bore stability, emphasizing the analysis of stress dynamics around the wellbore. It is crucial to understand how CO₂ injection affects mechanical stress fields, which could potentially induce structural deformations and compromise well integrity. A detailed examination of stress distribution around the wellbore, as illustrated in **Figure 40**, is essential. This will aid in identifying potential risks such as fracturing or leakage, critical to ensuring the safety and effectiveness of CO₂ sequestration efforts.

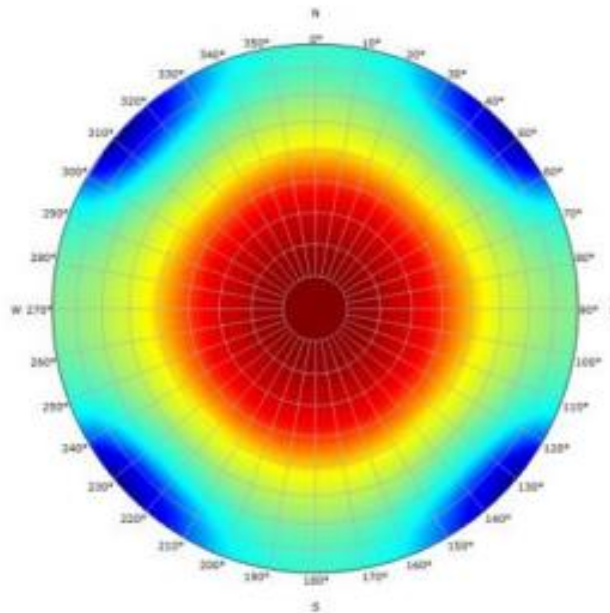


Figure 40: Stress distribution around borehole [60]

5.2.2 Advanced Wormhole Prediction:

Improve simulation tools to accurately predict the formation, dimensions, and properties of wormholes. The complex and varied nature of wormholes, as shown in **Figure 41**, has significant implications on the mechanical properties and structural integrity of the rock formation [61]. A comprehensive understanding of wormhole geometries is vital for predicting changes in porosity and permeability, essential for effective reservoir management and operation. Accurate modeling of these intricate structures allows engineers to better anticipate fluid flow patterns, optimize injection strategies, and address potential risks associated with uneven fluid distributions or unexpected pressure variations within the reservoir.

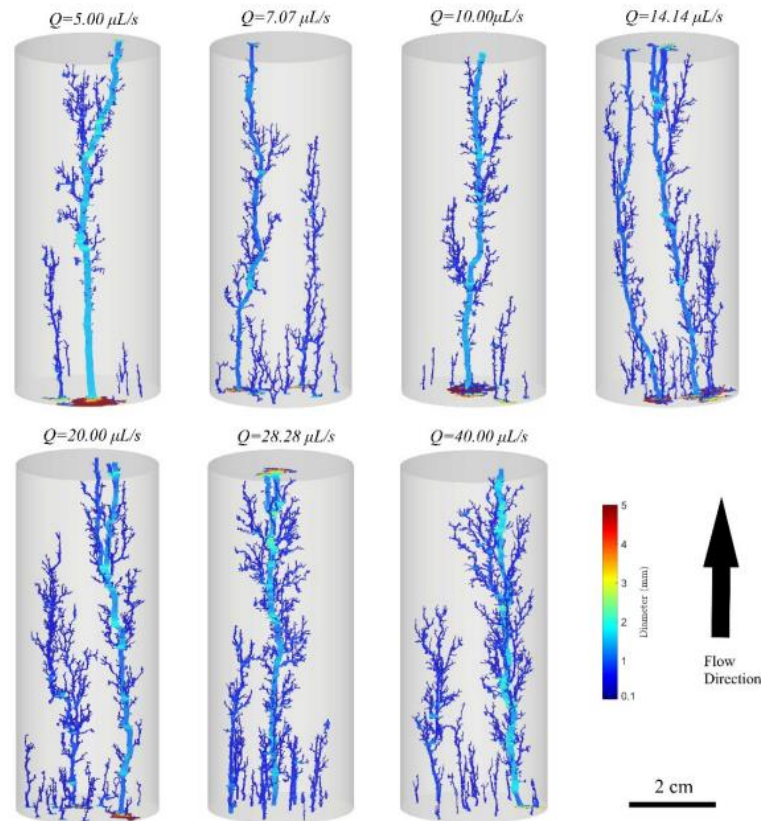


Figure 41: Complex wormhole geometries [61]

5.2.3 Modeling Complex Conditions:

It is important to expand model scope to include mixed lithology aquifers, high temperature and high-pressure conditions, as well as variations in CO₂ purity. This will improve predictive capabilities of numerical models for better assessments of CO₂ sequestration projects in saline aquifers. Further research on generating wormholes and using lithology-specific geomechanical models will help optimize injection strategies, reduce risks, and ensure long-term security and effectiveness of CO₂ storage.

By addressing these areas, future research can significantly advance the field of CO₂ sequestration, improving the reliability and efficiency of sequestration projects.

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VITAE

Name : Haidar Ahmed Almajed

Nationality : Saudi

Date of Birth : 3/23/1995

Email : Haidar.Majed@kfupm.edu.sa

Address : 31982, Al Hasa, Eastern province, Saudi Arabia

Academic Background : BSc. in Petroleum Engineering 2019 (King Fahd
University of Petroleum & Minerals - KFUPM)

Publications:

- 1- Algarni, S., Aljawad, M. S., **Al-Maijd, H.**, Alajmei, S., Abdulraheem, A., & Al-Shehri, D. (2023). Stability of carbonate rocks containing acid wormholes under high confining pressures. Rock Mechanics and Rock Engineering. <https://doi.org/10.1007/s00603-023-03568-w>.
- 2- Aidagulov, Gallyam , Gwaba, Devon , Kayumov, Rifat , Sultan, Abdullah , Aly, Moustafa , Qiu, Xiangdong , **Almajed, Haidar** , and Mustapha Abbad. "Effects of Pre-Existing Fractures on Carbonate Matrix Stimulation Studied by Large-Scale Radial Acidizing Experiments." Paper presented at the SPE Middle East Oil and Gas Show and Conference, Manama, Bahrain, March 2019. doi: <https://doi.org/10.2118/195153-MS>.