

**DEPOSITIONAL CONTROLS ON CO₂ STORAGE IN
CARBONATE RESERVOIRS:
FROM SUBSURFACE TO SIMULATION**

BY
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DHAHRAN, SAUDI ARABIA

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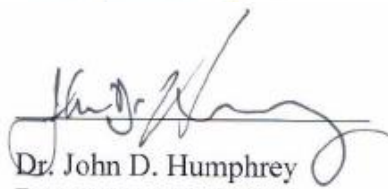
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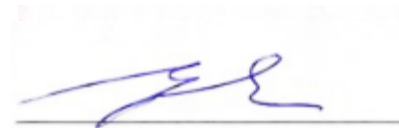


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For my dearest wife, whose unwavering love and support have been my guiding light through every journey and challenge, I dedicate this with boundless gratitude and affection.

To my precious children, you are the heartbeats of my life and the source of endless joy. May this dedication serve as a testament to the boundless love and pride I hold for each of you.

And to my beloved parents, whose sacrifices and wisdom have shaped me into the person I am today, I offer this dedication with deepest reverence and gratitude for your unwavering love and guidance.

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LIST OF ABBREVIATIONS

UKM	:	Upper Kharaib Member
FA	:	Facies Association
RT	:	Rock Type
ScCO₂	:	Supercritical CO₂

ABSTRACT

Full Name : Sani Yusmananto

Thesis Title : Depositional Controls on CO₂ Storage in Carbonate Reservoirs: From Subsurface to Simulation

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The significant release of CO₂ gases into the atmosphere, associated with Anthropocene activities, has been attributed to the rapid increase in global today's temperature. Significant efforts have been attempted to capture CO₂ and use depleted reservoirs as permanent subsurface storage for CO₂. In the Middle East, while the stacked Mesozoic carbonate reservoirs may act as an ideal target to safely store CO₂, our understanding on how depositional facies controls CO₂ trapping mechanisms in heterogenous carbonate reservoirs remains limited. This study utilizes subsurface open data from the COSTA Model (2022) to characterize the carbonate reservoir model of the Lower Cretaceous Upper Kharaib Member (UKM).

The main objectives include investigating the impact of depositional heterogeneity on identifying CO₂ storage sites and trapping mechanisms in heterogeneous carbonate reservoirs, proposing preliminary geological criteria for carbon storage based on facies distribution, and modelling the effects of CO₂ injection at a field scale on subsurface dynamics within the Upper Kharaib Carbonate Reservoirs, particularly in a deep saline aquifer context.

The results reveal four distinct facies associations (FA1-FA4) in the Upper Kharaib Member (UKM). Facies associations FA1 and FA2 (Shoal and Inner Ramp), predominantly found in the upper part of the reservoir, exhibit excellent reservoir properties, suggesting their significant potential for CO₂ structural trapping. These facies have an average thickness of 60 ft, with porosity and permeability ranging from 20-35% and 50-1000 mD, respectively. The Middle Ramp Facies (FA3), mainly present in the middle to lower part of the reservoir, covers about 60% of the UKM's total thickness. It has moderate to low reservoir quality, offering potential for residual/capillary trapping mechanisms, with an average net thickness of 100 ft and porosity-permeability ranging from 10-25% and 5-50 mD, respectively. The Outer Ramp Facies (FA4) has the thinnest average thickness of 10 ft and the poorest reservoir quality, with porosity less than 5% and permeability below 1 mD.

Additionally, reservoir simulation results indicate increased calcite dissolution, a lower reservoir pH profile, and higher reservoir pressure due to CO₂ injection. The facies-based modeling approach highlights the vertical stacking pattern variation and heterogeneity of potential trapping mechanisms. Residual trapping is generally more significant in the Middle Ramp Facies, while structural trapping is more prevalent in the Upper Ramp and Shoal Facies. These insights can inform a more effective design for CO₂ storage across the carbonate platform.

This research significantly advances our quantitative understanding of CO₂ storage in carbonate reservoirs, specifically in the Upper Kharaib Carbonate Reservoirs. The insights gained can inform effective reservoir management strategies, optimizing CO₂ storage

while minimizing subsurface and environmental risks. By uncovering the relationship between CO₂ injection, subsurface dynamics, and facies-based trapping mechanisms, this study provides a foundation for responsible decision-making and CO₂ storage operations in the Middle East and beyond. It underscores the significance of considering carbonate reservoir quality and heterogeneity in designing CO₂ injection projects, contributing to sustainable carbon management and enabling more efficient climate change mitigation initiatives especially in the Middle East region.

ملخص الرسالة

الاسم الكامل: ساني يوسمانانتو

عنوان الرسالة: ضوابط الترسيب على تخزين ثاني أكسيد الكربون في خزانات الكربونات: من تحت السطح إلى المحاكاة

التخصص: جيولوجيا

تاريخ الدرجة العلمية: مايو 2024

الإطلاق الكبير لغازات ثاني أكسيد الكربون في الغلاف الجوي، المرتبط بأنشطة الحقبة الأنثروبوسينية، يُعزى إلى الزيادة السريعة في درجة حرارة الأرض اليوم. وقد بُذلت جهود كبيرة لاحتجاز ثاني أكسيد الكربون واستخدام المكامن المستنفدة كأماكن تخزين دائمة تحت سطح الأرض لثاني أكسيد الكربون. في الشرق الأوسط، على الرغم من أن المكامن الكربونية المتكدسة من العصر الطباشيري الأوسط قد تكون هدفًا مثاليًا لتخزين ثاني أكسيد الكربون بأمان، فإن فهمنا لكيفية تحكم الطبقات الرسوبية في آليات احتجاز ثاني أكسيد الكربون في المكامن الكربونية غير المتجانسة لتوصيف نموذج المكامن (COSTA (2022 لا يزال محدودًا. تستخدم هذه الدراسة بيانات مفتوحة من النموذج من العصر الطباشيري السفلي (UKM) الكربونية لعضو خريب العلوي.

تشمل الأهداف الرئيسية دراسة تأثير التباين الترسيبي على تحديد مواقع تخزين ثاني أكسيد الكربون وآليات الاحتجاز في المكامن الكربونية غير المتجانسة، واقتراح معايير جيولوجية أولية لتخزين الكربون بناءً على توزيع الطبقات الرسوبية، ونمذجة تأثيرات حقن ثاني أكسيد الكربون على نطاق الحقل على الديناميكيات تحت السطحية داخل المكامن الكربونية لعضو خريب العلوي، وخاصة في سياق المياه الجوفية المالحة العميقة.

في عضو خريب العلوي (FA1-FA4) تكشف النتائج عن وجود أربع مجموعات مميزة من الطبقات الرسوبية (الضفة والمنحدر الداخلي)، التي تتواجد بشكل رئيسي في FA2 و FA1 تظهر المجموعات الرسوبية (UKM). الجزء العلوي من الخزان، خصائص ممتازة، مما يشير إلى إمكانياتها الكبيرة في احتجاز ثاني أكسيد الكربون الهيكلي. تتمتع هذه الطبقات بسمك متوسط يبلغ 60 قدمًا، وتتراوح المسامية والنفاذية بين 20-35% و 50-1000 ملي

، التي تتواجد بشكل رئيسي في الجزء الأوسط (FA3) دارسي، على التوالي. أما الطبقات الرسوبية للمنحدر الأوسط إلى السفلي من الخزان، فتغطي حوالي 60% من السمك الكلي لعضو خريب العلوي. تمتاز بجودة خزان معتدلة إلى منخفضة، مع إمكانية لآليات الاحتجاز المتبقي/الشعري، بسمك صافي متوسط يبلغ 100 قدم وتتراوح المسامية فهي (FA4) والنفاذية بين 10-25% و 5-50 ملي دارسي، على التوالي. أما الطبقات الرسوبية للمنحدر الخارجي الأرق بمتوسط سمك يبلغ 10 أقدام، وتعرض أدنى جودة للخزان، حيث تقل المسامية عن 5% والنفاذية عن 1 ملي دارسي.

بالإضافة إلى ذلك، تُظهر نتائج محاكاة الخزان زيادة في انحلال الكالسيت، وانخفاض في ملف الأس الهيدروجيني للخزان، وزيادة في ضغط الخزان نتيجة حقن ثاني أكسيد الكربون. يكشف النهج القائم على النمذجة بالطبقات عن التباين في نمط التراص العمودي وتفاوت آليات الاحتجاز المحتملة. يكون الاحتجاز المتبقي عمومًا أعلى في طبقات المنحدر الأوسط بينما يكون الاحتجاز الهيكلي أكثر انتشارًا في طبقات المنحدر العلوي والضفة. يمكن أن تسهم هاتان الآليتان في تصميم أفضل لتخزين ثاني أكسيد الكربون عبر المنصة الكربونية.

تساهم هذه الدراسة بشكل كبير في فهمنا الكمي لتخزين ثاني أكسيد الكربون في المكامن الكربونية، وبشكل خاص في المكامن الكربونية لعضو خريب العلوي. يمكن أن تسهم النتائج المكتسبة في استراتيجيات إدارة الخزانات بشكل فعال، مما يحقق تحسینًا في تخزين ثاني أكسيد الكربون مع تقليل المخاطر تحت السطحية والبيئية. من خلال الكشف عن العلاقة بين حقن ثاني أكسيد الكربون والديناميكيات تحت السطحية وآليات الاحتجاز القائمة على الطبقات الرسوبية، توفر هذه الدراسة أساسًا لاتخاذ قرارات مسؤولة وعمليات تخزين ثاني أكسيد الكربون في الشرق الأوسط وما وراءه. تؤكد هذه الدراسة على أهمية النظر في جودة المكامن الكربونية وتباينها في تصميم مشاريع حقن ثاني أكسيد الكربون، مما يساهم في إدارة الكربون بشكل مستدام وتمكين مبادرات أكثر كفاءة للتخفيف من تغير المناخ خاصة في منطقة الشرق الأوسط.

CHAPTER 1

INTRODUCTION

1.1 Background

The rapid increase in global today's temperature is attributed to significant volume of greenhouse gases emission, particularly CO₂, into the atmosphere due to various Anthropocene activities (IPCC, 2021). One of the main contributors is hydrocarbon exploration and production activities. Hence, oil and gas industry should play a pivotal role in reducing global carbon emission. Several methods have been implemented, including injecting CO₂ back to subsurface either for storage in deep saline aquifer or enhance oil recovery purpose (Donda, F, 2011, Brydie et al. 2014, Lu et al., 2012, Saini 2017, Temitope 2016). Several geological reservoirs can serve as repositories for CO₂ storage, including depleted or nearly depleted oil and gas reservoirs, unmineable coal seams, salt caverns, and deep saline aquifers within sedimentary basins (Fig. 1.1). Among these options, deep saline aquifers hold particular significance due to their extensive geographical coverage and substantial global storage potential within sedimentary basins (Koide et al., 1992; IPCC, 2005). The Middle East contributes approximately 8% to global CO₂ capture capacity with three commercial CCS facilities: Uthmaniyah (0.8 MMtpa CO₂-EOR, Saudi Arabia), Al Reyadah (0.8 MMtpa CO₂-EOR, Abu Dhabi), and Ras Laffan (2.1 MMtpa CCS, Qatar) (Global CCS Institute, 2023 and S&P Global, 2022). In addition, The United Arab Emirates (UAE) and Saudi Arabia have made significant pledges by setting net-zero targets for 2050 and 2060, respectively. These ambitious objectives act as drivers for the rapid integration

of CCS technologies, offering a clear path toward transitioning to a low-carbon future (Global CCS Institute, 2023).

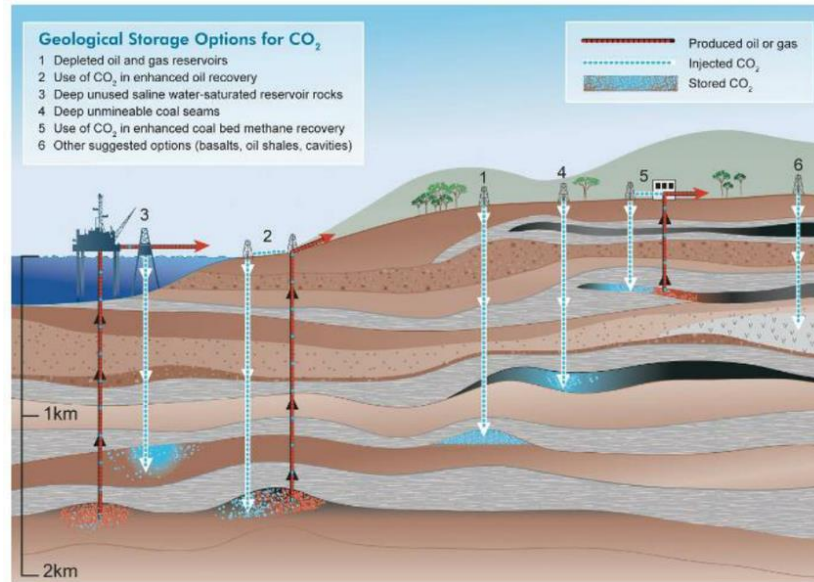


Figure 1. 1 Illustration of several geological storage options for CO₂. (IPCC, 2005)

Given the existing carbon capture infrastructure, industrial facilities, accessible natural CO₂ storage sites, and forthcoming initiatives in the GCC nations, the region has the potential to become a leading global center for CCS. Furthermore, CCUS holds considerable promise across various industrial sectors in the GCC countries and is poised to contribute significantly to the decarbonization efforts of hard-to-abate industries (Fig. 1.2). According to research conducted by Ye et al. in 2023, Saudi Arabia alone possesses a potential saline aquifer storage capacity of approximately 432 Gigatons.

The Middle East region presents a highly promising prospect for the secure sequestration of CO₂ in the subsurface due to the presence of stacked Mesozoic carbonates. These carbonates exhibit an ideal combination of reservoir properties, sealing capabilities, and trapping mechanisms, rendering them well-suited for safely storing CO₂ in the subsurface

(Vahrenkamp et al., 2021). Despite notable advancements in understanding alterations to rock properties at the near-wellbore and pore scale due to CO₂ injection in carbonate reservoir (Han et al., 2018; Seyyedi et al., 2020; Xu et al., 2017), a critical aspect necessitating attention is the seamless incorporation of these findings within a broader geological conceptual framework, supported by numerical simulations conducted at a field scale level. It is crucial to address the existing gap in integration to establish a cohesive approach to incorporating geological facies descriptions within the framework of carbon storage monitoring. Furthermore, it is essential to comprehend the effects of CO₂ injection at the field scale on subsurface dynamics and the profile of potential trapping mechanisms in the Upper Kharaib Carbonate Reservoirs, specifically within the context of a deep saline aquifer.

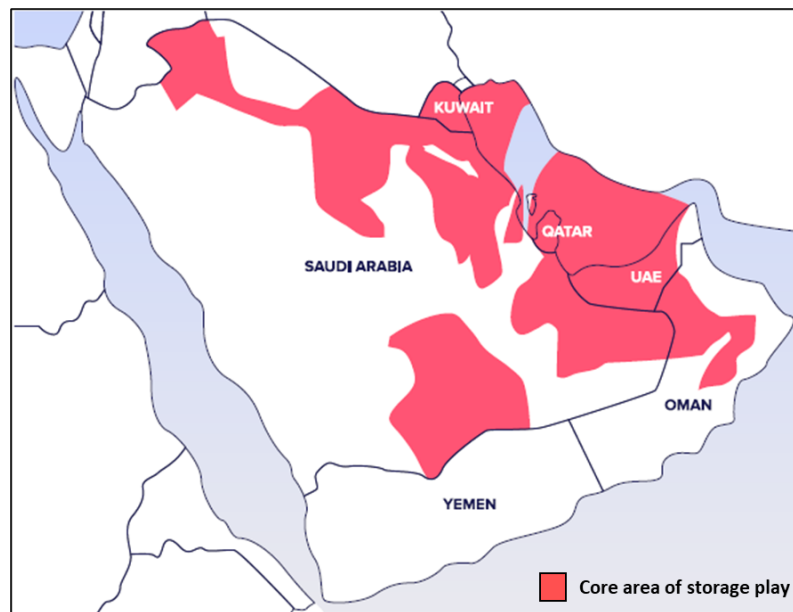


Figure 1. 2 Core area of storage play in the Middle East region. (Global CCS Institute, 2022)

Carbonate reservoirs are recognized for their higher chemical reactivity compared to clastic reservoirs. When CO₂ is injected into the water-bearing section of a depleted gas reservoir, reactions occur, leading to the formation of carbonic acid as CO₂ dissolves in water. This acid subsequently interacts with the carbonate rocks, potentially resulting in the precipitation or dissolution of minerals, which can either decrease or enhance the porosity and permeability of the rocks (Izgec et al, 2008, Luquot and Gouze, 2009, Smith et al, 2013, Masoudi et al, 2013, and Tutolo et al, 2014).

This study aims to contribute to the responsible and effective utilization of subsurface CCS modelling and evaluation for mitigating greenhouse gas emissions. By integrating geological and reservoir data, as well as facies-based modelling techniques, a comprehensive modelling and simulation framework characterizes CO₂ plume migration-trapping mechanism patterns based on depositional facies-reservoir quality and identifies key factors influencing subsurface conditions. The study sheds light on the intricate relationship between CO₂ injection and subsurface dynamics, providing valuable insights that can optimize CO₂ injection strategies and facilitate informed decision-making in CCS projects. CCS Modelling allows us to optimize injection strategies and predict the impact of CO₂ injection on subsurface dynamics and CO₂ plume profiles.

The integration of interdisciplinary approaches can aid in the development of accurate models for characterizing subsurface properties and uncertainties in predicting and monitoring carbon capture and storage projects. While numerous laboratory experiments have been conducted to observe CO₂ injection in both carbonate and siliciclastic reservoirs, limited efforts have been made to link these experiments within field scale combined with

reservoir or facies distribution. Consequently, the modelling of such experiments can facilitate improved prediction and injection placement for CCS projects.

1.2 Statement of problem

Storing carbon dioxide (CO₂) securely in carbonate rocks, despite its considerable potential, poses substantial challenges. The main challenges lie in the inherent depositional heterogeneity characteristic of carbonate reservoirs and post alteration diagenetic processes. These geological formations, composed primarily of carbonate minerals like calcite and dolomite, exhibit diverse structures and compositions due to varying depositional environments over time. This natural heterogeneity complicates the reliable containment of CO₂, as the behaviour of the gas within such reservoirs can vary significantly. Understanding and overcoming these challenges are crucial for developing effective and sustainable strategies for carbon capture and storage, ensuring that stored CO₂ remains securely trapped underground.

Numerous laboratory experiments have been conducted to investigate the injection of carbon dioxide (CO₂) at the wellbore scale, examining its impact on both carbonate and siliciclastic reservoirs. These experiments have provided valuable insights into the behaviour of CO₂ within smaller-scale geological formations. However, a significant gap in knowledge exists, as there have been limited efforts to integrate these laboratory findings into a larger field-scale context, particularly when considering the intricacies of reservoir or facies distribution and stacking patterns. This lack of comprehensive field-scale integration at least in the public literature, especially in the context of carbonate reservoirs,

hinders our ability to extrapolate and apply findings from controlled laboratory settings to real-world scenarios. Understanding the broader geological context at a field scale is essential for developing accurate and effective strategies for carbon capture and storage initiatives, ensuring their success on a larger scale.

In the Middle East, the difficulty in accessing subsurface data, attributed to confidentiality concerns, poses a challenge in obtaining comprehensive datasets. Any accessible subsurface data, even if partially synthetic, holds significant value, particularly for academic purposes. This study aims to address these challenges by developing methodologies to amalgamate such datasets, ultimately providing valuable insights, enabling better-informed decisions, and enhancing the efficiency of reservoir analysis in the region.

1.3 Objectives

This study aims to depict the depositional controls and subsurface dynamics of CO₂ injection in carbonate reservoir, specifically focusing on the Lower Cretaceous Upper Kharaib Member. The specifics of the objectives are outlined below:

- To perform adequate geological characterizations on carbonate reservoir model of the Lower Cretaceous Upper Kharaib Member from subsurface open data COSTA Model (2022).
- To gain insights on the impact of depositional heterogeneity in determining the potential CO₂ storage sites and potential trapping mechanisms in heterogeneous carbonate reservoirs

- To propose a set of preliminary geological criteria for carbon storage in carbonates based on its facies distribution
- To Model the impacts of CO₂ Injection (Field Scale) on reservoir heterogeneity, Subsurface Dynamics and Potential Trapping Mechanisms Profile in the Upper Kharaib Carbonate Reservoirs – Deep saline aquifer case

CHAPTER 2

LITERATURE REVIEW

2.1 Carbonate Rocks

Approximately 60% of global oil and 40% of gas reserves are believed to be stored in carbonate reservoirs (Sheng, 2013). In addition, the Middle East stands out for its substantial carbonate deposits, accounting for roughly 70% and 90% of oil and gas reserves respectively (Global CCS Institute, 2015). Nevertheless, carbonates display significant heterogeneity in characteristics like permeability, porosity, and fluid flow mechanisms within localized portions of the reservoir, presenting characterization difficulties.

Carbonate sediments typically originate in shallow and warm oceans through two main processes: direct precipitation from seawater and or biological extraction of calcium carbonate from seawater to form skeletal material. The resulting sediment consists of particles with diverse sizes and shapes, creating various depositional textures. These sediments might be cemented by encrusting organisms or laid down as unconsolidated sediment, prone to displacement by currents of the ocean. (Lucia, 1999)

Understanding the heterogeneous nature of these rocks and their fluid containment, along with flow properties within the porous and possibly fractured rocks, requires a focused approach. This entails thorough examination of pore-size distribution, fluid saturation, permeability, reservoir lithology, rock texture, and inherent fracture networks across various scales. Fracture pathways, spanning between tens up to several hundred meters wide and height, stretching across kilometers, act as principal conduits for fluid movement.

These pathways can exhibit permeability values thousands of times higher than the surrounding rock matrix, significantly impacting oil, gas, and water production, as well as drilling operations (Global CCS Institute, 2015).

2.1.1 Carbonate Petrophysical Properties

Bulk density, porosity, and permeability are contingent upon fundamental characteristics, namely mineralogical composition, texture, fabric, and diagenesis. Among these, porosity and permeability stand out as pivotal variables that dictate reservoir quality, hence garnering significant attention for CO₂ storage endeavours. Rocks are usually classified based on their fundamental properties such as porosity, which help determine their depositional environments. However, porosity classification may not directly relate to how the rocks were formed due to some alterations were taking place post deposition. (GCI, 2015).

Porosity could be assessed directly or indirectly through samples of core and several borehole logging tools. Permeability, on the other hand, could be measured as the proportionality in Darcy's equation coefficient, which governs fluid flow via porous medium. This parameter is directly measured from core data and serves as a crucial metric against which many reservoir quality assessments are made.

Porosity in reservoir rock varies according to texture, fabric, and fracture geometry. In clastic rocks, porosity is primarily influenced by factors such as grain shape, sorting, and packing, while in carbonate rocks, growth of fabric and microstructure of skeletal which

usually affect inter-grain, intragrain porosity, and microporosity. In addition, diagenesis processes play a crucial role, as they can either fill pores with cement, compact them, dissolve them (dissolution), or create new pores through recrystallization or replacement.

Berg (1970) demonstrated the geometric relationship between grain size and pore size using identical spheres packed together, resulting in approximately 30% porosity. Modern carbonate sediments (i.e., loose material) typically exhibit porosities ranging from 40% to 70%, whereas ancient rocks typically have porosities ranging from 0.1% to 40% (Choquette & Pray, 1970). The mechanisms leading to porosity reduction can be intricate, often involving cementation, compaction, or a combination of both processes.

Lucia's classification (1983) of porosity type of carbonate rocks, as depicted in Figure 2.1, developed from research undertaken at Shell Companies back in the 1960s. The classification of Lucia highlights the petrophysical significance of isolated and connected vuggy porosity, in which pores larger than the surrounding framework grains. These vugs may originate as interparticle, moldic type of pores, intraparticle, or intercrystalline pores and then evolved through dissolution and become vuggy type of pores. Lucia's classification also highlights the porosity-permeability, particle size, and capillary pressure relationship—a concept that was recognized early on by Craze (1950) and Bagrintseva (1977). This method acts as an initial approach for "rock typing" or assessing reservoir zones according to their petrophysical features.

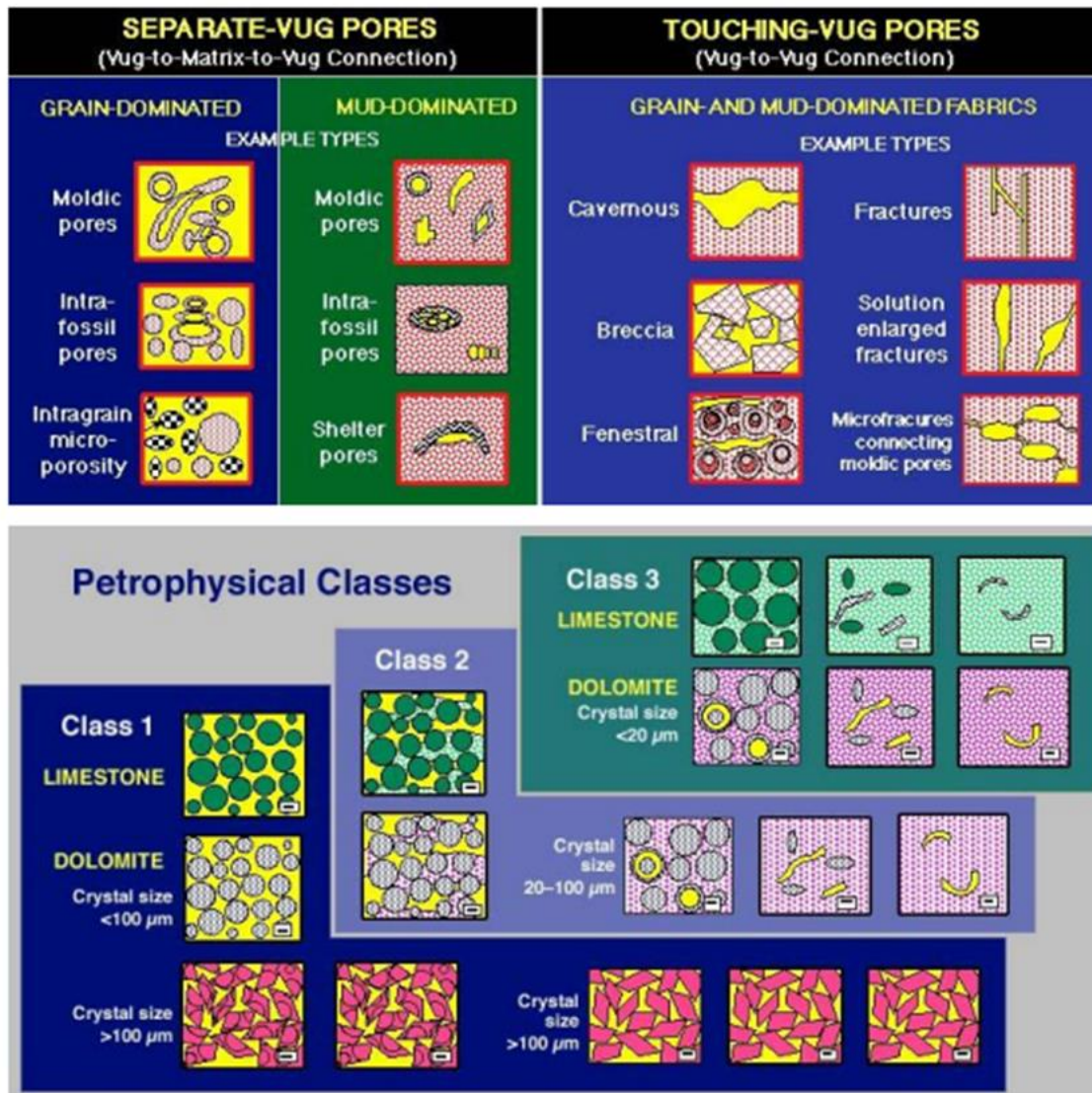


Figure 2. 1 Lucia's (1983) categorization of carbonate porosity holds particular significance as it highlights the considerable impact of interparticle porosity (resulting from grains or crystals) and distinct or interconnected vuggy porosity on various petrophysical properties of reservoirs.

To obtain initial broad estimates of permeability, it's necessary to consider porosity-permeability relationships. However, it's important to recognize that actual permeability is influenced by additional factors, notably pore size and connectivity, which aren't fully

represented by porosity alone. Consequently, these relationships are subject to high uncertainty and must accommodate these supplementary factors (GCI, 2015).

While discrete hydraulic methods like mini tests are available, they are expensive. Reservoir geologists seek a correlation between porosity and permeability through log analysis techniques. However, this endeavour is often risky due to the intricate nature of the porosity-permeability relationship, particularly in carbonates with their complex and heterogeneous pore networks (Figure 2.2).

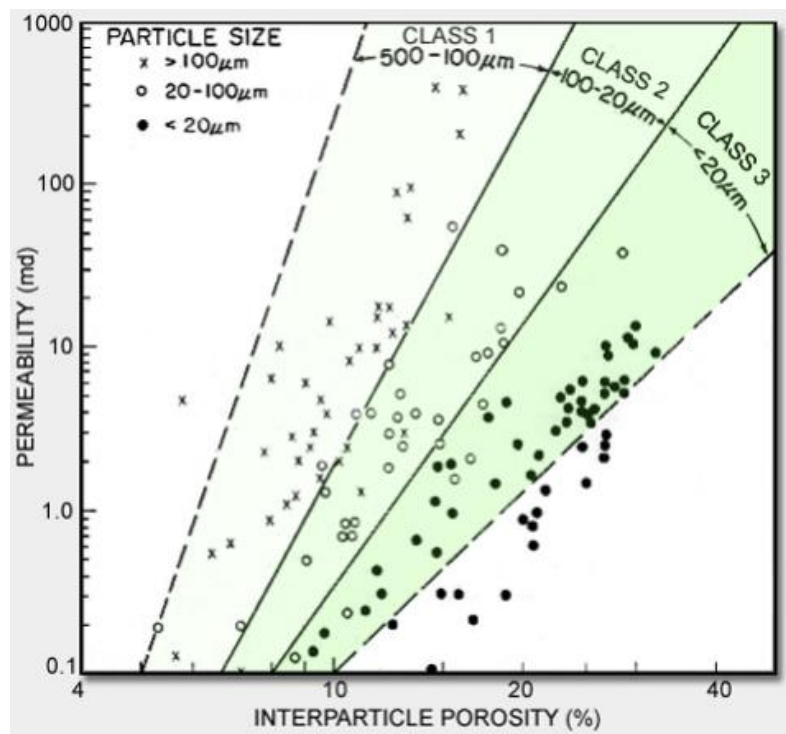


Figure 2. 2 Permeability (logarithmic scale) plotted against porosity (arithmetic scale) and grain size, according to Lucia (1995).

Carbonate pore systems defy simple classification into distinct pore shapes and pore throats; instead, they exhibit scaled in different ways, intricate pore structures. Although several pore classifications have been proposed based on observable textures, such as those by Choquette and Pray (1970), Mousavi et al. (2013), Lønøy (2006), and Lucia (1995), they do not directly address the flow properties of rocks, whether in single-phase or multi-phase conditions.

The petrophysical attributes of carbonate rocks and their distribution in the subsurface are shaped by factors such as sediment grain size, type, fabric, depositional facies, subsequent diagenetic and structural events. Carbonate rocks are highly reactive in nature, often undergo significant syn- to post-depositional alterations. Diagenetic processes like dissolution, cementation, compaction, neomorphism, and dolomitization can modify porosity and permeability, consequently impacting the features of the carbonate rocks (Flügel, 2004 and Lucia, 2007).

Within carbonate rocks, excluding mudstones, two distinct types of porosity contribute to their petrophysical attributes, each exerting varying effect: Micro-porosity, also known as micro-connected porosity, is consistently present within the matrix and allochems. In addition, Macro-connected porosity, occasionally encountered between allochems or intergranular, and occasionally within dissolution vugs, provided they are sufficiently numerous to interconnect.

2.2 Upper Kharaib Member, Abu Dhabi, UAE

2.2.1 Geological Framework

From the Berriasian to Late Barremian, the eastern Arabian Plate experienced a period of geological stability without significant tectonic activity (Alsharhan et al., 2000). Over the course of approximately 20 million years, carbonate formations were deposited, which exhibited a consistent and uniform nature that persisted over long distances (Christian, 1997). However, during the overlying Aptian Shu'aiba Formation's deposition, the development of intra-shelf basins occurred, which were filled in multiple stages (Bromhead et al., 2021).

The data for this study was sourced from subsurface records in onshore and offshore UAE. In this area, a sequence of carbonate platforms was formed, which was characterized by laterally extensive ramp systems (Murriss, 1980). Rub Al-Khali basin is dominated by the cyclic deposition of Cretaceous-aged carbonates and shales (van Buchem et al., 2013). In this study, our focus is on the Upper Kharaib Formation (Late Barremian) which composed predominantly of shallow-marine limestones (Sugden & Standring, 1975).

During the Lower Cretaceous period, the study area was part of a broad shallow marine platform with no significant land mass developed in the adjacent area (Pacheco et al., 2019) (Fig. 2.3). The Upper Kharaib Member is part of the Thamama Group and distributed widely across the Middle East forming a prolific reservoir in UAE, Qatar, Oman, Iraq, and Kuwait (van Buchem et al., 2013).

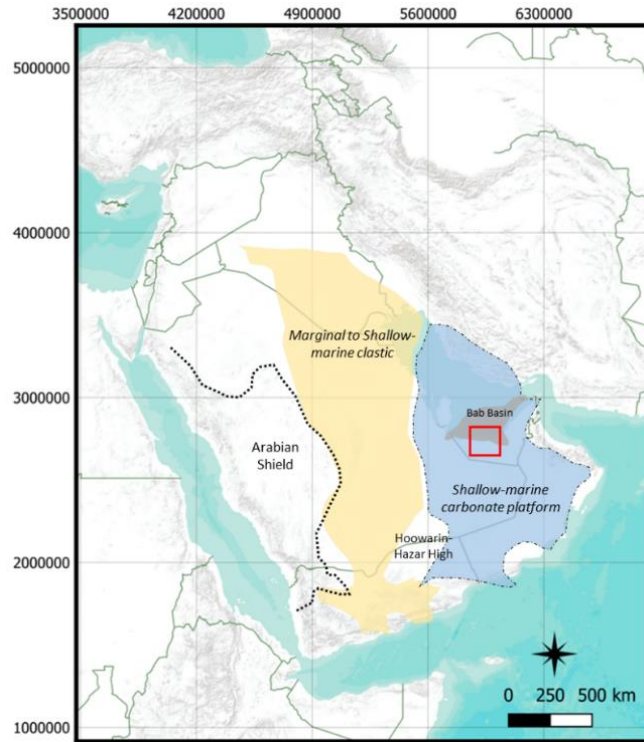


Figure 2. 3 Location of study area in red box and simplified Paleogeography map during Lower Cretaceous time (after van Buchem et al., 2013)

The comprehensive high resolution stratigraphic architecture of KharaiB formation was presented and described by van Buchem (2002) as basis of our stratigraphic framework understanding. Overall, the Upper KharaiB Member was deposited under a moderate energy, shallow water environment on a broad eastward dipping carbonate ramp (Strohmenger et al., 2006). The type of reservoir in the Thamama group is well known to be a single cycle of shoaling upward sequence, which the upper part of Upper KharaiB was dominated by Rudist grainstone facies (Fig. 2.4).

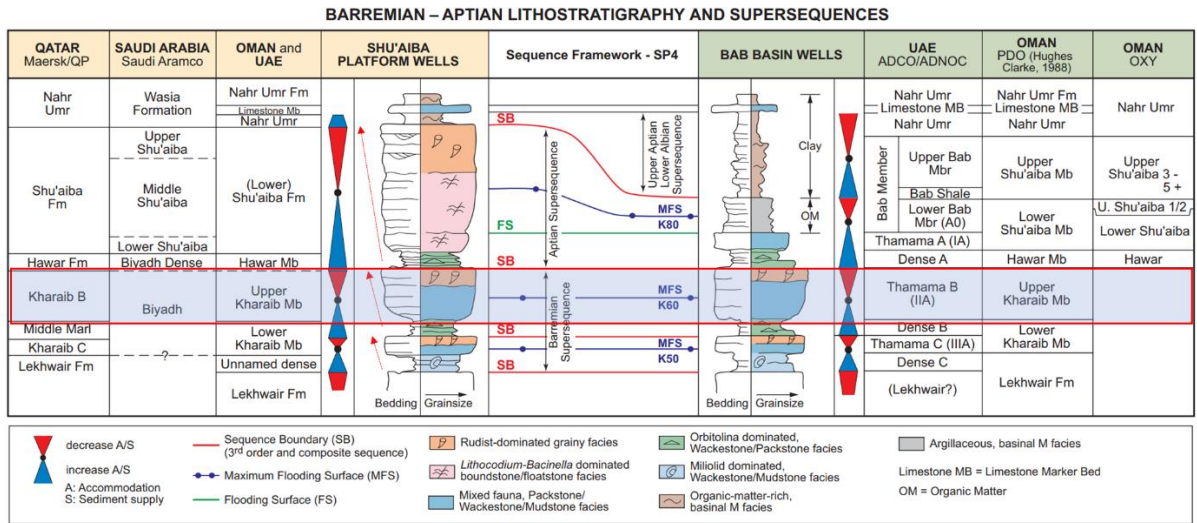


Figure 2. 4 Lithostratigraphy of study area highlighting Upper KharaiB interval as broad layer cake bedding and single shoaling upward succession. (Buchem et al., 2013)

2.3 CO₂ sequestration in Carbonate Reservoir

Carbonate reservoirs stand out as promising options for CO₂ sequestration due to their significance as hosts for the majority of the world's oil reserves, particularly notable in the Middle East. This makes them compelling storage targets, especially when coupled with Enhanced Oil Recovery (EOR) operations. Additionally, the recent discovery of deep-water oil fields along the Brazilian coast in the South Atlantic Ocean, referred as the Pre-Salt region, consists of carbonate reservoirs. CO₂ injection is already underway in these reservoirs, such as the Lula field in the Santos Basin, utilizing CO₂ extracted from the Pre-Salt reserves, known for their high CO₂ content (GCI, 2014 and Ketzer, 2015).

However, carbonate minerals exhibit high reactivity (Pokrovsky et al., 2009) and often create highly heterogeneous reservoirs (Lucia, 2007)), making them susceptible to notable

alterations upon CO₂ injection. These alterations may impact integrity, injectivity, and ultimately, storage safety (Bildstein et al., 2009). Furthermore, changes in rock porosity and permeability can affect storage capacity. Therefore, understanding between CO₂, formation water, and rock interactions and its implications in carbonate reservoirs is crucial.

2.3.1 Interactions between CO₂ and geological media

Upon injection into a reservoir, carbon dioxide induces alterations in both pore pressure and fluid chemistry inside the reservoir (Kampman et al., 2014) (Fig. 2.5). Near the injection wells, CO₂ undergoes dissolution into the resident reservoir fluids, leading to a decrease in pH, often causing mineral dissolution and consequent changes in porosity and permeability (Andreani et al., 2009, Bacci et al., 2011). It is essential to quantify these processes and its impact on the hydraulic properties of the reservoir to comprehend the evolution of transport accurately (Ketzer et al., 2015).

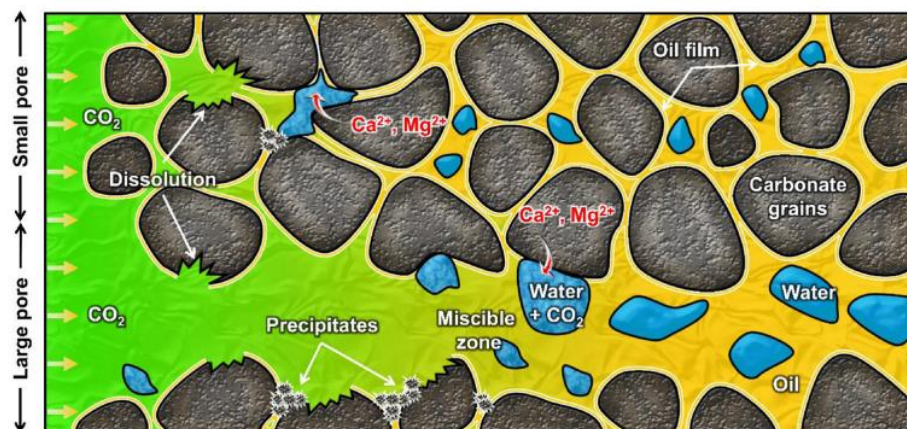
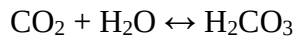


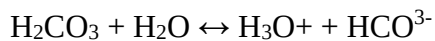
Figure 2. 5 Diagram illustrating the distribution of fluids and reaction mechanisms in a carbonate reservoir during CO₂ flooding (Han et al., 2018).

The dissolution of CO₂ into brines is a rapid process, occurring within minutes to hours, resulting in a swift decrease in the brine pH level or aqueous phase concentrations and altering the distribution of various dissolved materials (Gaus, 2010, Kharaka et al., 2013). Models based on experimental data can quantify CO₂ solubility in brine, while the subsequent reactions between dissolved CO₂, brine, and also rock-forming minerals are complex and less precisely defined (Duan and Sun, 2003, Portier and Rochelle, 2005). Some of these reactions may be advantageous, facilitating the chemical trapping of CO₂ as dissolved species or leading to the formation of carbonate minerals (Gaus, 2010, Kampman et al., 2014). However, others could be detrimental, possibly jeopardizing the integrity of both the reservoir and sealing formations by dissolving minerals that constitute the rock (Bachu et al., 1994, Gunter et al., 2004, Bachu, 2008, Bildstein et al., 2010).

The chemical reactions triggered by CO₂ dissolution in formation water are well-documented (Ortoleva et al., 1998). Initially, the dissolution process results in major acidification of the medium through the development of carbonic acid:



This acid subsequently dissociates, producing bicarbonate ions:



The bicarbonate in solution undergoes reactions with two-valent cations to form carbonate minerals through precipitation, given that aqueous medium acidity is at an adequate level (pH ranging from neutral to alkaline); alternatively, the species stay dissolved. The creation of calcium, magnesium, or iron carbonates under elevated pH conditions is anticipated to be the predominant mechanism through which CO₂ is permanently stored in a secure state.

Calcite Dissolution : $\text{CaCO}_3 + \text{H}_2\text{CO}_3 \leftrightarrow \text{Ca}^{2+} + 2\text{HCO}_3^-$

Dolomite Dissolution : $\text{CaMg}(\text{CO}_3)_2 + \text{H}_2\text{CO}_3 \leftrightarrow \text{Ca}^{2+} + \text{Mg}^{2+} + 2\text{HCO}_3^-$

Divalent cations that are dissolved could already exist in the brine or may arise from primary rock minerals dissolution due to CO_2 injection (Gaus, 2010, Gunter et al., 2004). The degree of mineral trapping correlates immediately with the concentration of these cations dissolved in the brine and the medium pH level (Bachu et al., 1994).

In carbonate rocks, the reduction of porosity and permeability primarily stem from the calcite and salt precipitation. This happens due to increases in Cl^- ions concentration and pH in the brine, respectively, often brought about by desiccation (Kaszuba et al., 2003). Brine desiccation, a phenomenon extensively recorded, is anticipated to happen in close proximity to the injection well. When CO_2 is injected in a dehydrated state and interacts with reservoir brine, some water molecules dissolve in the saturated CO_2 . With high injection rates, significant amounts of water could be transferred to the CO_2 phase, resulting in the concentration of dissolved species in the brine (Kaszuba et al., 2003). This concentrated brine then initiates rapid precipitation reactions involving minerals like carbonates, sulphates, and evaporites (Pauwels et al., 2007).

The processes through which precipitates affect permeability are relatively less understood and pose challenges for prediction compared to dissolution effects. Several factors influence whether precipitation takes place within pore spaces. Additionally, the material that has precipitated might either stay in position or migrate to other locations based on flow dynamics (Crandell, 2012). Grasping the relationship between chemical interactions and their outcomes on porosity and permeability remains a significant hurdle. Nonetheless,

this aspect has gained prominence due to its pivotal role in understanding the repercussions of geochemical reactions triggered by CO₂ (Luquot and Gouze, 2009, Luquot et al., 2004). Hence, thorough characterization of any storage site before the injection phase is imperative (Gaus, 2010, Chadwick et al., 2006).

Most of the time, the investigation of geochemical interactions among CO₂, fluids, and minerals in reservoirs or caprocks heavily depends on laboratory experiments and numerical simulation tools (Ketzer et al., 2009). The modelling of pore scale in CO₂-induced reactions and experimental analysis of pore space geometry alterations under geological storage conditions hold potential for improved comprehension (Gaus, 2010). Furthermore, examining CO₂ reservoirs and studying the features and these formations diagenesis offer additional insights (Bickle et al., 2013).

Kumar et al. (2004) conducted a compositional reservoir simulation study focusing on CO₂ sequestration in a deep saline aquifer. This study explored various parameters affecting CO₂ sequestration mechanisms, such as the ratio of vertical to horizontal permeability, residual gas saturation, salinity, temperature, aquifer inclination angle, and mineralization. Using the GEM simulator from the Computer Modelling Group, the study revealed that residual gas saturation significantly influences CO₂ sequestration at the pore level. Additionally, aquifer dip and horizontal to vertical permeability ratio emerged as crucial factors affecting gas migration, thereby impacting CO₂ dissolution in brine and mineralization. Tables and references detailing CO₂ solubility, mineral reactions, and correlations to determine residual gas saturation based on porosity values were provided.

Kartikasurja et al. (2008) investigated CO₂ sequestration in an aquifer, focusing on injecting CO₂ extracted from offshore gas fields in Malaysia. The study involved geological assessment of aquifer formations and also reservoir engineering for CO₂ injection with limited reservoir data. Sensitivity analyses determined the number of injection wells needed, while geo-mechanical calculations coupled with flow simulation predicted caprock failure risks, emphasizing the importance of Retention of gas residues in aquifers with low permeability and the potential of water injection to increase this trapping mechanism.

2.3.2 CO₂ trapping mechanism

CO₂ injection into deep saline aquifers for sequestration purposes undergoes various trapping mechanisms, including structural, residual, solubility, and mineral trapping (IPCC 2005; Bachu 2003). Various numerical simulations have been developed to forecast the degree of every trapping mechanism under varying circumstances (Prevost et al., 2005). Typically, CO₂ is injected as a supercritical fluid (scCO₂), saturating the interstitial space around the well as it displaces brine during injection. Initially, injection often targets the lowest reservoir layers to facilitate efficient brine "drainage" through buoyant displacement. Due to its lower density compared to brine, scCO₂ ascends buoyantly until reaching a geological seal rock (Bachu 2008). Underneath the seal layer, the CO₂ accumulates and is retained through structural trapping mechanisms (Bachu et al. 2007) as illustrated by figure 2.6. Additionally, some CO₂ dissolves into formation water when in

contact with the phases, contributing to storage via the solubility trapping mechanism (Bachu et al. 1994).

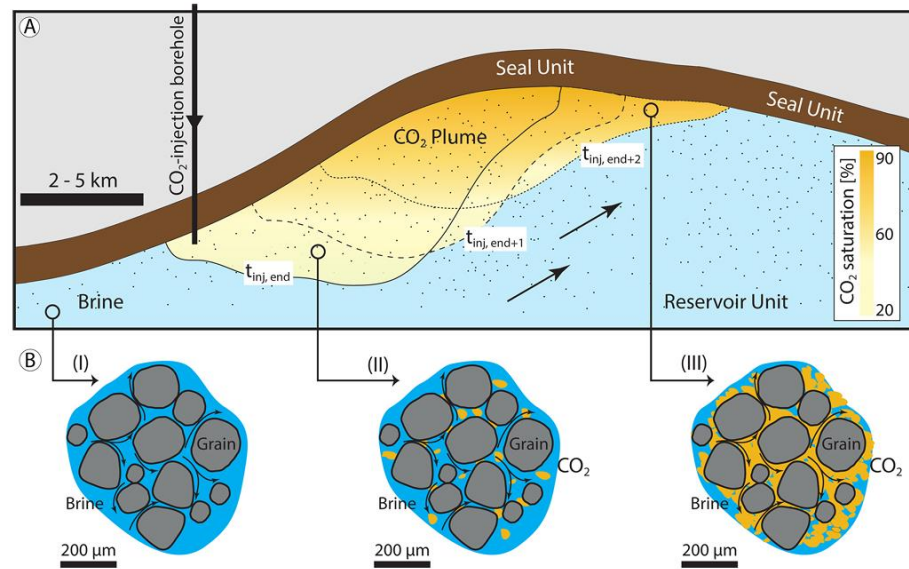


Figure 2. 6 Diagram showing CO₂ sequestration in a saline aquifer, where injected CO₂ tends to move updip due to the non-horizontal nature of caprocks. After CO₂ injection ends, the entire CO₂ plume typically follows this updip movement (Hefny et al., 2020).

According to Nghiem et al. in 2004, as CO₂ dissolves into the brine, its dissolution rate depends on pressure, temperature, and salinity state. This leads to an increase in brine density, causing the CO₂-saturated brine to descend due to gravity, potentially mixing with unsaturated brine and altering the CO₂ plume's extent. As denser fluids re-enter the lower regions of the supercritical CO₂ plume, where higher permeability layers exist, they trap and trap CO₂ pockets within an uninterrupted brine phase (Bachu 2008; Juanes et al. 2006). This trapped CO₂ categorized as residual trapping mechanism, crucial for understanding CO₂'s long-term fate (Bachu et al. 2007).

Some amount of dissolved CO₂ breaks down into bicarbonate within the aqueous brine, leading to geochemical reactions with fluid-rock components, leading to dissolution and precipitation of various minerals (Gunter et al. 1993). All these reactions, known as CO₂, brine, and rock interactions, lead to precipitation of calcite materials, categorized as mineral trapping (Bachu and Adams 2003). Although these reactions may occur slowly, over hundreds of years, they are considered the most secure mechanism for CO₂ storage due to the precipitate's stability.

The supercritical CO₂ beneath the seal rock typically persist as fluid reservoir within the formation and tends to rise due to buoyancy, potentially posing a leakage risk depending on seal rock properties. In an ideal sequestration site, the sealing rock ought to possess minimal permeability and significant water retention via capillary action. However, there's still a possibility of CO₂ diffusion into the seal rock (Bildstein 2010). The storage's security relies entirely on the seal's integrity over an extended period, ensuring the lack of natural fractures, fissures, or areas of high permeability in the cap (Kumar et al. 2005).

Residual trapping known as the confinement of a fluid as a result of capillary forces in a snap-off process (IPCC, 2005; Juanes et al., 2006; Pentland, 2011; Jalil et al., 2012; Raza et al., 2016b, 2016c). Pentland (2011) identified two processes at the pore scale that control the extent of residual trapping. The first process is due to imbibition, which involves competition for filling between the pore and the throat. In addition, at reservoir scale, imbibition predominates at the end of the migrating CO₂ plume, where brine, condition in wetting phase, imbues the migration non-wetting CO₂ phase. As the amount of CO₂

decreases below a certain threshold, it becomes trapped by the capillary pressure and it ceases to flow (Ennis-King and Paterson, 2001; Holtz, 2002).

The second process regulating residual trapping is due to the snap-off process, occurring during the imbibition process, as the water preferentially replenishes the tiniest pore voids. The extent of non-wetting phase progressively occupies smaller pores, with the degree of trapping dictated by local capillary forces (Pentland, 2011). It is important to note that thin films are present exclusive to highly wetted systems, and the snap-off mechanism may be entirely absent or reduced in intermediate-wet media (Kimbrel et al., 2015). Consequently, strongly water wet systems exhibit increased potential for residual trapping compared to intermediate or oil-wet formations (Iglauer et al., 2015; Al-Menhali and Krevor, 2015, 2016).

Essentially, residual trapping of CO₂ emerges as the most effective mechanism among various trapping mechanisms, better than dissolution trapping or mineral trapping mechanisms (Kimbrel et al., 2015). This mechanism significantly affects the speed and degree of plume movement, immobilization, and storage safety (Krevor et al., 2015). Several parameters, including characteristic of rock-fluid, geological settings, and injection conditions, are associated with residual trapping (Raza et al., 2016a, 2016c). Considering these diverse parameters, assessing the residual trapping potential of a reservoir prior to CO₂ injection appears challenging. This likely explains the scarcity of studies focused on determining residual trapping at a field scale. Figure 2.7 (Adapted from the IPCC report, 2005) qualitatively illustrates the enhancement of storage security over time.

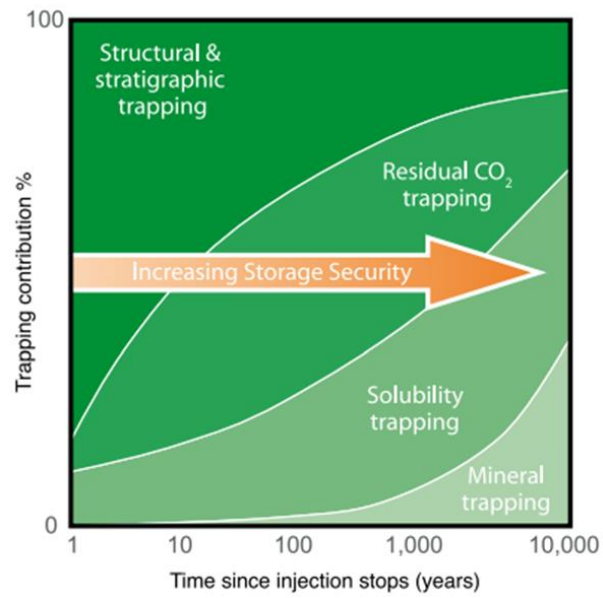


Figure 2. 7 The long-term security of CO₂ storage concerning trapping mechanisms over time (IPCC, 2005).

CHAPTER 3

METHODOLOGY

The methodology of this study is separated into two different processes. The first one is the reservoir characterization, which is including stratigraphy and depositional analysis, well log data analysis, grain texture approach analysis and extensive porosity-permeability cross-plot. The second one is the reservoir simulation and Modelling, which is modelling and simulation workflow using several numbers of parameters.

3.1 Reservoir Characterization

This study is using a publicly accessible carbonate reservoir model from the Late Cretaceous Upper Kharaib Member (COSTA MODEL; Costa et al., 2022) which consists primarily of measured field data (logs and Core data from 17 wells), and pre-defined static-dynamic models. The dataset comprises a mixture of real (i.e., Gamma Ray, Resistivity, Neutron-Density, and Sonic logs) and synthetic data (i.e., depth, maps, static-dynamic models). Recognizing the constraints of the Costa model, which result from the amalgamation of both real and synthetic data, it is important to note that despite these limitations, the data continue to offer valuable insights into subsurface storage. Furthermore, even with some alterations to the information, the data still retain comparable geological conditions. (Costa et al., 2022).

Within the COSTA model, we also identified the existence of a pseudo-facies or rock-typing methodology that was developed through the application of petrophysical methods and calculations. In a somewhat distinct approach aimed at enhancing the geological foundation of our analysis, this study leverages well log data, encompassing critical parameters such as GR, density, and core porosity-permeability, to carry out an extensive facies' analysis. This analysis is further enriched by a thorough examination of relevant literature (Ehrenberg and Wu 2019, Pachecho et al. 2019, El-Wazir et al. 2015, van Buchem et al. 2010, Strohmenger et al. 2004) on the sedimentology and stratigraphy of the Upper Kharaib Member in the broader Eastern Arabian Plate region. By employing this method, our objective is to provide a geologically-informed representation of the reservoir's characteristics.

We employ the Windland r35 equation (1) as a proxy for the texture-based porosity-permeability relationship, enabling the classification of grainy, mix, and muddy textures within the carbonate reservoir (Dernaika et al., 2019).

$$\log r35 = 0.732 + 0.588 \log K_{air} - 0.864 \log \phi \text{ core} \quad (1)$$

where:

r35 is the pore throat radius at 35% mercury saturation (micron)

ϕ is the porosity (%)

K is the uncorrected air permeability (mD)

We divided into three categories for our data; Grainy texture which has the r35 or pore throat radius value $> 3 \mu\text{m}$, mix texture which has the r35 or pore throat radius value between $1\text{-}3 \mu\text{m}$, and muddy texture which has r35 value $< 1 \mu\text{m}$.

Subsequently, a porosity-permeability crossplot has been conducted to depict the relationship between carbonate facies and reservoir properties, grain texture, and its diagenetic signature (Farooq et al., 2023). Extensive literature review has also been conducted as an additional information on seal properties and general vertical reservoir facies succession, in which this information is essential to produce a new Facies Association scheme to reflect related depositional environment. Then, the isopach map of each Facies Association is generated to show lateral thickness variation within the dataset. Finally, the screening matrix of carbon storage criterion and possible model for CO₂ trapping mechanism for Upper Kharaib is presented as a summary of overall evaluation.

3.2 Reservoir Modelling Construction

In order to understand the influence of lateral and horizontal variations in the reservoir on the migration patterns and distribution of CO₂, this study employs an approach involving the creation of reservoir models divided into three different cases based on reservoir characterization result and conceptual model. Each case considers various geological and physical factors, such as reservoir structure, rock properties, and internal baffle zones, which directly affect the behaviour of CO₂ within the reservoir.

- The first case may encompass reservoirs with relatively homogeneous lateral characteristics with various vertical value as layer cake model, where the properties spread evenly within each layer.

- The second case is similar to case 1. It may consider the presence of significant internal baffle zones, such as zones with relatively low permeabilities (0.1 mD), which can affect slowing down CO₂ vertical migration within the reservoir.
- Meanwhile, the third case may explore a combination of complex lateral and horizontal variations, incorporating a 3D geological model derived from well data to delineate facies and associated properties (porosity and permeability).

By modelling these three cases, we can gain deeper insights into how CO₂ migration patterns respond to reservoir structure and heterogeneity. The results of this analysis will aid in the development of more effective reservoir management strategies and strengthen our understanding of the potential distribution of CO₂ within the reservoir environment.

3.2.1 Case 1 – Layer Cake Model

In the first case, a layer cake model is depicted, wherein the vertical variations are represented by layers derived from average values from all wells and correlated with depositional facies, while maintaining a constant value horizontally (Figure 3.1). This model depicts a coarsening-shoaling upward trend, where reservoir properties generally improve upwards, as commonly observed in UKM reservoirs. Additionally, Table 3.1 shows the parameter set up for the grid

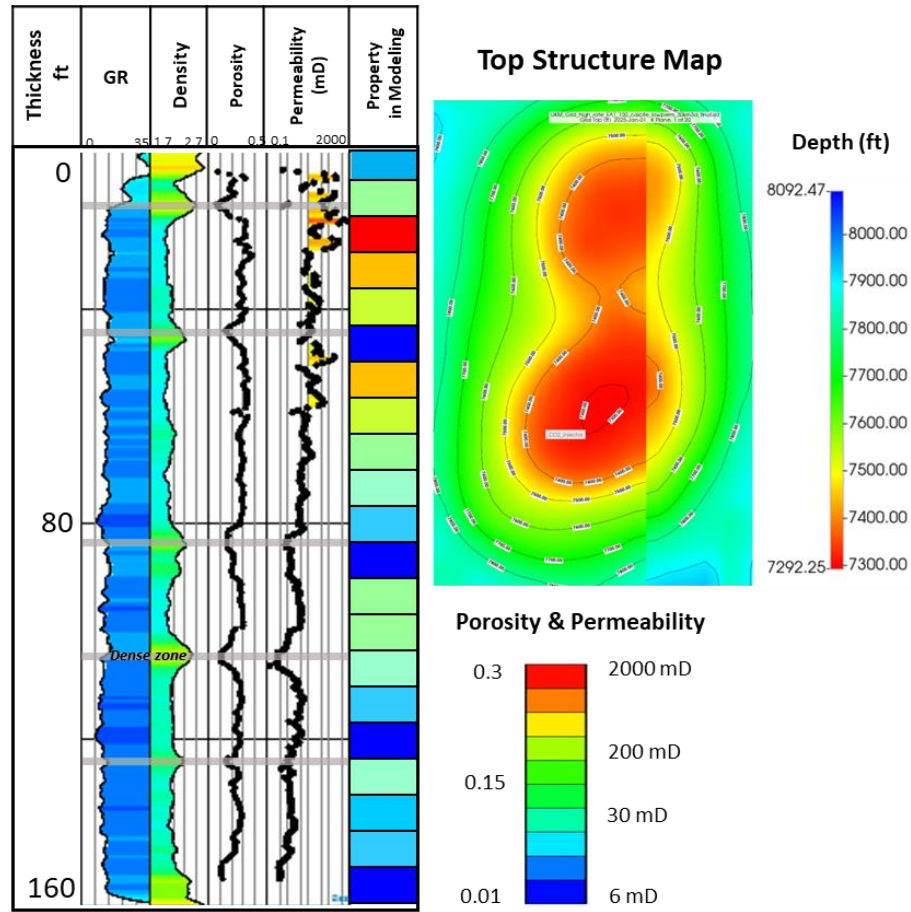


Figure 3. 1 The method for grid construction in both Case 1 and Case 2.

Case 1	
Grid	Layer Cake Model
Structure Map	Synthetic Anticline
Properties Distribution	Vertical variation only
Reservoir Thickness, ft	160
Total Layers	20
Baffle layers	4
Baffle permeability, mD	6-9 mD

Table 3. 1 Summary of grid construction for Case 1

3.2.2 Case 2 – Layer Cake & 0.1 mD Baffle layers

The second case is similar to Case 1, but for the internal baffle zone or dense zone, the lowest horizontal permeability value is set to 0.1 mD (Table 3.2) to conduct sensitivity analysis on how low permeability layers affects and slows down the vertical migration of CO₂.

Case 2	
Grid	Layer Cake Model
Structure Map	Synthetic Anticline
Properties Distribution	Vertical variation only
Reservoir Thickness, ft	160
Total Layers	20
Baffle layers	4
Baffle permeability, mD	0.1 mD

Table 3. 2 Summary of grid construction for Case 2

3.2.3 Case 3 - 3D Geological Model

The third case is a static model where 3D modelling is conducted, with the distribution of facies resulting from reservoir characterization based on existing well data (Table 3.3). In geological concept, this third case is the one that most closely resembles geological descriptions because it honours both lateral and vertical variations originating from wells, and then properties are distributed spatially using statistical modelling, as commonly practiced in reservoir modelling in the oil and gas industry.

Several steps were conducted to build and reconstruct the model as follow:

- Identification and correlation of well markers within the reservoir to determine the presence of geological zones in the dataset.
- Generation of a top structure map grid using depth information from well markers, creating a simple pseudo 3D map framework in the absence of seismic data (without fault).
- Upscaling of rock type, porosity, and permeability logs to capture variations within wells with a resolution suitable for accelerating simulation run times.
- Modelling and distribution of facies-rock types to visualize lateral and vertical variations in 3D based on geological interpretation and conceptual understanding.
- Modelling and distribution of properties to allocate porosity and permeability values throughout the reservoir.

Case 3	
Grid	3D Geological Model
Structure Map	Well Marker Interpolation
Properties Distribution	3D Property Modelling
Reservoir Thickness, ft	3D Structural Modelling
Total Layers	26
Reservoir Zones	6

Table 3. 3 Summary of grid construction for Case 3

3.3 Reservoir Simulation

CMG-GRID software was employed to construct a simplified grid model of the Upper Kharaib reservoir for Case 1 and Case 2, while Petrel software was employed to construct 3D geological model for Case 3. In designing the grid, critical factors such as geological interpretation, facies associations, and vertical succession patterns were considered. Specifically, in Case 3, the actual log values from wells were utilized for calibration and

property distribution within the reservoir. The goal was to develop a grid that accurately represented the key geological features of the reservoir while ensuring efficient computational performance.

After the completion of the grid framework and the construction of the property model, the next step is to input several parameters such as reservoir rock-fluid parameters (Costa, 2022), brine (El Wazir, 2015) and mineral composition into the Process wizard module for CCS within the CMG-GRID software, as shown in the Table 3.4. Another crucial aspect is that the simulation model was configured for CO₂ injection in a deep saline aquifer scenario.

The subsequent stage involves selecting various options for CCS modelling by activating the PITZER model for high salinity cases (Feistel and Marion, 2007), as well as activating the rock geochemical reaction model and the CO₂ trapping model through relative permeability hysteresis as shown by the curve in Figure 3.2.

Rock-Fluid Properties	
Rock compressibility, 1/psi	1E-06
Reservoir Temperature, C	121
Water Density, lb/ft3	65.34
Water Salinity, ppm	157,000
Initial Reservoir Pressure, psi	4400
Reference Depth, ft	7300
Initial pH	7.5

CCS Activity model	PITZER
Brine Composition, ppm	
Ca ²⁺	15000
Mg ²⁺	1200
Na ⁺	47000
SO4 ²⁻	654
Cl ⁻	110000
Mineral Composition, %	
Calcite	99.9
Dolomite	minor
Anhydrite	minor
Hysteresis Parameters	
Hysteresis model	Linear
CO ₂ Hysteresis	LAND
Maximum residual gas saturation	0.15

Table 3. 4 Reservoir and CCS model parameters essential for the simulation.

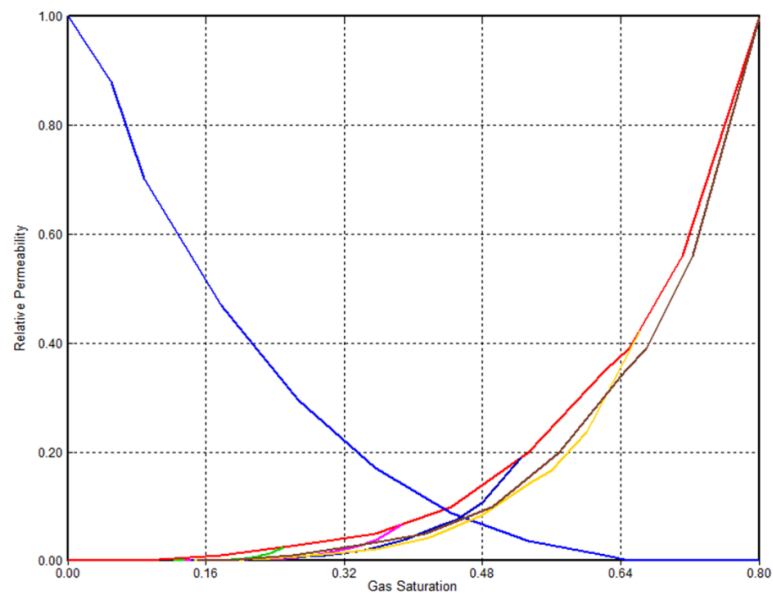


Figure 3. 2 The relative permeability curve utilized in the model to account for hysteresis.

For this project, the gas (hydrocarbon compounds) and oil saturation are both set to zero, necessitating the insertion of a placeholder table to facilitate model execution. Figure 3.2 illustrates the relative permeability curves utilized for the CO₂-water system in this model.

The study did not incorporate capillary pressure within a CO₂-water system. Further investigation is required to enhance the characterization of CO₂ flow in a saline aquifer and obtain accurate values for relative permeability and capillary pressure.

The simulation of CO₂ injection was conducted using the CMG-GEM software CCS workflow. Nghiem (2004) developed the GEM module specifically for CO₂ sequestration. The simulation and Modelling methods for solubility, residual gas, and mineral trapping rely on the compositional equation of state and greenhouse gas simulator with the geochemical option.

For all three cases, the simulation model setup included a constant injection rate of 30,000 m³/day over the initial 25-year period, followed by a 200-year monitoring phase (Table 3.5). Perforation points were established for each facies association, all wells are vertical, well locations were selected, and initial subsurface conditions and constraints were set. The simulation results were extensively analysed and compared across the various facies. This analysis focused on parameters such as CO₂ plume migration, changes in reservoir pressure and properties, mineral precipitation and dissolution, as well as the mechanism of CO₂ entrapment. These analyses provided predictions and valuable insights into the likelihood of different CO₂ phenomena occurring within the Upper Kharaib carbonate reservoir, based on facies distribution at various injection points.

Case 1 and Case 2			
Injection Well	FA1	FA2	FA3
Well Placement	Flank	Flank	Flank
Perforation Interval (I, J, K)	10 , 32, 3-4	10 , 32, 7-8	10 , 32, 13-14
Porosity value	0.25-0.3	0.1-0.2	0.1-0.15
Permeability value, mD	700-2000	30-200	10-15
Start of Injection, year	2025	2025	2025
Injection duration, years	25	25	25
Monitoring period, years	200	200	200
Maximum injection rate (m3/day)	30000	30000	30000

Case 3			
Injection Well	FA1	FA2	FA3
Well Placement	Flank	Flank	Flank
Perforation Interval (I, J, K)	24, 27, 5-6	19, 12, 8-9	16, 27, 21-22
Porosity value	0.25-0.3	0.25-0.3	0.25-0.3
Permeability value, mD	100-200	100	5-10
Start of Injection, year	2025	2025	2025
Injection duration, years	25	25	25
Monitoring period, years	200	200	200
Maximum injection rate (m3/day)	30000	30000	30000

Table 3. 5 Well injection parameters for Case1, Case 2, and Case 3.

CHAPTER 4

RESULTS

4.1 Facies Association

In general, based on well logs and core data, the Upper Kharaib Member can be sub-divided into four different Facies Associations (FA), representing restricted platform interior (subtidal to inner shoal) and open platform (shoal to outer ramp). FA1 or Inner Shoal-Shoal Facies Association dominated by rudist-skeletal-algal rich grainstone-packstone facies which indicating restricted to high energy environment. FA2 or Upper Ramp Facies Association is dominated by coated grain algal, skeletal rudstone – floatstone facies represent high-medium energy environment. The presence of FA1 and FA2 consistently manifests in nearly all wells, primarily confined to the upper section of the Upper Kharaib member. FA3 or Middle Ramp Facies Association mainly consisting of packstone to wackestone facies which reflecting medium to low energy environment. The FA3 are mainly distributed in the middle to lower part of UKM. Lastly is FA4 or Outer-ramp to basinal Facies Association which mainly dominated by mudstone and burrowed wackestone facies and related to low energy environment. The FA4 also characterized by relatively high density, low porosity and low permeability. The overall succession of Upper Kharaib Member represented by a single large-scale cleaning-upwards cycle and dominated by aggradation parasequences, showing gradational depositional transition from relatively distal to more proximal environment (Figure 4.2b).

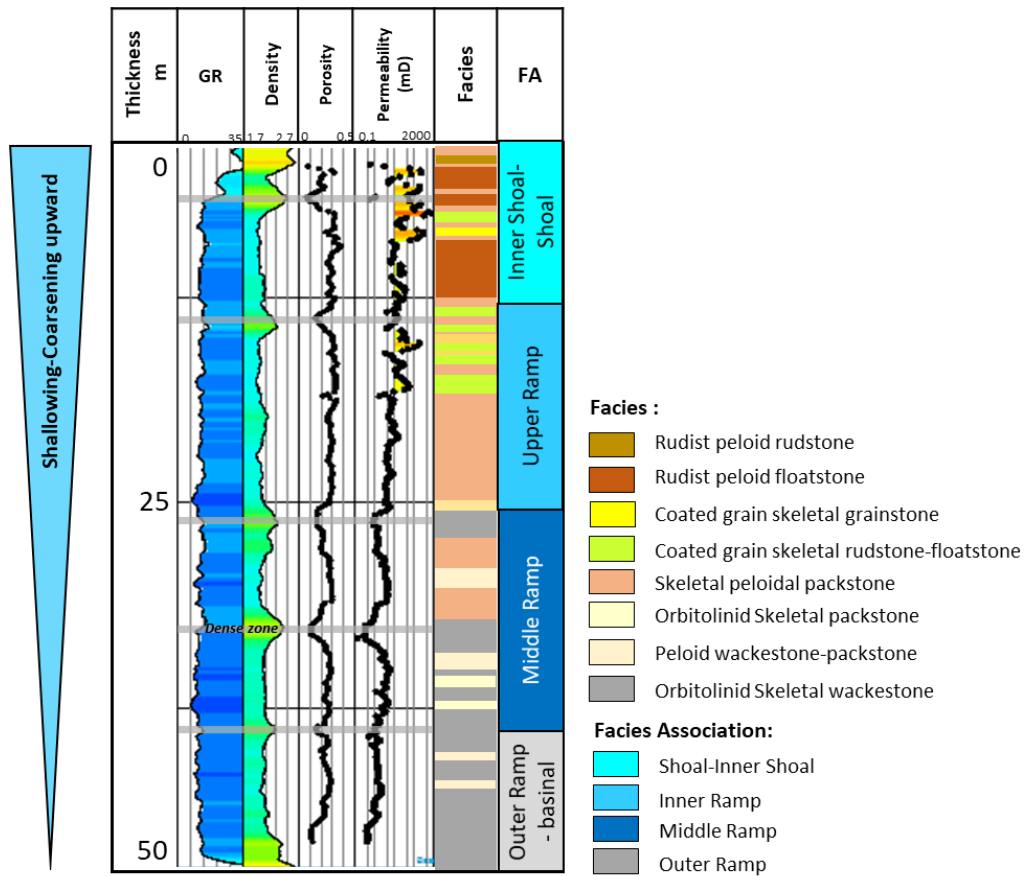
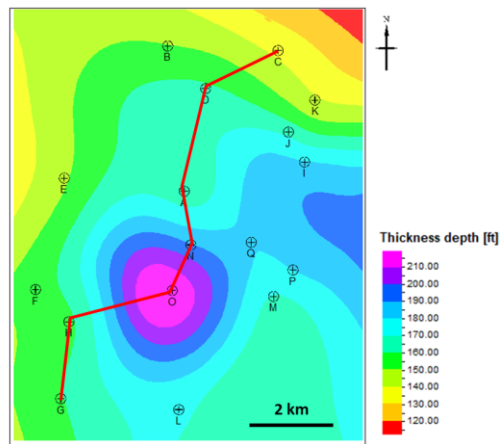


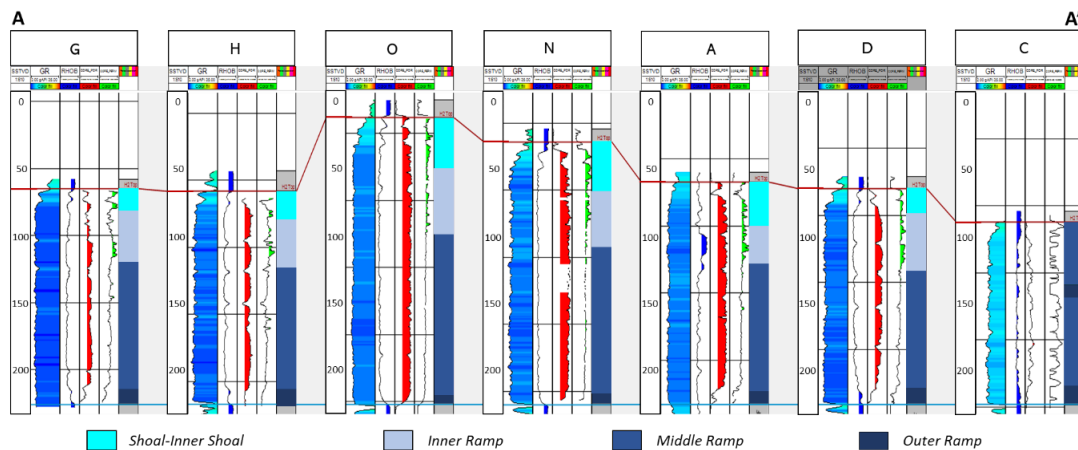
Figure 4. 1 Classification of Upper Kharai reservoir lithofacies (El-Wazir et al., 2015) and their correlation with depositional environment through type log analysis and facies association grouping.

In nearly all wells, the permeability log trend indicates an improvement towards the top reservoir that corresponds with the observed and interpreted shallowing upward trend of facies association (Fig. 4.1). Meanwhile, the total porosity log does not exhibit any specific trends or significant changes from the bottom to the top of reservoir. In addition, we observe five high dense zones in the density log curve which also characterized by low porosity and low permeability values within the reservoir (Fig. 4.1).

The well correlation depicted in Figure 14a. illustrates that the upper Kharaiib reservoir exhibits thickness variation ranging from 140 to 220 feet. The wells situated towards the northern region exhibit distinct GR log characteristics, including a reduction in reservoir thickness and a decline in both log porosity and permeability values, indicative of a decrease in reservoir quality. In addition, The GR (specify the value range) log values of the Upper Kharaiib carbonate reservoir exhibit a blocky and relatively uniform distribution, except for the HW-5 well (Figure 4.2b).



(a)



(b)

Figure 4. 2 a. Gross thickness Map of Upper Kharaib reservoir within study area. b. South-North Well correlation displays Facies Association Interpretation and distribution.

The general trend is thinning and more basinal facies towards north.

4.2 Exploratory Data Analysis – Well logs

Core porosity and permeability were used to determine rock quality and its correlation with Facies Association. Below is the histogram of Core Porosity and Core Permeability for each FA.

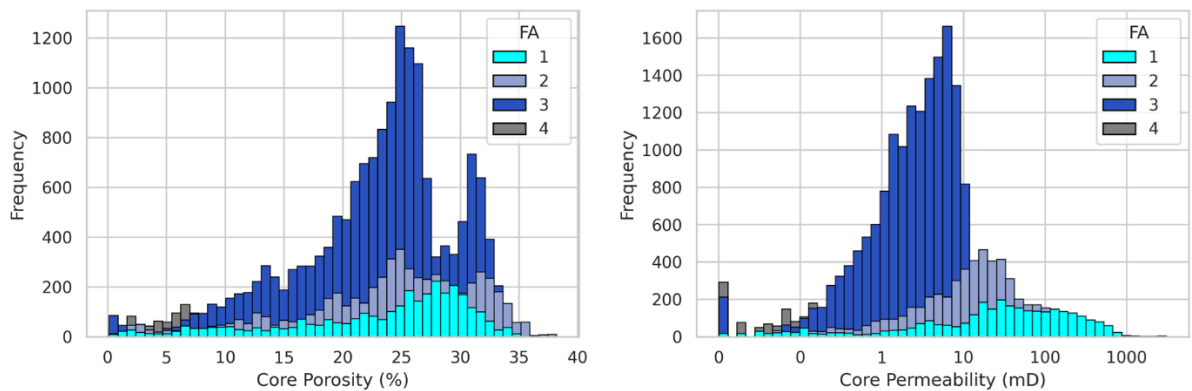


Figure 4. 3 Histogram of Core porosity and permeability on each Facies Association

In Figure 4.3 above, for FA1 cores, the primary porosity falls within the range of 25% to 30%, with mean, median, and standard deviation values of 24%, 25%, and 7.9, respectively. Simultaneously, the core permeability lies in the range of 10 to 1000 mD, with mean, median, and standard deviation values of 106 mD, 32 mD, and 208, respectively. Moving on to FA2 cores, the porosity spans from 20% to 35%, with mean, median, and standard deviation values of 23.7%, 25%, and 7.6, respectively. The core permeability for FA2 ranges from 1 to 100 mD, with mean, median, and standard deviation

values of 39 mD, 15 mD, and 84.5, respectively. FA3 demonstrates a porosity range of 10% to 33%, with mean, median, and standard deviation values of 23%, 24%, and 6.6, respectively. The permeability for FA3 ranges from 0.1 to 10 mD, with mean, median, and standard deviation values of 4.3 mD, 2.9 mD, and 8.46, respectively. In contrast, FA4 exhibits the lowest quality, featuring a porosity range of 0.1% to 11%, with mean, median, and standard deviation values of 9%, 10%, and 6.2, respectively. The permeability for FA4 ranges from 0.001 to 2 mD, with mean, median, and standard deviation values of 0.9 mD, 0.2 mD, and 6.13, respectively. The figure below (Table 4.1) provides a summary statistic of the log curve from all wells.

	DEPT	CORE_PERM	CORE_POR	DT	GR	NPHI	PHIE	RHOB
mean	8605.97	21.79	20.34	76.40	14.08	0.17	0.19	2.38
std	262.18	84.38	9.38	13.22	8.36	0.09	0.10	0.17
min	7820.00	0.01	0.09	41.35	3.95	-0.01	0.00	2.08
25%	8458.40	0.72	14.55	65.08	9.56	0.11	0.13	2.26
50%	8634.10	3.33	23.00	79.70	11.28	0.20	0.23	2.33
75%	8789.90	9.40	26.88	87.43	14.89	0.25	0.27	2.49
max	9114.00	3076.15	38.20	101.03	69.89	0.39	0.35	2.79

Table 4. 1 Summary statistics derived from well logs across all wells.

Based on the findings depicted in the crossplot below (Fig. 4.4), a notable trend emerges across the majority of wells, indicating a negative correlation between Neutron Porosity (NPHI) and Bulk Density (RHOB). This observation implies that areas characterized by higher density rock formations tend to coincide with lower neutron porosity readings. It is worth noting that neutron porosity serves as an indirect indicator of the overall porosity within the rock formations.

Moreover, the color representation in the plot indicates the Gamma Ray (GR) values. It's observed that areas with low GR values are predominantly situated within zones characterized by relatively lower density and higher neutron porosity values.

High GR $\rightarrow$ High Density $\rightarrow$ Low NPHI

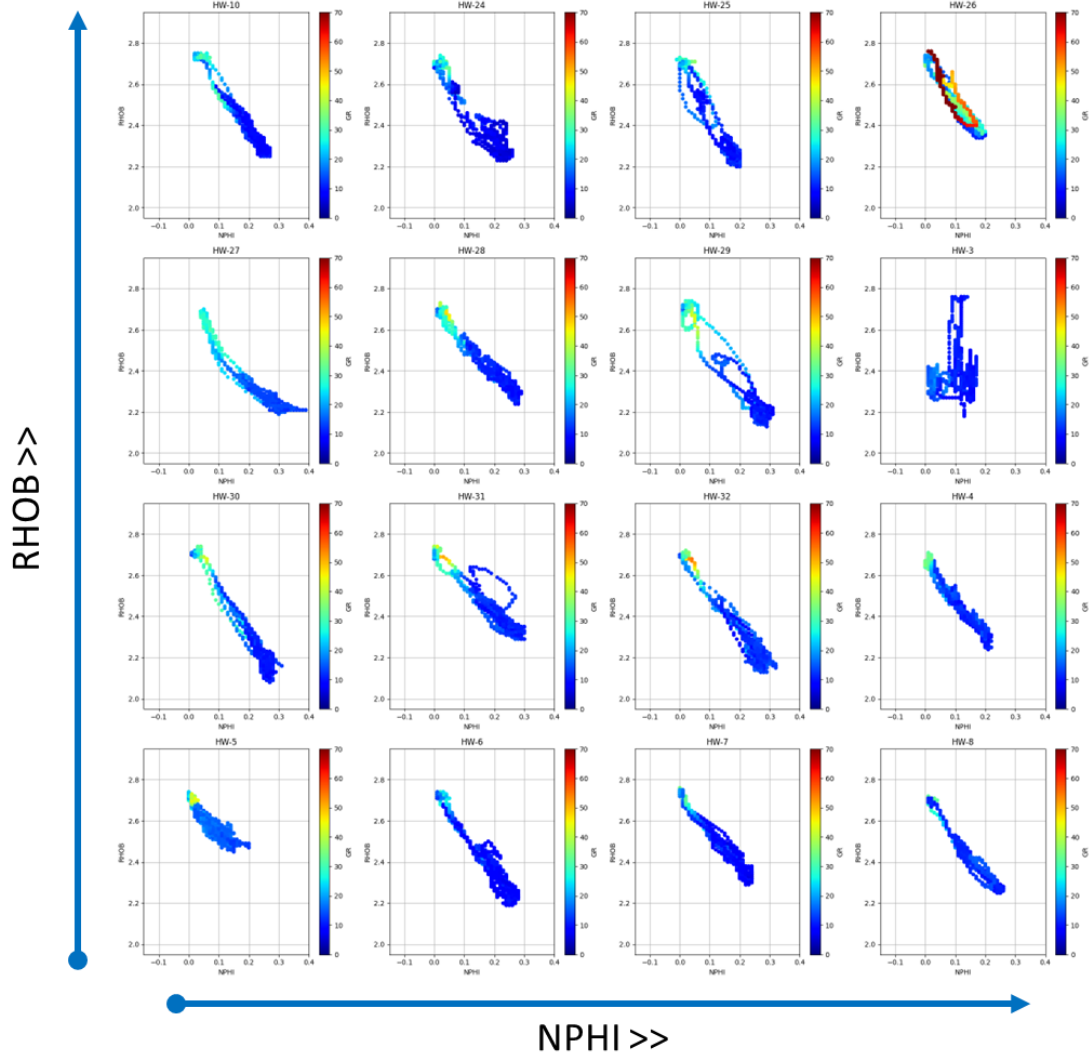


Figure 4. 4 The correlation between NPHI and RHOB plotted on a crossplot across all wells.

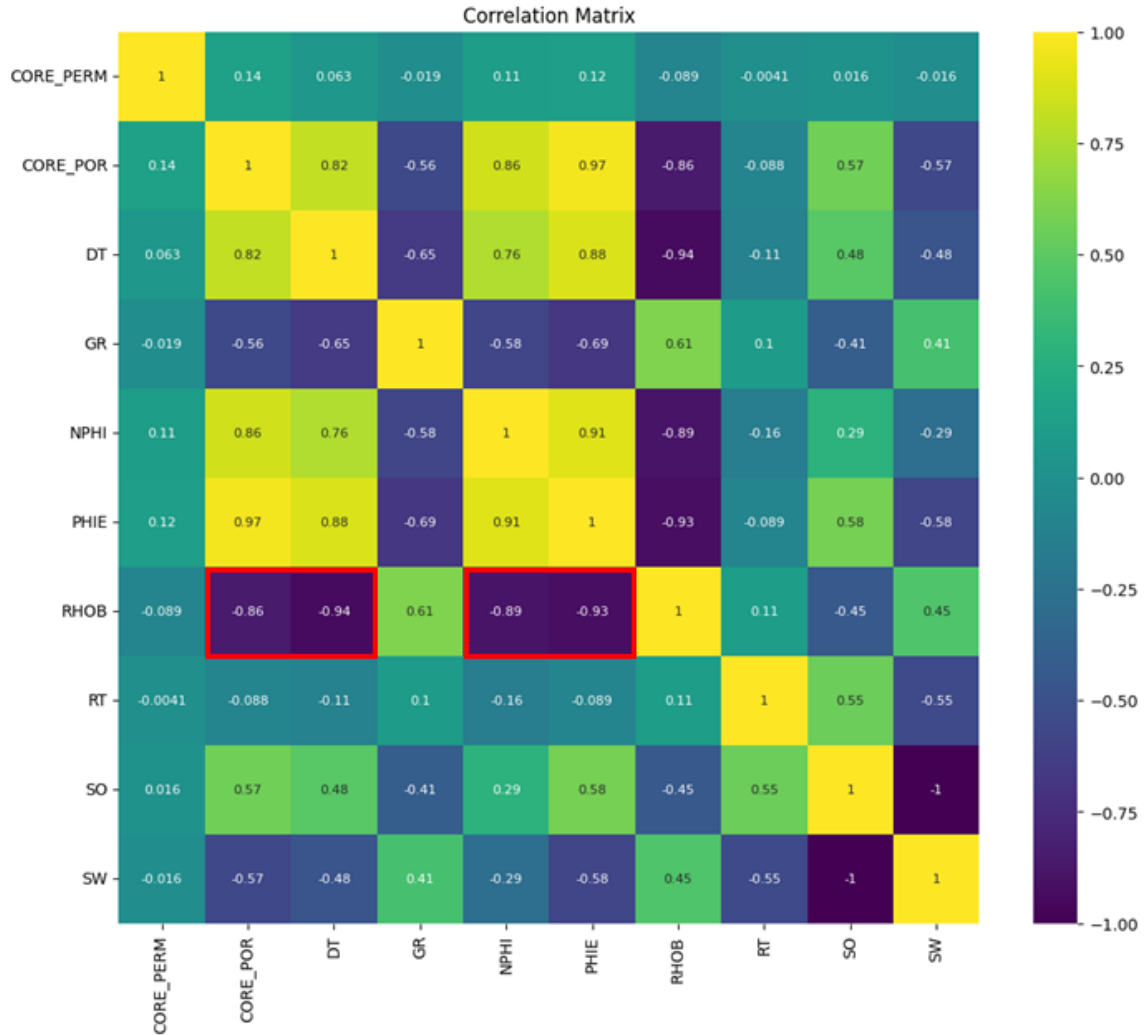


Figure 4. 5 A heatmap illustrating the correlation matrix of all available well logs. Dark blue color representing the negative correlation, and yellow color indicating positive correlation.

The Bulk Density (RHOB) exhibits a significant negative correlation with Porosity ($\emptyset$), registering a correlation coefficient of -0.86, and with Sonic (DT), recording a correlation coefficient of -0.94. This indicates that higher bulk density values are associated with lower core porosity, and sonic velocities within the formations (Fig. 4.5). Conversely, RHOB exhibits a relatively positive correlation with Gamma Ray (GR) values with correlation

coefficient of -0.61, suggesting that regions with higher bulk density tend to coincide with high GR readings.

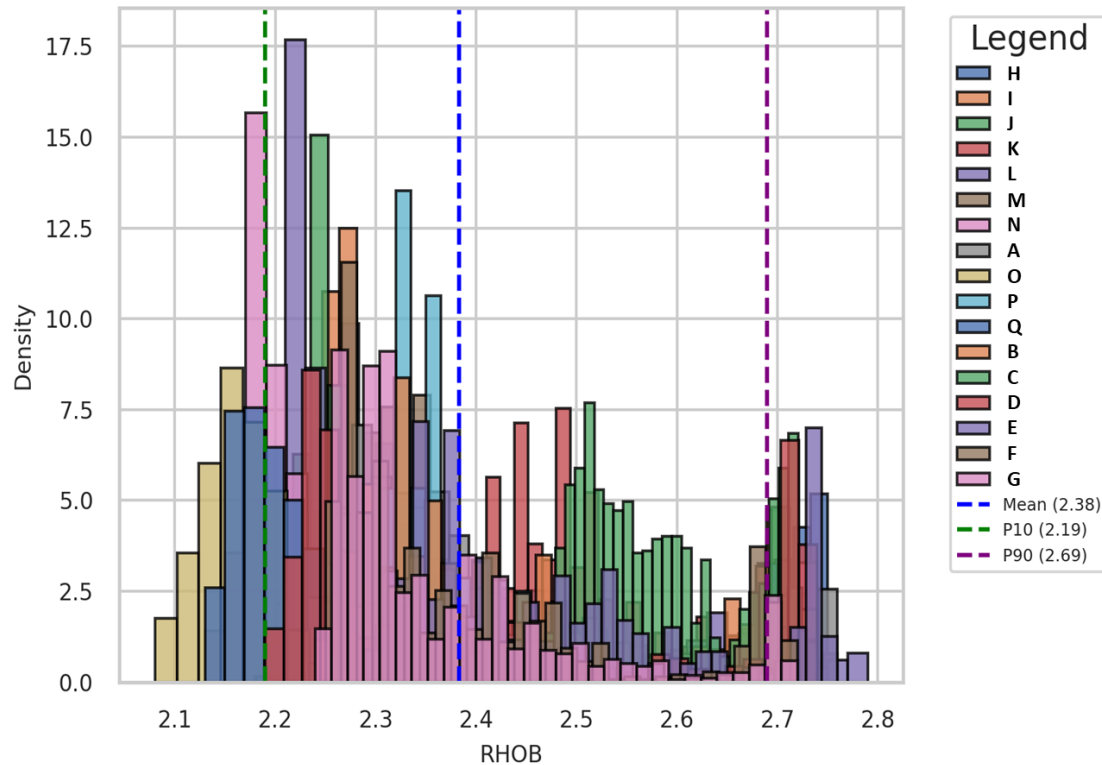


Figure 4. 6 Histogram displaying the density values for each well in the dataset.

From the histogram above (Fig. 4.6), we can observe a varied spectrum in each well, with some wells predominantly exhibiting density values (RHOB) between 2.2 and 2.4 g/cc, while others have a distribution of density values ranging from 2.5 to 2.75 g/cc. For example, in certain wells, such as Well C, denser rock formations (2.45 – 2.75 g/cc) are observed compared to others. This discrepancy and variation in rock density may indirectly signify variations in dominant lithology and potentially reflect different depositional settings and also diagenetic signature, such as proximal versus distal environments. The denser rock formations could suggest the presence of lithologies with higher mineral

content or compactness or cementation, which may be indicative of specific depositional environments or sedimentary facies and post diagenetic event. Further investigation into the lithological composition and depositional history of these formations can provide valuable insights into the geological processes and depositional settings that influenced the formation of the observed rock densities.

4.3 Rock Type and Porosity-Permeability Correlation

Windland r35 equation (1) were used as a proxy to represent the texture of the limestone reservoir based on porosity and permeability value. The crossplot in Figure 4.7 and figure 20 indicating the positive correlation between grain texture and Facies Association. The limestone with a grainy texture is connected to the Inner Shoal-Shoal Facies Association (FA1) and Inner Ramp (FA2). The limestone exhibiting a mixed texture is predominantly associated with FA2 and FA3. Meanwhile, the limestone characterized by a muddy texture is primarily linked to the Middle Ramp (FA3) and FA4.

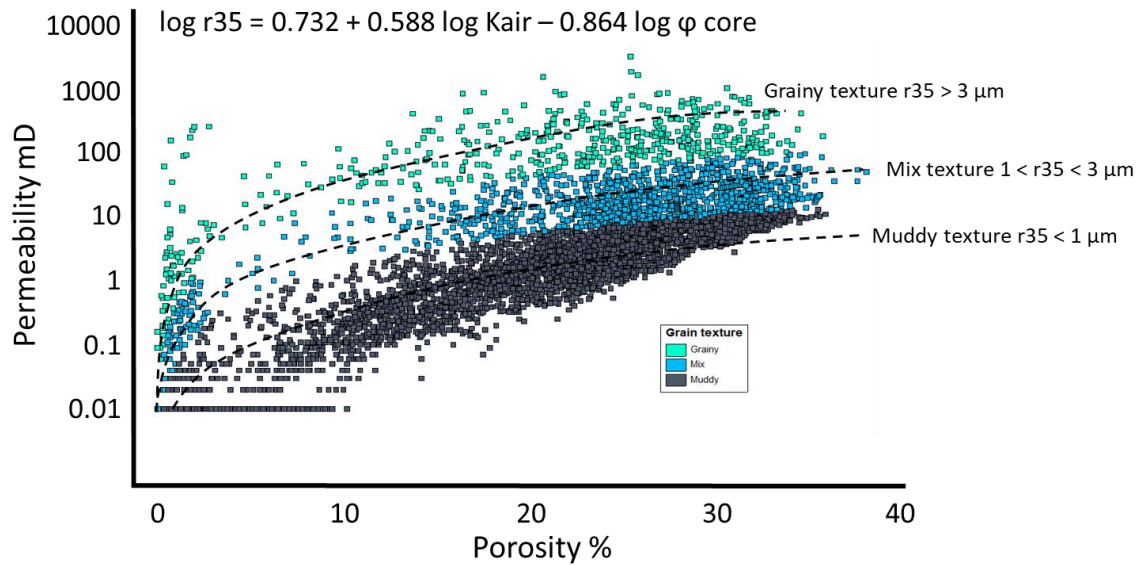


Figure 4. 7 Porosity-permeability cross-plot based on grain texture of Winland r35 (pore throat radius) cutoff.

In addition, the Facies Association scheme also reflecting similar trend that suggest shallowing-upward succession from distal to more relatively proximal facies (Fig. 4.8).

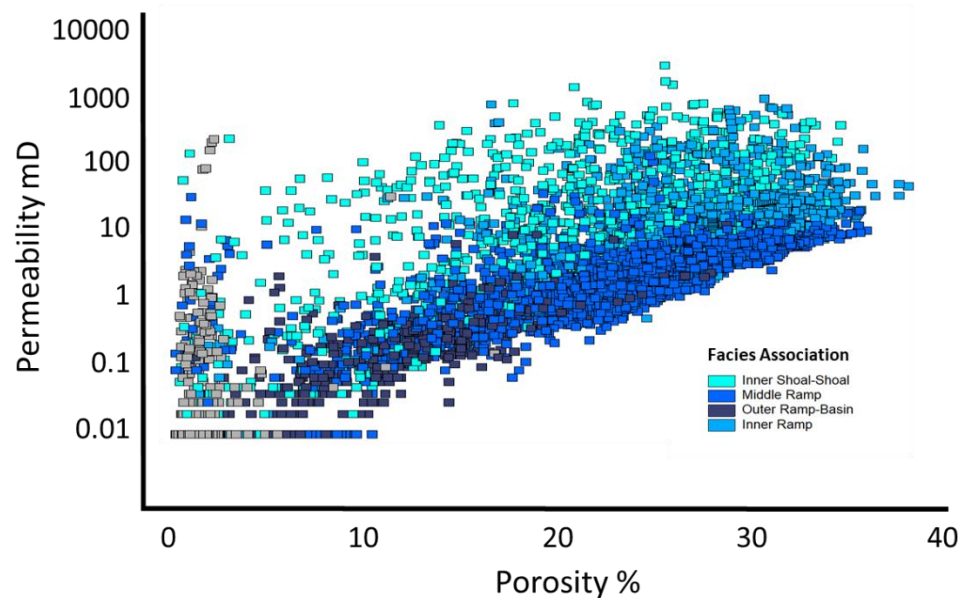


Figure 4. 8 The relationship between porosity and permeability in the Upper KharaiB reservoir has been analyzed through the interpretation of Facies Association.

The similarity between grain texture and facies scheme serves as the basis for creating a rock-type scheme based on reservoir quality derived from porosity and permeability values. Using the same equation, Winland R35, a total of 10 Rock Types were generated, as illustrated in the Figure 4.9.

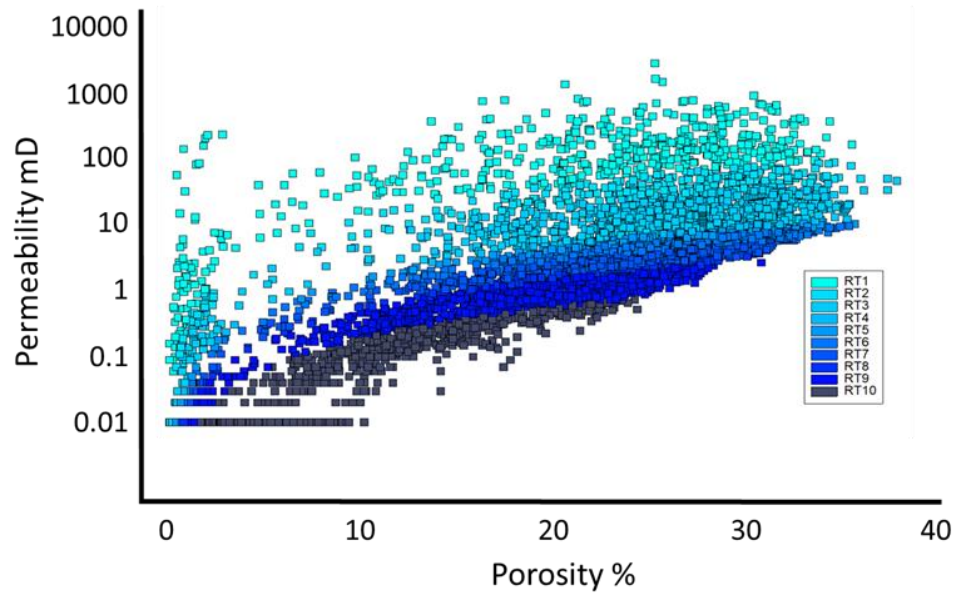


Figure 4. 9 Rock Type classification generated based on Winland R35 equation

Rock type (RT) 1 denotes the highest reservoir quality, whereas RT 10 indicates the lowest reservoir quality. Through this analysis, it is noted that the transformation of lithofacies into rock types shows a positive correlation with the Facies Association scheme.

4.4 Diagenetic Signature

As shown in Figure 4.10, the analysis indicates that a significant portion of data points with high porosity and permeability are associated with grain-dominant facies and relatively low cementation percentages. This observation suggests that these data predominantly originate from the Inner Shoal-Shoal to Inner Ramp facies association (FA1 and FA2). Conversely, data points from the Middle Ramp facies (FA3) mostly fall under mud-dominant facies, with cementation degrees ranging from low-moderate to moderate-high. Data points corresponding to the Outer Ramp facies (FA4) exhibit low porosity and permeability values and are classified as mudstone with very high cementation percentages. This mud-rich fabric is typically found in the lowermost section of the Upper Kharaiib reservoir.

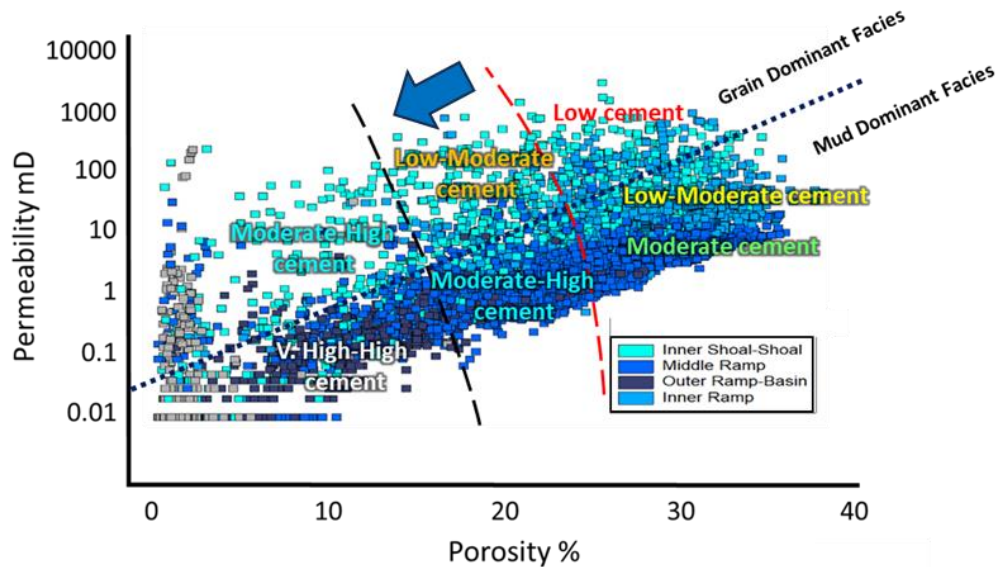


Figure 4. 10 The combination of facies grain texture, cementation level, and the porosity-permeability plot derived from FA core data is illustrated. The blue arrow indicates an increasing degree of cementation.

Our analysis highlights that the Inner shoal-shoal Facies Association shows the most ideal target for carbon storage (Table 4.2). this FA host the best reservoir properties compared to other. In addition, further assessment also shows that the middle ramp facies association could act as an additional target for storing CO₂ in this carbonate reservoir based on its laterally continuous thick succession (up to 150 ft) and moderate petrophysical properties (Ø:10-30% and K:0.1-50 mD). The injection of CO₂ will likely create and enhance the permeability of Middle Ramp facies by the processes of mineral dissolution around wellbore due to acidic character of liquid phase CO₂ in the subsurface (Middle Ramp Facies).

Carbonate Reservoir (Criteria Parameter)	Facies Association				Positive indicator
	FA1	FA2	FA3	FA4	
Upper Kharaib Reservoir					
Net Thickness (m)	8	15	30	4	The thicker the better
Depth (m)	>2000	>2000	>2000	>2000	>800 m
Porosity (%)	10-30	10-30	10-30	<10	>10%
Permeability (mD)	100-2000	10-500	0.1-10	<0.1	>100 mD
Diagenetic signature	Low cement	Low-med cement	Med-high cement	Very High cement	
Type Of Potential CO ₂ Trapping	Structural	Structural	Residual	Internal baffle	

Table 4. 2 A matrix outlining the criteria for carbon storage in the Upper Kharaib Reservoir, based on the associated lithofacies. (After Chadwick, 2008)

4.5 CO₂ Sequestration Modelling

4.5.1 Simulation Results Case 1

The model grid was established to have dimensions of 2.4 x 4 km², featuring a total thickness of 160 ft distributed uniformly across 20 layers. The reference depth was defined at -7300 ft. Each individual grid cell was sized at 300 x 300 x 8 ft. The porosity permeability distribution within the grid was designed to follow a coarsening upward pattern in the vertical direction, while remaining constant laterally (Figure 4.11).

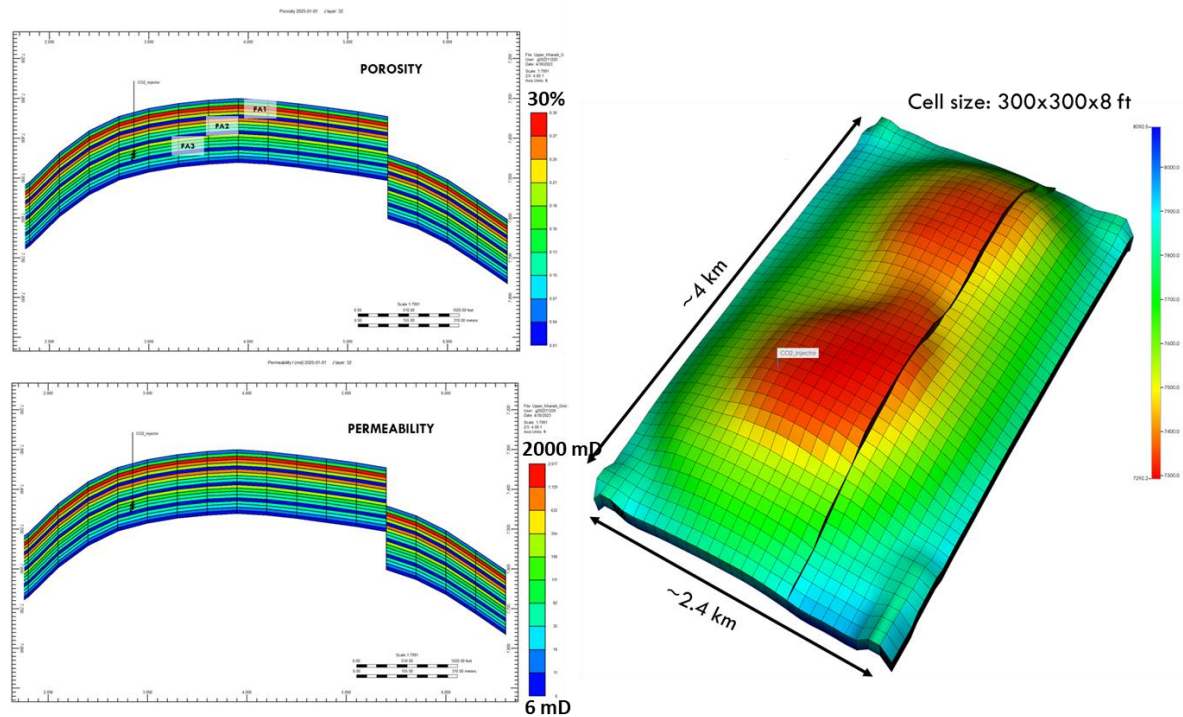


Figure 4. 11 The diagram presents a visual representation of the vertical succession in the Upper Kharaib carbonate platform, along with the model grid illustrating the arrangement of porosity distribution based on the facies association profile (red: high porosity-permeability; blue: low porosity-permeability).

4.5.1.1 CO₂ Gas Saturation

The post-injection results were monitored at various facies association levels on each perforation. After a 200-year monitoring period, the plume profile revealed the following outcomes: the maximum gas saturation, reaching approximately 0.88. The figure 24. illustrates the lateral movement of the CO₂ plume towards the crestal area following the dipping direction of the structure. The distribution of FA1 is located at the top of the geological model, resulting in a relatively short distance between the injection point and the top of the structure or seal rock.

The total amount of injected CO₂ continuous for 25 years is consistent across all injection point cases, equal to 7.88×10^9 gmole or 420 Mt of CO₂. The Lower Zone Middle Ramp FA (FA3) exhibited a predominant presence of residual trapping (indicated by the color cyan) for CO₂, whereas the Inner Shoal-Shoal FA (FA1) showcased a prevalence of structural trapping (indicated by the color red) at the crestal point. The Upper Ramp FA (FA2) demonstrated an intermediate scenario, with a combination of residual trapping and a slight dominance of structural trapping for CO₂ (Fig. 4.12).

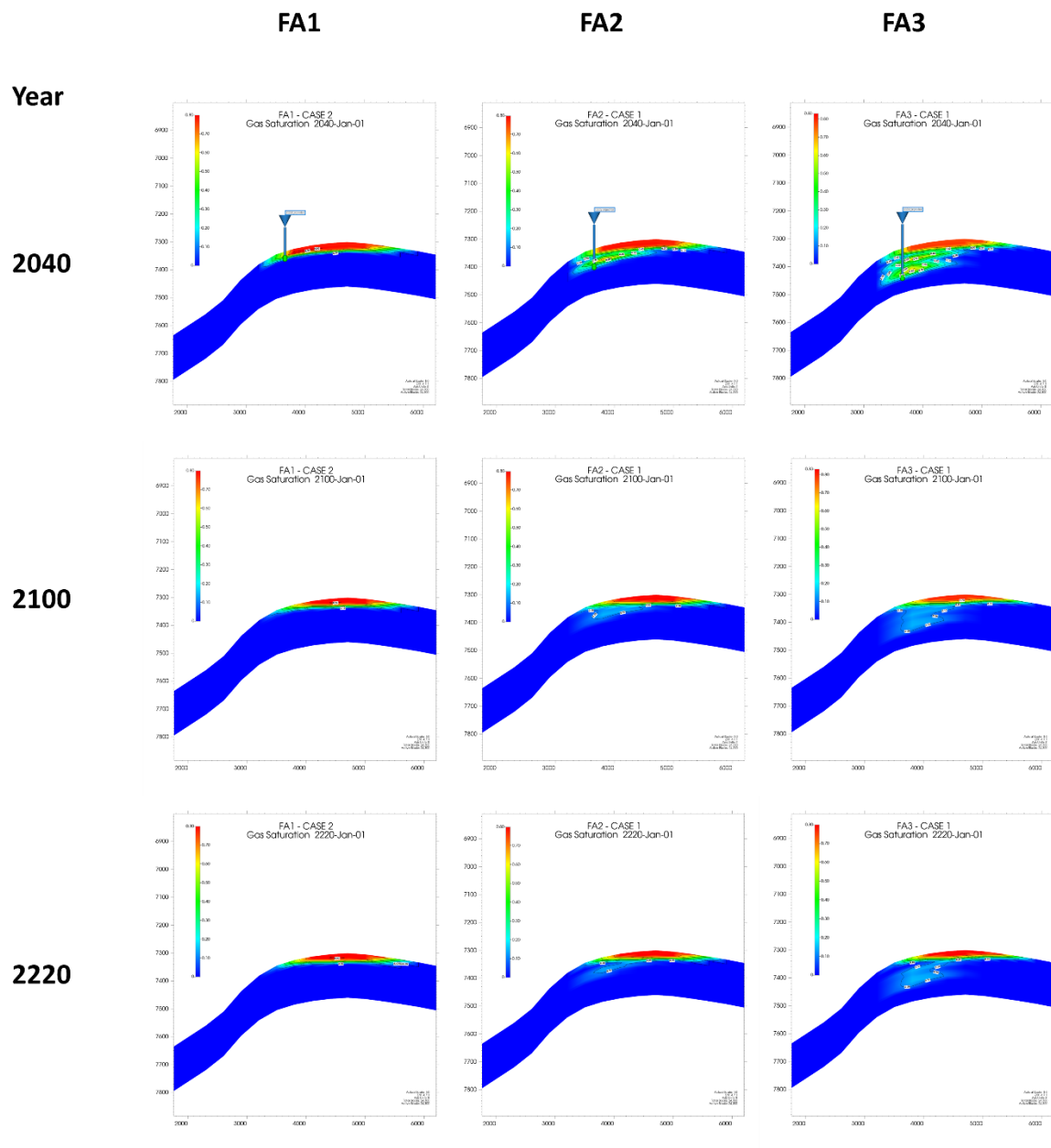


Figure 4. 12 The disparity in CO₂ gas saturation profile posts the injection in each Facies Association – Case 1.

4.5.1.2 Mineral (Calcite) Dissolution

The three injection point cases illustrate the occurrence of calcite dissolution both during and after CO₂ injection. At each injection point, the maximum values of calcite dissolution (gmole) or mineral mole changes are FA1= -2.57e^8 , FA2= -3.27e^8 , and FA3= -3.6e^8 .

The Figure 4.13 demonstrates a comparison of dissolution distribution patterns in cross-section. These distribution patterns reveal the extent of dissolution reaching towards both the crestal and down flank directions from the injection well.

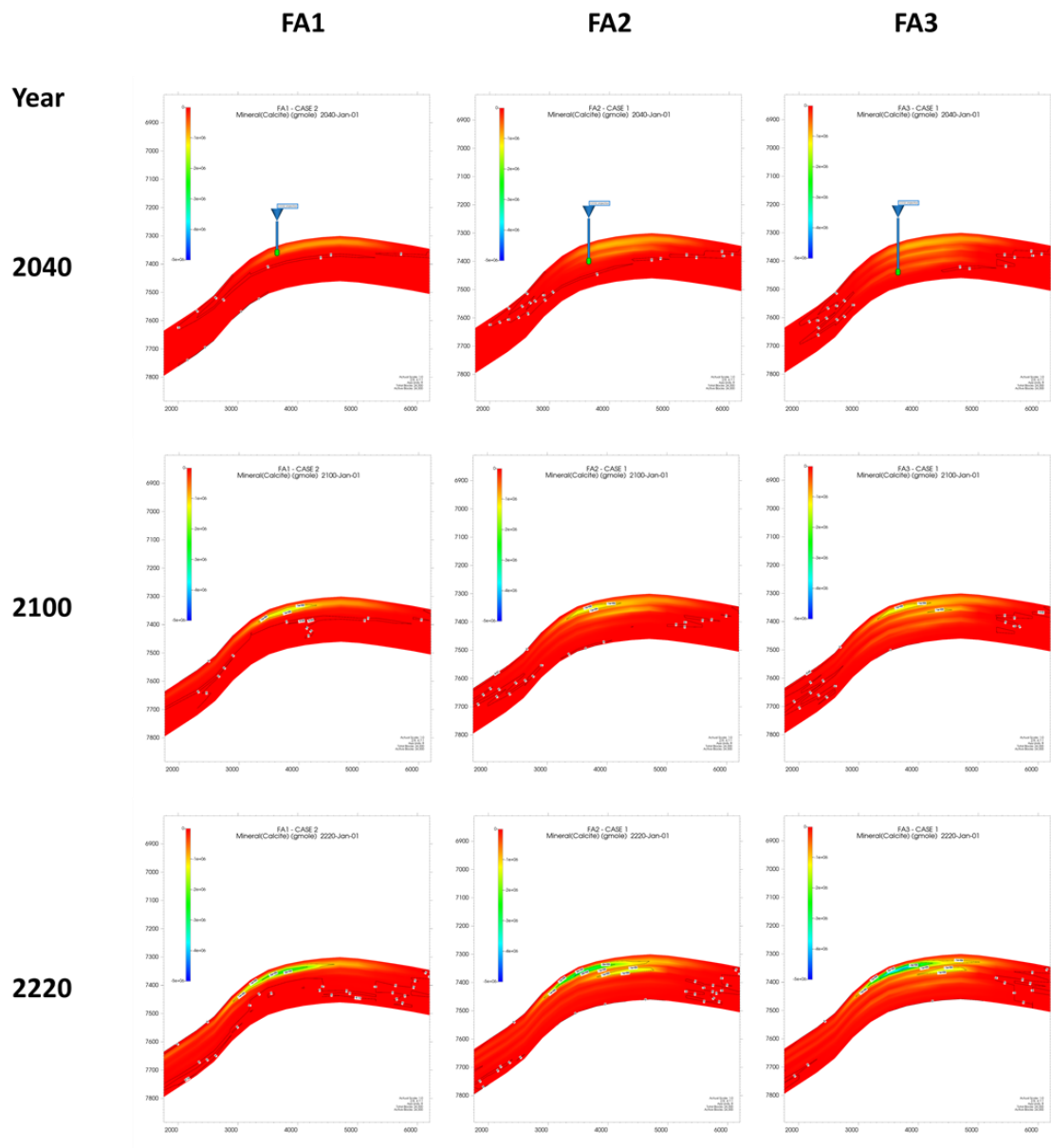


Figure 4. 13 The disparity effect in calcite dissolution posts the injection in each Facies Association – Case 1.

4.5.1.3 Effect on pH and CO₂ dissolved in brine

The initial pH value in the reservoir stands at 7.5. Typically, CO₂ injection, both during and after the process, leads to a decrease in the pH value. Over a monitoring period of 200 years, FA1 exhibits a pH profile around 6 at the crestal area and between 6.5 to 7 in the flank region. FA2, on the other hand, presents the lowest pH value recorded at 5.8, with a predominant pH of 6 from the crestal region extending down to the middle and lower parts of the reservoir around the well injector. This region is enveloped by pH values ranging from 6.5 to 7 in the outer ring. FA3 showcases a similar trend to FA2 with the lowest recorded pH value at 5.6; however, it demonstrates a broader and lower distribution compared to the former two cases, as illustrated in Figure 4.14.

Comparing the injection results, FA3 demonstrates a more pronounced impact on the lateral and vertical distribution of lower pH levels compared to FA1 and FA2. Water mole fraction of CO₂, or CO₂ dissolved in brine, is depicted below for all three cases. The maximum fraction of CO₂ dissolved in brine reaches 1.1%. Similar to the pH profile, FA3 exhibits a broader and wider distribution around the crestal and down flank regions of the reservoir (Fig. 4.15).

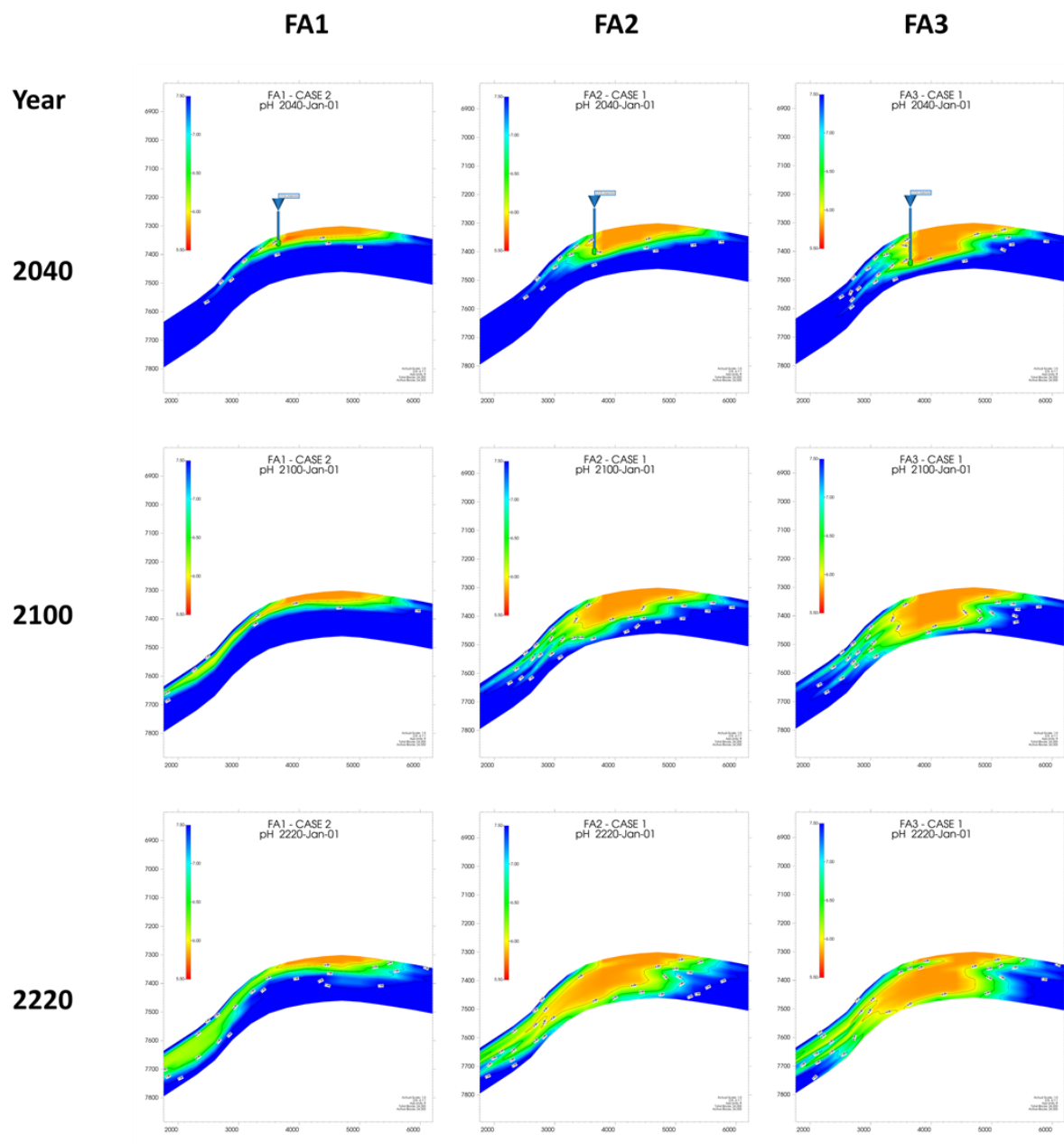


Figure 4. 14 The disparity effect in pH profile posts the injection in each Facies

Association – Case 1

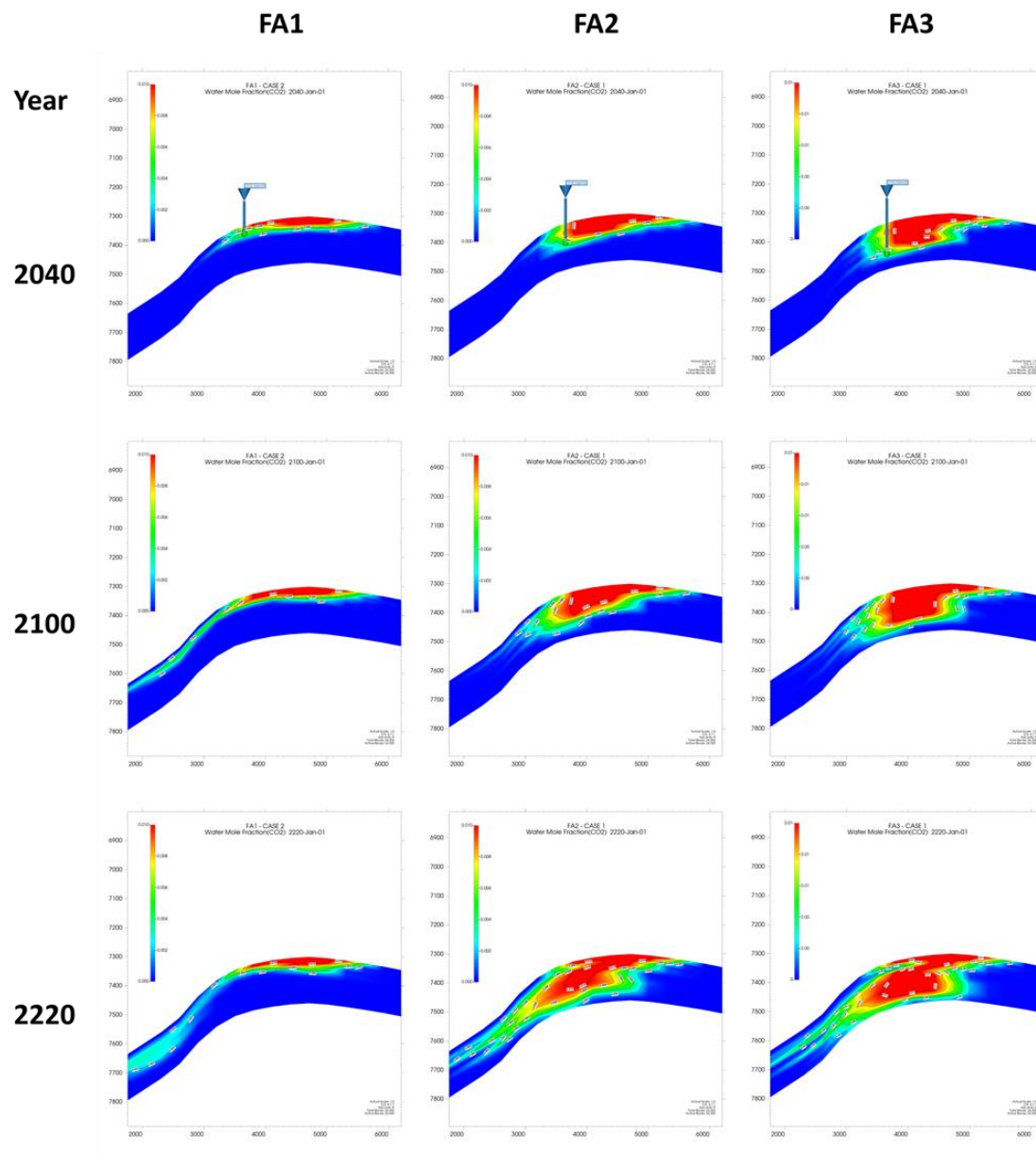


Figure 4. 15 The disparity effect in CO₂-dissolved posts the injection in each Facies

Association – Case 1

4.5.1.4 Trapping Mechanism Profile

All three cases demonstrate that the predominant form of CO₂ trapping is structural or supercritical trapping. The highest recorded values of CO₂ in the supercritical state, in terms of mole, are 7.57e⁹ in FA1, 7.48e⁹ in FA2, and 7.41e⁹ in FA3. Additionally, the maximum values of dissolved CO₂ are 3.07e⁸ in FA1, 4.2e⁸ in FA2, and 4.95e⁸ in FA3.

Mineral trapping is evidenced by negative values across all three cases, indicating ongoing mineral dissolution. At the conclusion of the year-long monitoring period, FA3 exhibits the highest dissolution value in mole at -3.72e⁸, followed by FA2 at -3.38e⁸, and FA1 at -2.66e⁸.

When comparing the injection cases individually for each category of CO₂ trapping mechanism, as indicated in the table below (Table 4.3), across all three injection cases, there is a consistent trend of decreasing structural trapping by approximately 2% from the year 2050 to 2220. Concurrently, mineral dissolution shows a 2% increase, residual trapping decreases by 1% in FA1 and 2% in FA2 and FA3, while dissolution trapping increases by 1% in FA1 and FA2, and by 2% in FA3 during this period.

FA1 – CASE 1				
Year	Trapping Mechanism (%)			
	Structural	Mineral	Residual	Dissolved
2050	89.37	-1.47	6.47	2.69
2100	88.52	-1.94	6.44	3.1
2220	87.71	-3.19	5.42	3.68

FA2 – CASE 1				
Year	Trapping Mechanism (%)			
	Structural	Mineral	Residual	Dissolved
2050	86.65	-1.79	8.2	3.36
2100	85.55	-2.36	8.16	3.93
2220	84.56	-3.99	6.49	4.96

FA3 – CASE 1				
Year	Trapping Mechanism (%)			
	Structural	Mineral	Residual	Dissolved
2050	84.8	-2.04	9.32	3.84
2100	83.15	-2.72	9.45	4.68
2220	82.28	-4.35	7.59	5.78

Table 4. 3 Comparison of trapping mechanism percentages between injection points FA1, FA2, and FA3, along with their evolution over time.

Furthermore, upon comparing the data at the end of the 2220 monitoring period, the discrepancy in structural trapping shows a 5% decrease in FA3 compared to FA1, and a 3% decrease in FA2 compared to FA1. Regarding mineral dissolution, FA3 exhibits a 1.3% higher rate compared to FA1, while FA2 shows a 1% increase relative to FA1. Residual trapping displays a 2% increase in FA3 compared to FA1 and a 1% increase in FA2 relative to FA1. Additionally, dissolution trapping demonstrates a 2% increase in CO₂ dissolution in FA3 compared to FA1, and a 1.3% increase in FA2 relative to FA1. For better

visualization, below is the graph comparison in trapping mechanism between FA1, FA2 and FA3 (Figure 4.16).

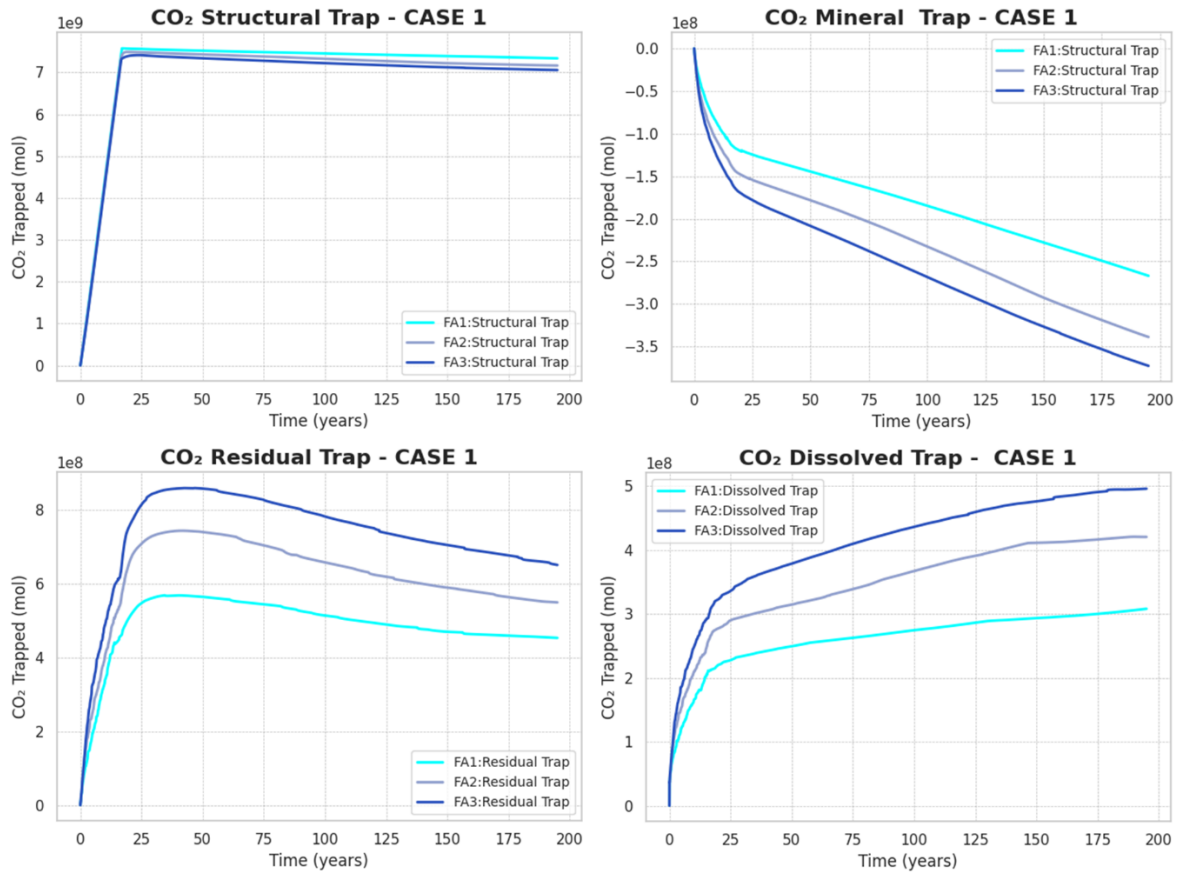


Figure 4. 16 A graphical representation illustrating the comparison of each trapping mechanism among FA1, FA2, and FA3.

4.5.2 Simulation Results Case 2

The model grid configuration mirrored that of Case 1, with the sole variation lying in the horizontal permeability value of the dense/baffle zone or layers, set at 0.1 mD. This adjustment was made deliberately to investigate the sensitivity of the system and evaluate its implications on the migration pattern of the plume.

4.5.2.1 CO₂ Gas Saturation

The post-injection results were monitored at various facies association levels on each perforation. After a 200-year monitoring period, the plume profile revealed the following outcomes: the maximum gas saturation, reaching approximately 0.88. The figure below illustrates the lateral movement of the CO₂ plume towards the crestal area following the dipping direction of the structure.

The total injected CO₂ volume remains consistent over the 25-year period across all injection points, totaling 1.16×10^{10} gmole or 420 Mt of CO₂. Within the Middle Ramp FA (FA3), residual trapping is notably prevalent (indicated by cyan-green colour), while in the Inner Shoal-Shoal FA (FA1), structural trapping is more prominent (indicated by red) at the crestal point. The Upper Ramp FA (FA2) shows an intermediate scenario, with both residual trapping and a slight dominance of structural trapping observed for CO₂ (Fig. 4.17).

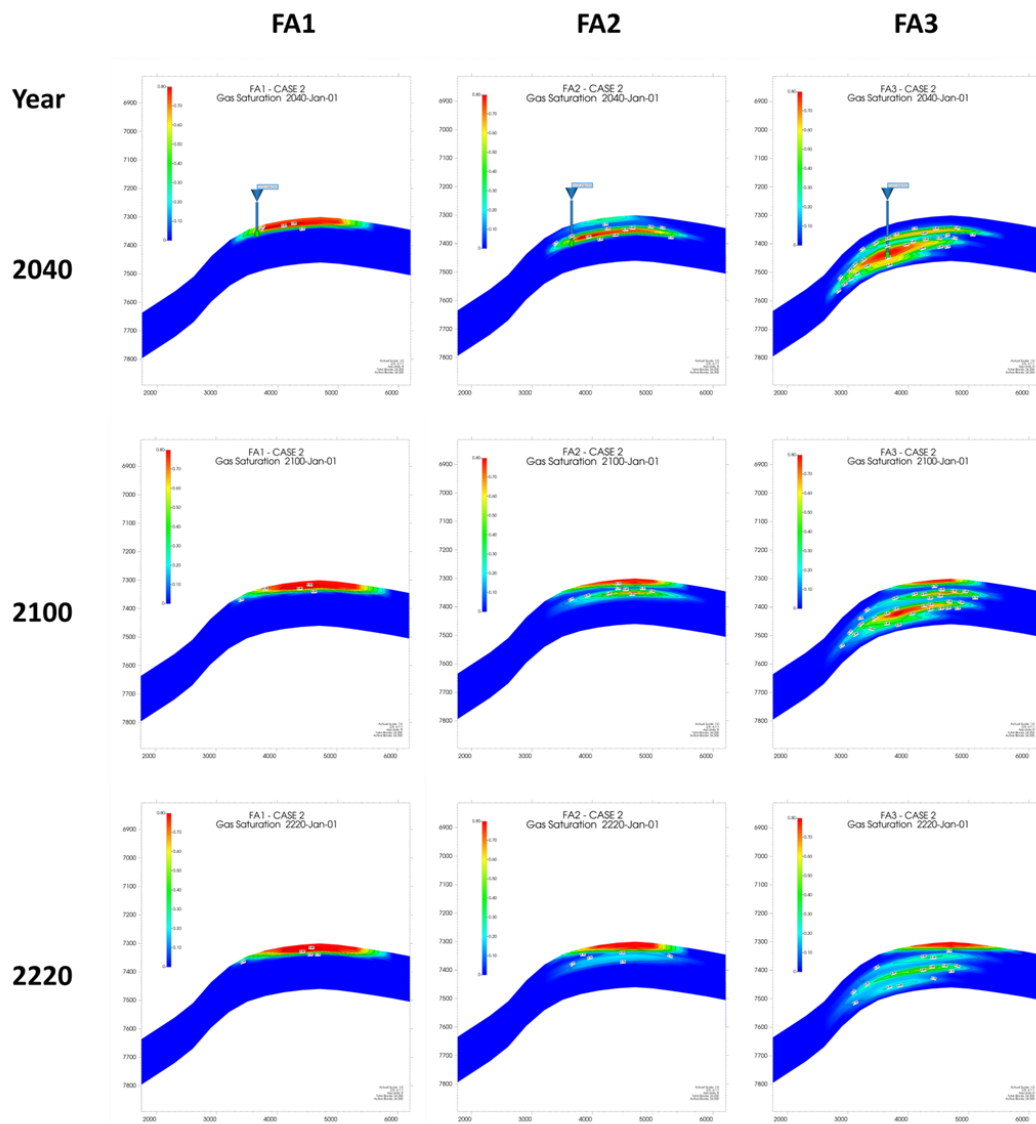


Figure 4. 17 The disparity in CO₂ gas saturation profile posts the injection in each Facies Association – Case 2.

4.5.2.2 Calcite mineral Dissolution

In all three injection scenarios, calcite dissolution is evident during and after CO₂ injection. The greatest levels of calcite dissolution or alterations in mineral moles are

recorded at each injection point as follows: FA1 = $-1.25e^8$, FA2 = $-2.49e^8$, and FA3 = $-2.71e^8$ calcite gmole.

The Figure 4.18 presents a contrast of dissolution distribution patterns in a cross-sectional view. These patterns unveil the reach of dissolution extending in both crestal and down flank directions from the injection well.

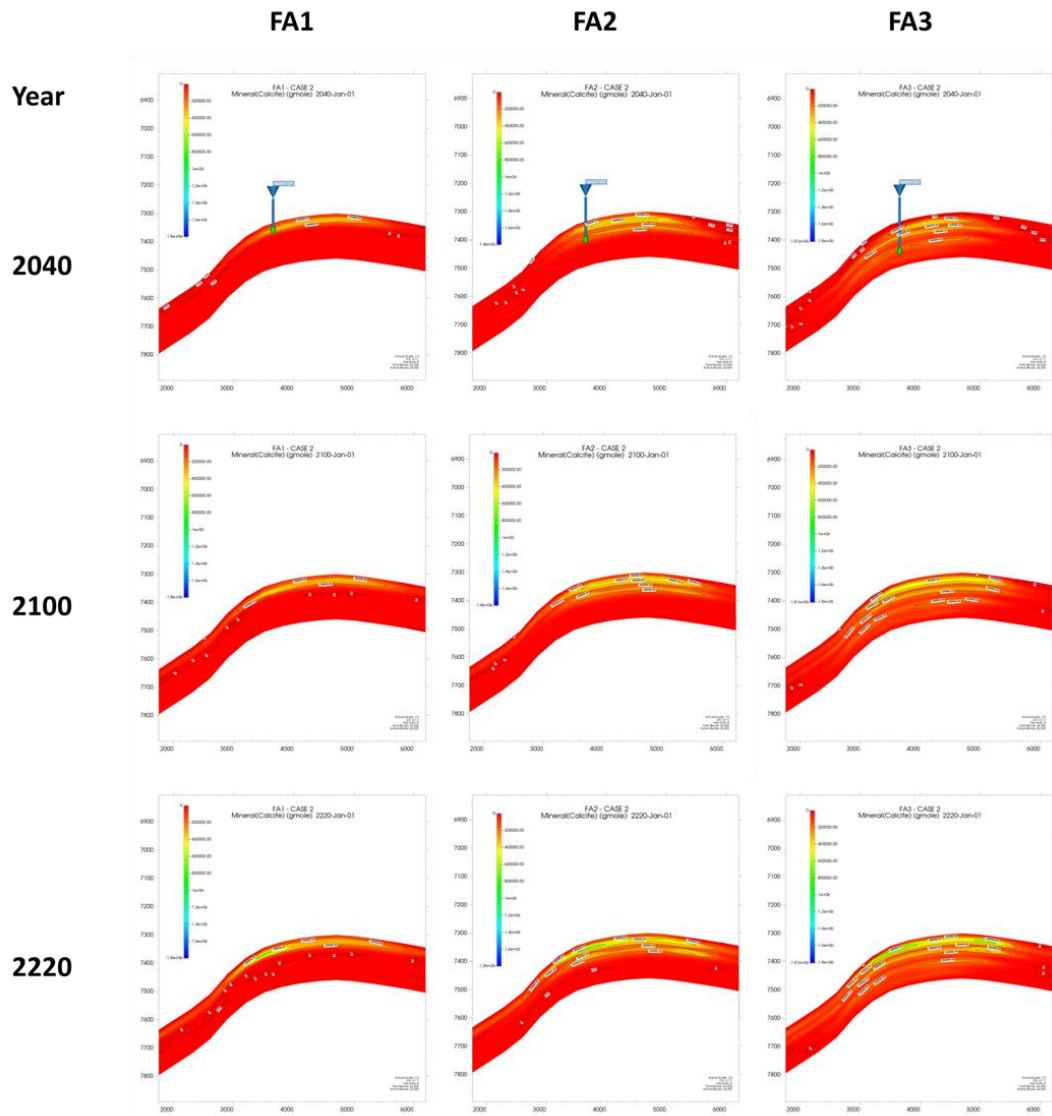


Figure 4. 18 The disparity effect in calcite dissolution posts the injection in each Facies Association - Case 2.

4.5.2.3 Effect on pH and CO₂ dissolved in brine

The reservoir's initial pH level is measured at 7.5. Upon CO₂ injection, both during and after the process, there is a noticeable decline in pH. Over a 200-year monitoring period, the pH profiles for FA1 indicate values around 5.3 at the crestal area and between 5.6 to 6 in the flank region. Similarly, FA2 shows a minimum pH value of 5.36, with a prevailing pH range of 5.5 to 6 extending from the crestal to the lower parts of the reservoir around the injection well. FA3 follows a comparable pattern to FA2, with the lowest recorded pH value also at 5.3. However, FA3 exhibits a more significant impact on both lateral and vertical pH distribution compared to FA1 and FA2, as depicted in Figure 4.19.

The water mole fraction of CO₂, or CO₂ dissolved in brine, is illustrated below for all three cases. The maximum fraction of CO₂ dissolved in brine reaches 2.5%. Consistent with the pH profiles, FA3 demonstrates a broader and more extensive distribution around both the crestal and down flank regions of the reservoir (Figure 4.20). This suggests that the injection of CO₂ in FA3 results in a more widespread dissolution and interaction with the brine compared to the other injection points.

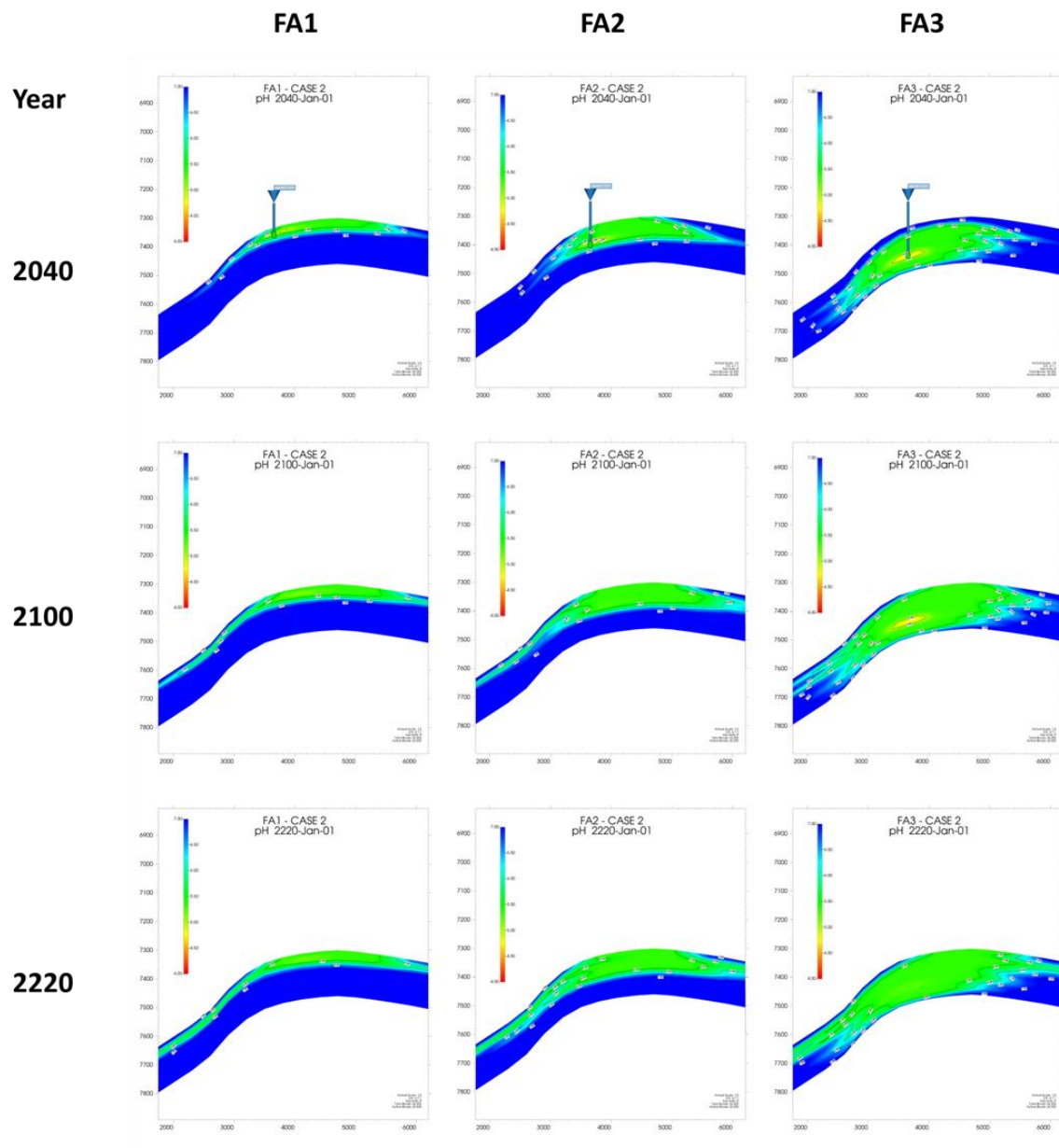


Figure 4. 19 The variation in pH profiles observed after injection in each Facies Association - Case 2.

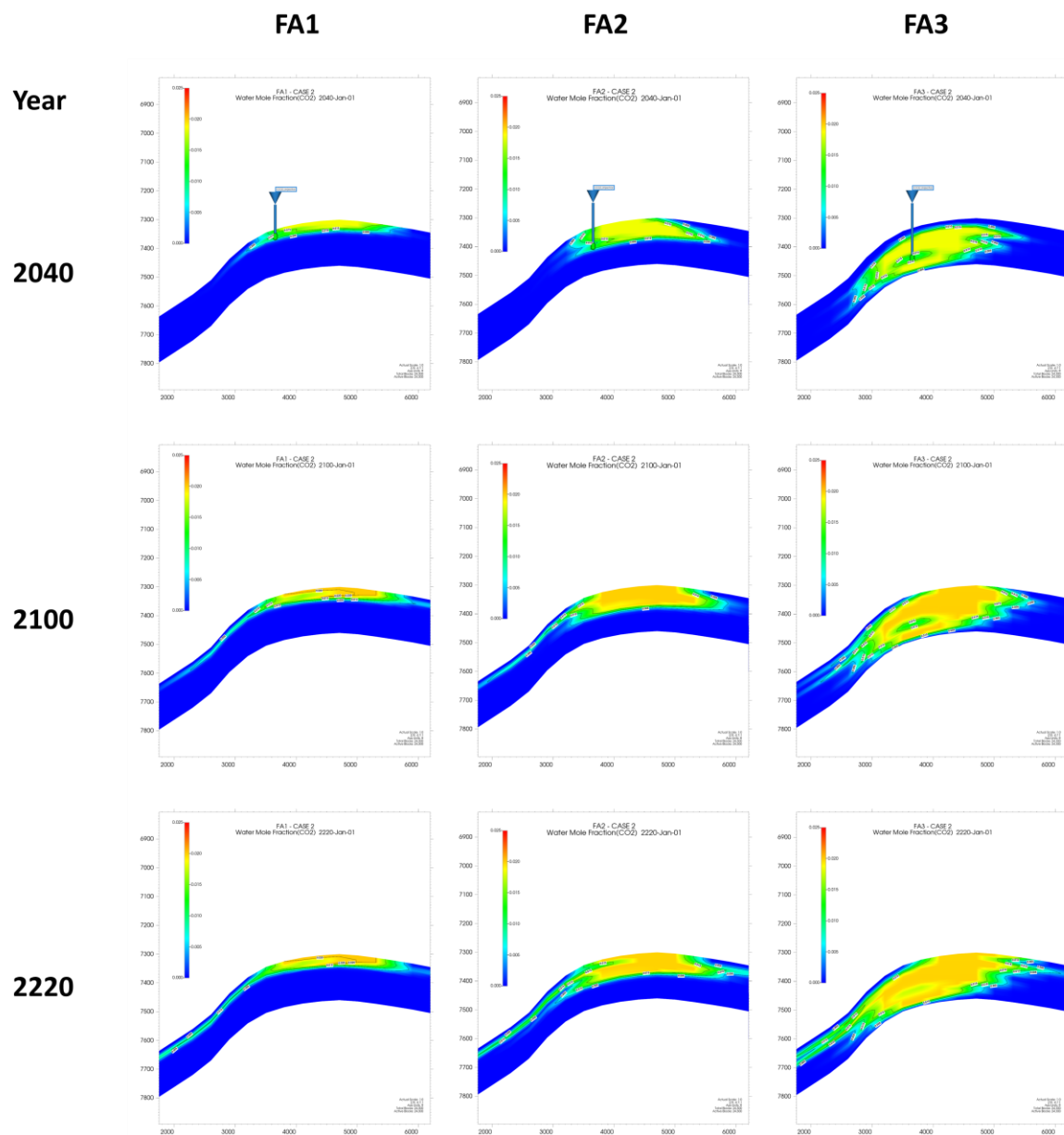


Figure 4. 20 The disparity effect in CO₂-dissolved posts the injection in each Facies

Association – Case 2

4.5.2.4 CO₂ Trapping Mechanism Profile

In all three scenarios, structural or supercritical trapping prevails as the primary form of CO₂ entrapment. The maximum recorded quantities of CO₂ in the supercritical phase are 1.1e^{10} mol in FA1, 1.02e^{10} mol in FA2, and 1.01e^9 mol in FA3. Moreover, the highest levels of dissolved CO₂ are observed at 0.82e^9 mol in FA1, 2.01e^9 mol in FA2, and 2.36e^9 mol in FA3.

Evidence of mineral trapping is indicated by negative values across all cases, signifying ongoing mineral dissolution. At the conclusion of the year-long monitoring period, FA3 demonstrates the highest dissolution value at -1.33e^8 mol, followed by FA2 at -2.61e^8 mol, and FA1 at -2.85e^8 mol.

For a detailed comparison of CO₂ trapping mechanisms within each injection scenario, please refer to the comprehensive breakdown provided in the following Table 4.4.

The data presented in the table above highlights a consistent trend of decreasing structural trapping over the years. Specifically, there is an approximate 2.8% decrease in structural trapping from the year 2050 to the year 2220 in FA1, an 11% decrease in FA2, and a 15.5% decrease in FA3. Meanwhile, mineral dissolution shows a slight increase of 0.4% in FA1 and a 0.8% increase in both FA2 and FA3. Residual trapping sees an increase of 0.8% in FA1, 5.8% in FA2, and 9% in FA3, while dissolution trapping increases by 1% in both FA1 and FA2, and by 2% in FA3 during this period.

FA1 - CASE 2				
Year	Trapping Mechanism (%)			
	Structural	Mineral	Residual	Dissolved
2050	88.87	-0.63	5.51	4.99
2100	86.96	-0.76	6.65	5.63
2220	86.03	-1.07	6.34	6.56

FA2 - CASE 2				
Year	Trapping Mechanism (%)			
	Structural	Mineral	Residual	Dissolved
2050	78.77	-1.08	9.96	10.20
2100	70.71	-1.34	15.67	12.28
2220	67.83	-1.88	15.76	14.53

FA3 - CASE 2				
Year	Trapping Mechanism (%)			
	Structural	Mineral	Residual	Dissolved
2050	78.11	-1.12	10.14	10.63
2100	67.34	-1.45	17.58	13.64
2220	62.55	-1.97	19.13	16.35

Table 4. 4 Comparison of trapping mechanism percentages between injection points FA1, FA2, and FA3, along with their evolution over time.

Comparing the data at the end of the year 2220 monitoring period, there is a 5% reduction in structural trapping in FA3 compared to FA1, and a 3% reduction in FA2 compared to FA1. In terms of mineral dissolution, FA3 exhibits a 1.3% higher dissolution compared to FA1, while FA2 shows a 1% higher dissolution relative to FA1. Residual trapping indicates a 2% higher residual in FA3 compared to FA1 and a 1% higher residual in FA2 relative to FA1. Additionally, dissolution trapping demonstrates a 2% higher CO₂ dissolution in FA3 compared to FA1, and a 1.3% higher dissolution in FA2 relative to FA1. For a clearer

visualization, the graph below illustrates the comparison in trapping mechanisms between FA1, FA2, and FA3 (Figure 4.21).

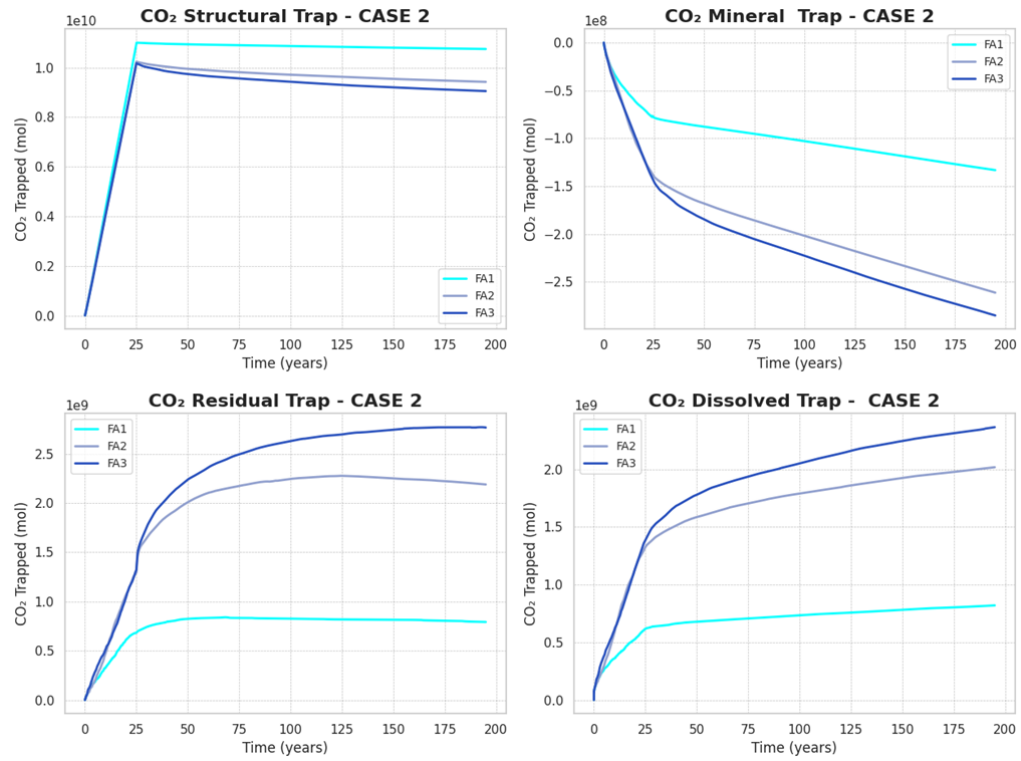


Figure 4. 21Figure 33. A graphical representation illustrating the comparison of each trapping mechanism among FA1, FA2, and FA3 – Case 2.

4.5.3 Simulation Results Case 3

4.5.3.1 3D Geological Grid Model

The model grid was established to have dimensions of 8 x 10 km², featuring average thickness of 165.7 ft and distributed by 3D structural framework modelling and based on well marker and consist of total 26 layers (Fig. 4.22). The reference depth was defined at - 7700 ft. Each individual grid cell was sized at 650 x 650 ft. The rock type distribution was modelled by facies modelling using Truncated Gaussian Simulation (TGS) while porosity-permeability distribution within the grid was modelled by 3D property modelling using SGS or Sequential Gaussian Simulation technique in order to get smooth gradation distribution both lateral vertical variation (Figure 4.23 and Figure 4.24).

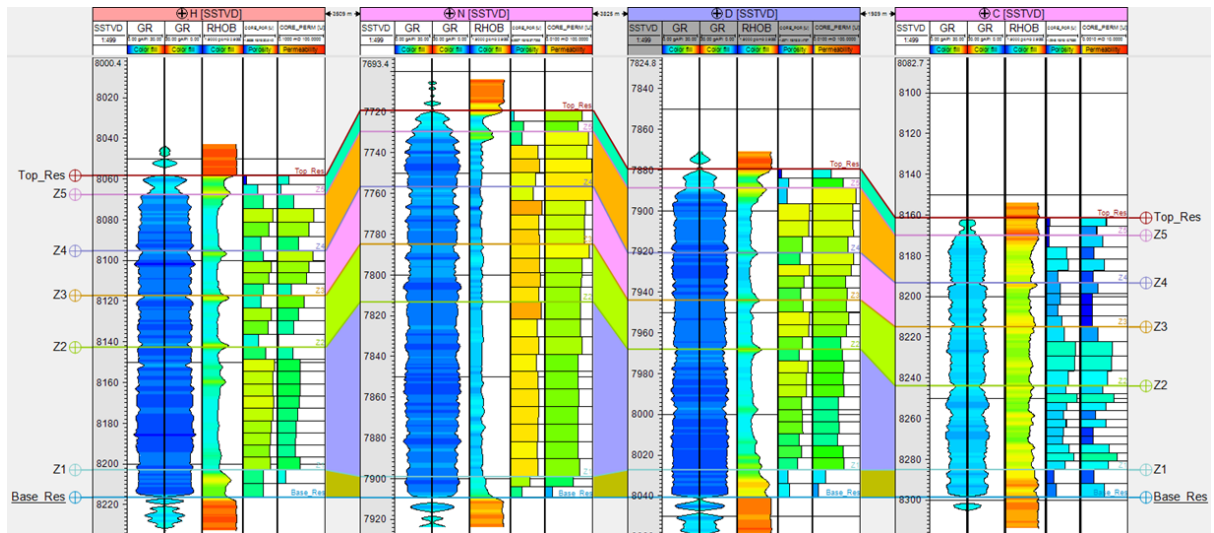


Figure 4. 22 Representation of the well marker and reservoir zone within the reservoir interval, alongside the upscaled logs of core porosity and permeability.

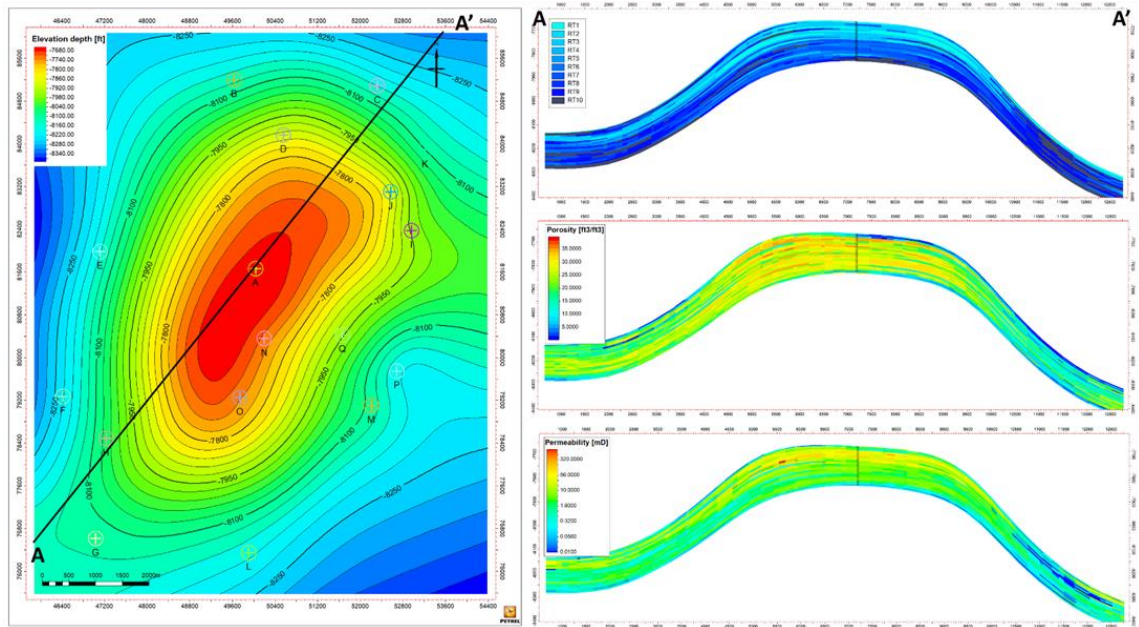


Figure 4. 23 The Grid Structural Map and a section of distributed Rock Type, Porosity, and Permeability profile.

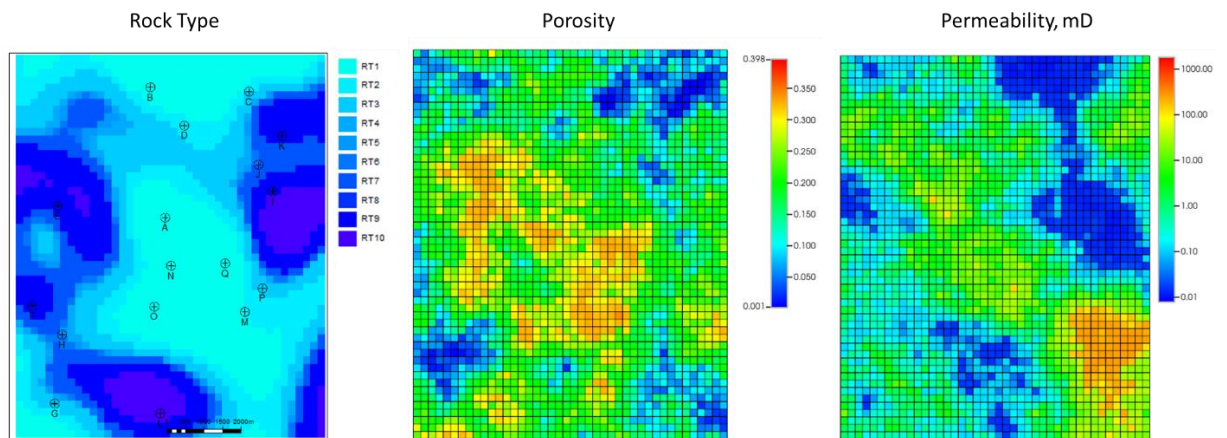


Figure 4. 24 An example displaying the spatial distribution of Rock Type, Porosity, and Permeability obtained through 3D facies and property modelling in a map view.

The histogram of Rock-Type (RT), porosity and permeability show a reasonable match between raw well logs, upscaled logs and the overall grid model and the differences are less than 5% (Fig. 4.25). In the overall model, the predominant percentages for RT are RT9, RT3, RT6, and RT7, with average porosity and permeability values of 0.2 and 10 mD respectively.

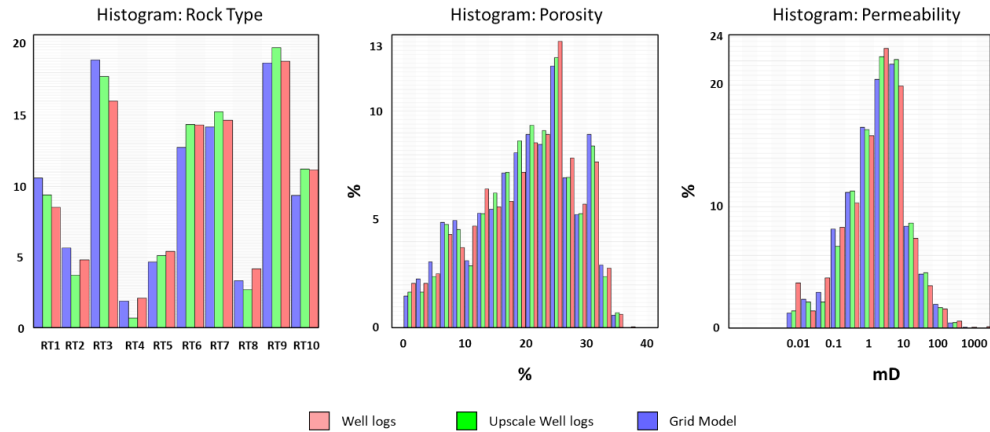


Figure 4. 25 The histograms of Rock-Type, Porosity, and Permeability in comparison between well logs, upscaled well logs and overall grid model.

Unlike cases 1 and 2, in case 3, due to the 3D distribution of its properties, the well placement for each injection scenario is different, as depicted in the image below (Figure 4.26).

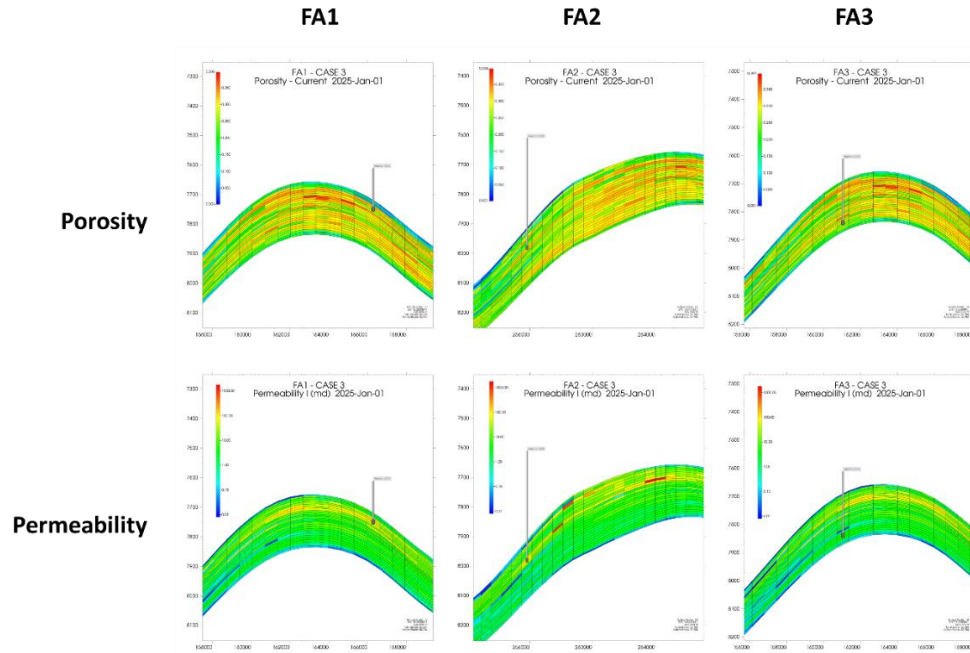


Figure 4. 26 Porosity and permeability profile around injection point cases based on
Facies Association and Rock Type

4.5.3.2 CO₂ Gas Saturation

The post-injection results were monitored at various facies association levels on each perforation. After a 200-year monitoring period, the plume profile revealed the following outcomes: the maximum gas saturation, reaching approximately 0.88. The figure below illustrates the lateral movement of the CO₂ plume towards the crestal area following the dipping direction of the structure. The distribution of FA1 is located at the top of the geological model, resulting in a relatively short distance between the injection point and the top of the structure or seal rock.

The total amount of injected CO₂ continuous for 25 years is consistent across all injection point cases, equal to 1.16e10 gmole or 420 Mt of CO₂. The Middle Ramp FA (FA3)

exhibited a predominant presence of residual trapping (indicated by the color cyan) for CO₂, whereas the Inner Shoal-Shoal FA (FA1) showcased a prevalence of structural trapping (indicated by the color red) at the crestal point. The Upper Ramp FA (FA2) demonstrated an intermediate scenario, with a combination of residual trapping and a slight dominance of structural trapping for CO₂ (Fig. 4.27).

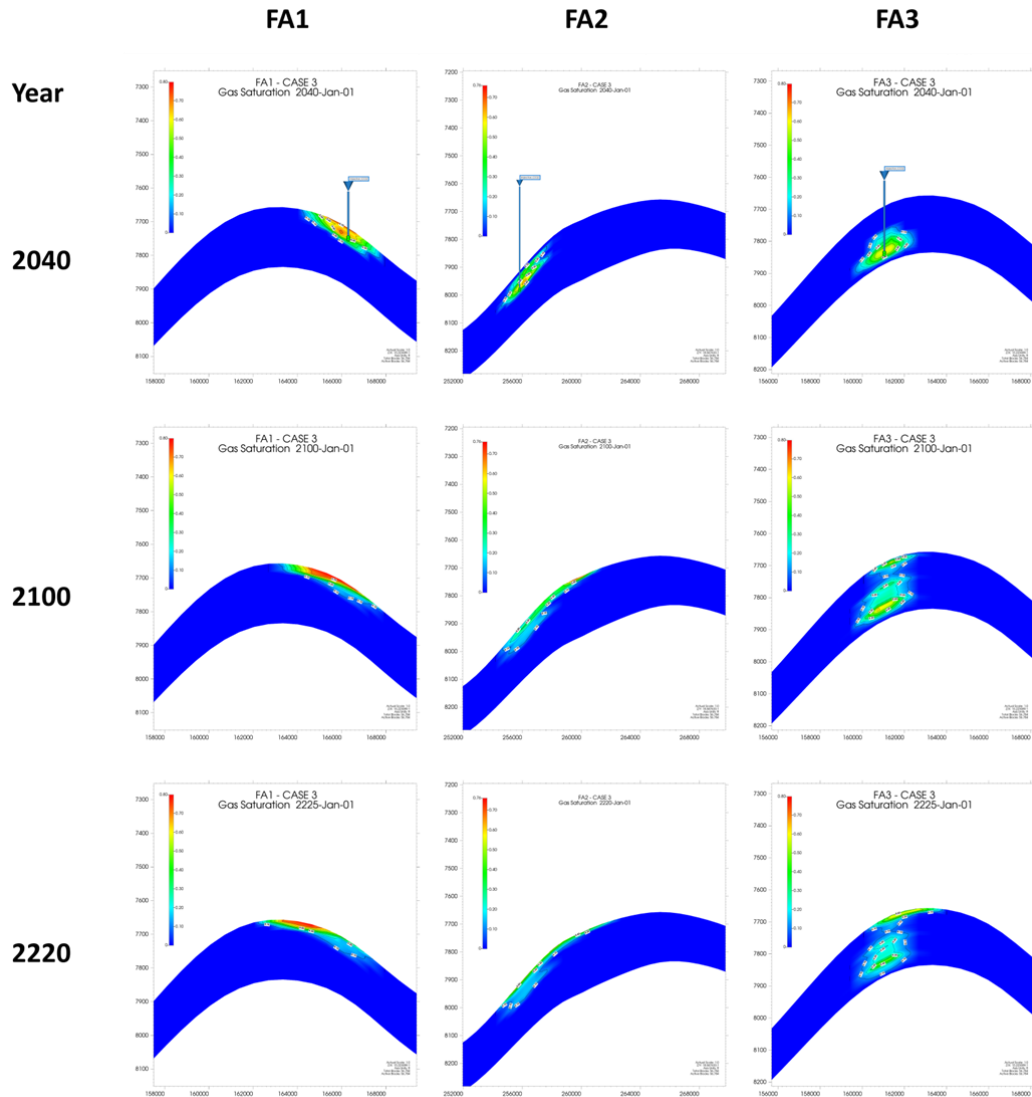


Figure 4. 27 The disparity in CO₂ gas saturation profile posts the injection in each Facies Association – Case 3.

4.5.3.3 Calcite mineral Dissolution

The three injection point cases illustrate the occurrence of calcite dissolution both during and after CO₂ injection. At each injection point, the maximum values of calcite dissolution (gmole) or mineral mole changes are FA1= -2.57e⁸, FA2= -3.27e⁸, and FA3= -3.6e⁸.

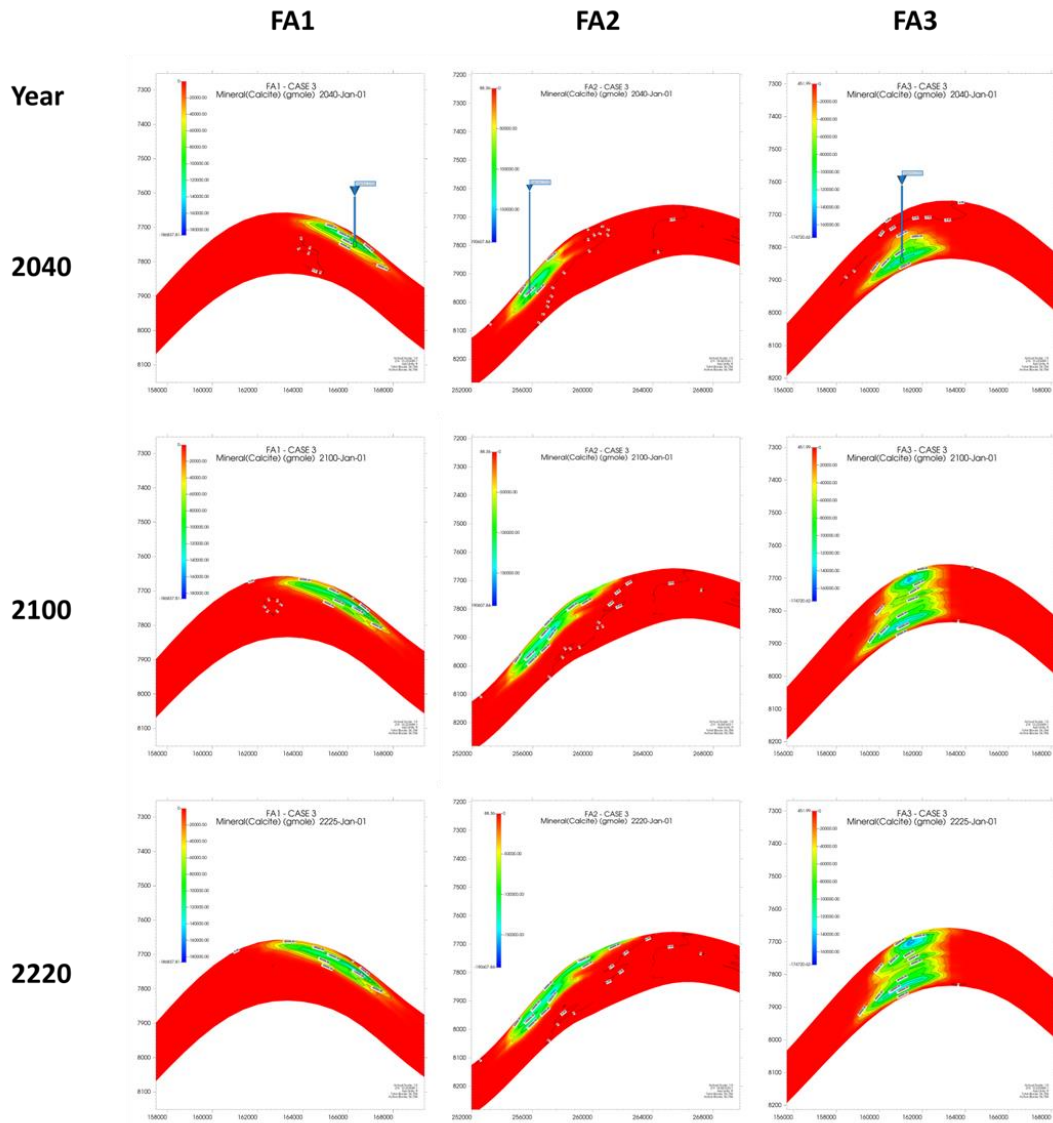


Figure 4. 28 The disparity effect in calcite dissolution posts the injection in each Facies Association – Case 3.

The Figure 4.28 demonstrates a comparison of dissolution distribution patterns in cross-section. These distribution patterns reveal the extent of dissolution reaching towards both the crestal and down flank directions from the injection well.

4.5.3.4 CO₂ dissolved in brine

Comparing the results, CO₂ injection in FA3 or low-quality Rock Type demonstrates a more pronounced impact on the lateral and vertical distribution of lower pH levels compared to FA1 and FA2. Water mole fraction of CO₂, or CO₂ dissolved in brine, is depicted below for all three cases. The maximum fraction of CO₂ dissolved in brine reaches 2.5%. in general, FA3 exhibits a broader and wider distribution around the crestal and down flank regions of the reservoir (Fig. 4.29).

4.5.3.5 CO₂ Trapping Mechanism Profile

All three cases demonstrate that the predominant form of CO₂ trapping is structural or supercritical trapping. The highest recorded values of CO₂ in the supercritical state are 1.05e10 mol of CO₂ in FA1, 0.96e⁹ mol of CO₂ in FA2, and 0.97e⁹ mol of CO₂ in FA3. Additionally, the maximum values of dissolved CO₂ are 2.92e⁹ mol in FA1, 4.38e⁹ mol in FA2, and 4.14e⁹ mol in FA3. Maximum values of residual trapping from the simulation are 2.77E⁹ mol in FA1, 4.85e⁹ mol in FA2, and 5.06e⁹ mol in FA3.

Like in Case 1 and Case 2, in Case 3 the mineral trapping is evidenced by negative values across all three cases, indicating ongoing mineral dissolution. At the end of the year-long monitoring period, FA3 exhibits the highest dissolution value at $-2.74e^7$ mol, followed by FA2 at $-3.17e^7$ mol, and FA1 at $-1.97e^7$ mol.

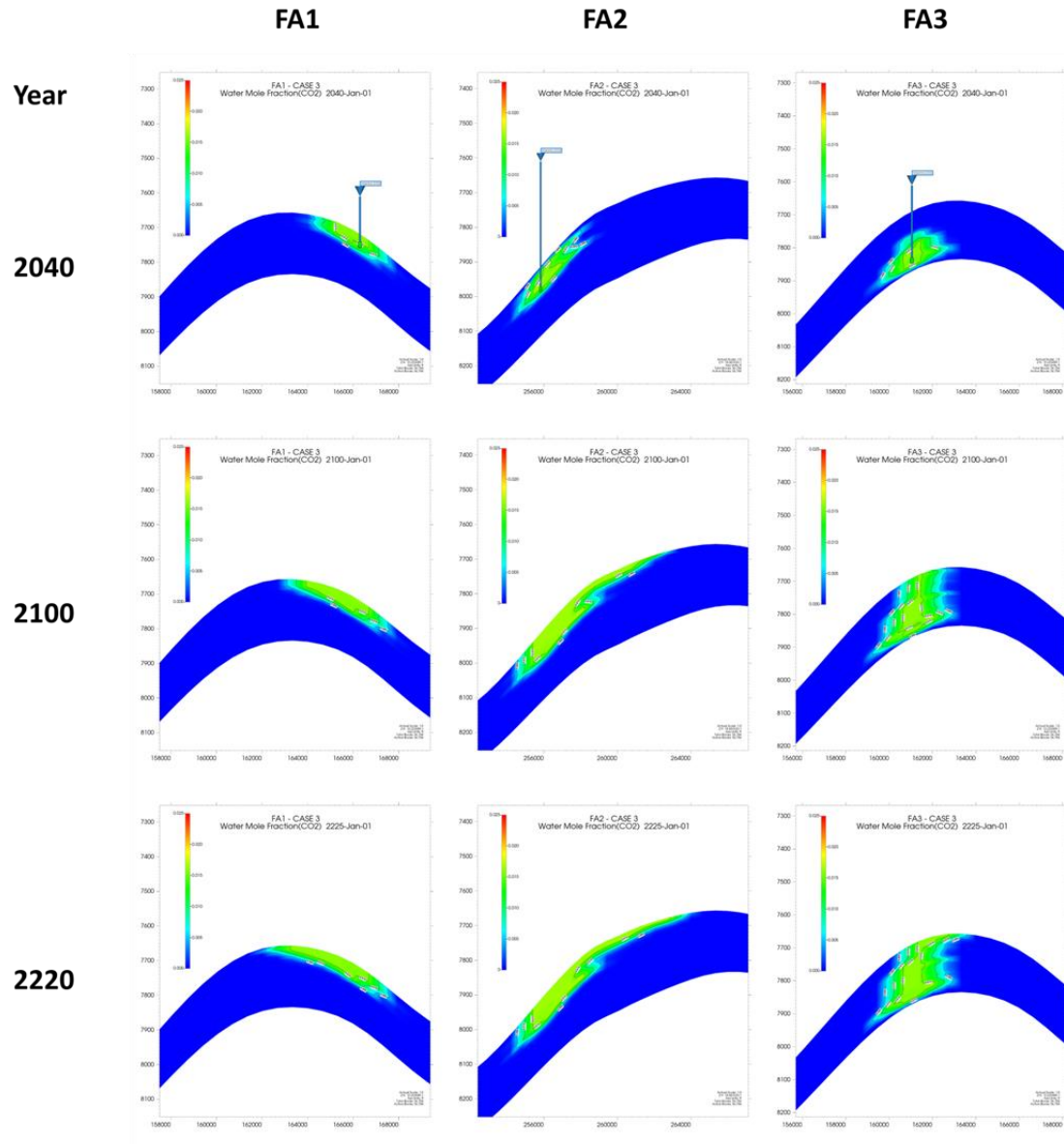


Figure 4. 29 The disparity effect in CO₂-dissolved posts the injection in each Facies

Association – Case 3

For a detailed comparison of CO₂ trapping mechanisms within each injection case, as shown in the Table 4.5, there is a consistent trend of decreasing structural trapping percentages across all three injection cases over the years. From 2050 to 2220, structural trapping decreases by 12.5% in FA1, 21.2% in FA2, and 21.5% in FA3. Meanwhile, mineral dissolution experiences subtle changes, with only a 0.01-0.04% increase, while residual trapping increases by 9.8% in FA1, 17.2% in FA2, and 18% in FA3. Dissolution trapping also sees an increase, by 2.8% in FA1, 4% in FA2, and 3.3% in FA3 during this period.

FA1 - CASE 3				
Year	Trapping Mechanism (%)			
	Structural	Mineral	Residual	Dissolved
2050	75.75	-0.10	8.09	16.06
2100	66.72	-0.12	15.24	17.92
2220	63.25	-0.13	17.82	18.81

FA2 - CASE 3				
Year	Trapping Mechanism (%)			
	Structural	Mineral	Residual	Dissolved
2050	68.18	-0.14	10.52	21.15
2100	51.65	-0.17	23.69	24.49
2220	46.94	-0.18	27.76	25.11

FA3 - CASE 3				
Year	Trapping Mechanism (%)			
	Structural	Mineral	Residual	Dissolved
2050	69.33	-0.13	10.42	20.13
2100	55.30	-0.14	22.82	21.73
2220	47.86	-0.15	28.59	23.40

Table 4. 5 Comparison of trapping mechanism percentages between injection points FA1, FA2, and FA3, along with their evolution over time – Case 3.

Comparing the data at the end of the 2220 monitoring period, there is a 15.4% lower structural trapping in FA3 compared to FA1, and an 16.3% lower in FA2 compared to FA1. Regarding mineral dissolution, FA3 exhibits a 0.02% higher value compared to FA1, while FA2 shows a 0.05% higher value relative to FA1. Residual trapping is 10.77% higher in FA3 compared to FA1 and 10.1% higher in FA2 relative to FA1. Additionally, dissolution trapping shows a 4.6% higher CO₂ dissolution in FA3 compared to FA1, and a 7.7% increase in FA2 relative to FA1. For a clearer visualization, the graph below provides a comparison of trapping mechanisms between FA1, FA2, and FA3 (Fig. 4.30).

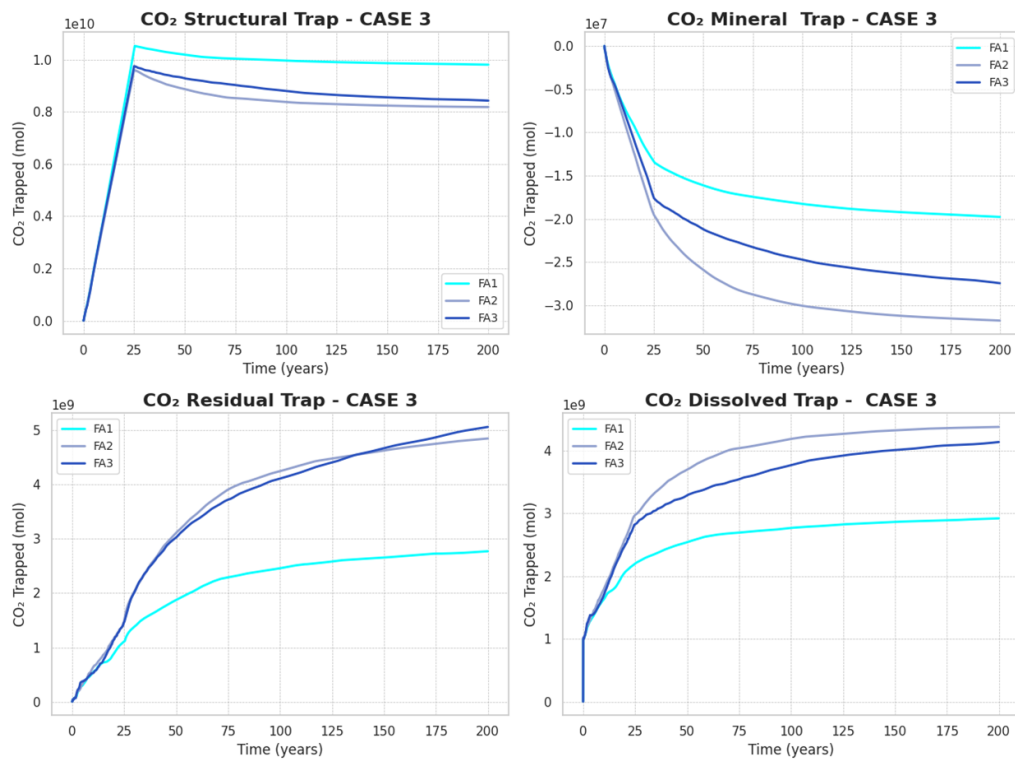


Figure 4. 30 A graphical representation illustrating the comparison of each trapping mechanism among FA1, FA2, and FA3.

CHAPTER 5

DISCUSSION

5.1 Depositional Environment

In the onshore UAE, the Upper Kharaib deposition occurred far from the shorelines and behind the shelf margin in low-relief areas. These intervals exhibit lateral continuity over extensive distances, indicating deposition in a relatively stable and widespread epeiric carbonate platform. This observation is supported by findings from previous studies conducted by Murris (1980), Alsharhan (1989), and van Buchem et al. (2013). The Upper Kharaib zone displays a shoaling trend from deeper-water, low-energy wackestone in its lower part to shallower-water, high-energy, grain-supported textures in its upper part. This trend is depicted as a transition from a muddy (FA4) to grainy, medium-energy ramp or an open muddy lagoon, with *Thalassinoides* burrows and tempestites upward into a grainy, high-energy ramp with rudist and ooid shoals (FA1) (van Buchem et al., 2013; Strohmenger et al., 2006). These align with previous research on diagenesis of Upper Kharaib reservoir conducted by Pacheco in 2017, which noted the diverse range of lithofacies present in the reservoir proved by the petrography or thin sections. On top of the reservoir, the rudists grainstone facies (FA1) are capped by thin rudist shoals, which have a locally planar to low-angle cross-laminated structure and are bioturbated. These shoals are believed to represent relatively the highest-energy facies and indicate shallow shoal development in the wave-affected zone (Strohmenger et al., 2006). In addition, the lateral variation from the well correlation in Figure 5 provides additional support to the

interpretation of a depositional environment transitioning towards more distal or basinal facies in the northern direction (Costa et al., 2022).

The thickest part of FA1 around crestal area is hypothesized to constitute a component of a minorly developed buildup or, alternatively, to be an area conducive to the formation of rudist grainy lithofacies during the Highstand System Tract (HST) parasequence. The current structural configuration or the anticline pattern observed in the Upper Kharaib reservoir is likely to be influenced by the surrounding natural lithofacies topography. This inference is supported by the isopach map of the Inner Ramp and Inner-Shoal Facies Association, which reveals a decrease in thickness towards the northern region, consistent with the regional geological context. On the other hand, Despite the generally low to moderate reservoir quality of FA3, its considerable thickness renders it conducive for long-term carbon dioxide (CO₂) storage, owing to its extensive lateral and continuous distribution in the lower-middle zone.

In most oilfields, the Upper Kharaib zone is divided several reservoir sub-zones by thin intervals of moderately lower porosity associated with greater frequency of stylolites or called dense or baffle zones (Ehrenberg and Wu, 2019). These sub-zone tops are correlatable between different fields throughout the Abu Dhabi area. As a comparison, the well-known Utsira massive sandstone from Sleipner CCS Project, shows the presence of nine internal barrier or baffle zones which responsible to create layer cake model of CO₂ plume profile (Cavanagh et al., 2014). It similarly observed in Upper Kharaib reservoir that there are possibly at least four potential baffle or dense zones identified from logs which consistent and observed in most of the wells. These dense zones might indicate cemented carbonates related to stylolites. Understand the vertical and lateral distribution of each FA

is one of the key types of information for injection well planning as well as Modelling the likelihood of post injection CO₂ plume profile.

The Kharaib Formation's Platform carbonates are recognized as one of the most significant hydrocarbon-bearing reservoirs in Abu Dhabi and the UAE. The Kharaib reservoir, along with its associated seal, the Hawar Mb., presents a compelling case for geological characterization in the study of potential carbon storage and utilization due to its noteworthy properties. In summary, The Carbonate equivalent of Kharaib Formation was widely spread deposited especially in the eastern basins from Eastern Saudi Arabia, UAE, Oman and Southwest of Iran (Murriss (1980), Alsharhan (1989), and Van Buchem et al. (2002), this could be an ideal case to gain some insights from this study and hopefully could be applicable to another carbonate reservoir in the Middle East Region.

5.2 CCS Rock Type Cluster

The Rock Type (RT) classification is utilized to distinguish a section of rock with uniform and foreseeable geological and petrophysical characteristics that may impact the distribution and flow of fluids. Typically, the reservoir properties of the Upper Kharaib reservoir have strong correlations with lithofacies, with diagenetic processes occasionally exerting influences that can enhance or diminish these properties. The most favorable reservoir quality is predominantly observed in the upper part, specifically within the Inner Ramp-Shoal-Inner Shoal Facies Association or other facies associated with high-energy water environments. The initial framework of lithofacies plays a crucial role in determining the distribution and pattern of reservoir quality, as well as the impact of diagenetic

overprint on porosity and permeability, which is later mostly enhanced by dissolution and reduced by cementation (Fig. 5.1).

In the context of CO₂ sequestration, Rock Typing may deviate from conventional approaches, as the focus is on understanding the behavior of rocks when subjected to CO₂ injection and predicting the impact on trapping mechanisms. Nevertheless, the fundamental principle remains consistent, whereby specific cutoff values of porosity and permeability are employed. A combined screening criterion for depleted reservoir has been presented by Reza et al. 2016, which basically combination of several previous work done by Kovscek (2002), Solomon (2006), and Chadwick et al. (2008) including parameters that need to be considered such as reservoir depth, storage capacity, formation thickness, permeability, and seal properties. This criterion is commonly used as first step of feasibility study or early screening to conduct further evaluation and for selection of suitable CO₂ storage sites.

Our analysis highlights that the Inner shoal-shoal Facies Association shows the most ideal target for utilizing CO₂ to improve enhanced oil recovery based on its storage capacity (Table 1.). this FA host the best reservoir properties compared to other. In addition, further assessment also shows that the middle ramp facies association could act as an additional target for storing CO₂ in this carbonate reservoir based on its laterally continuous thick succession (up to 50 m) and moderate petrophysical properties (ϕ :10-30% and K:0.1-50 mD). The injection of CO₂ will likely create and enhance the permeability of Middle Ramp facies by the processes of mineral dissolution around wellbore due to acidic character of liquid phase CO₂ in the subsurface (Middle Ramp Facies). The research conducted by Smith et al. in 2013, which assessed the reservoir's response to CO₂ injection in the

Weyburn-Midale project in Canada, indicates that most of the mineral dissolution occurred in the vicinity of the sample's entry point, spanning a few millimeters. According to Morad et al. (2018), the Upper Kharaib reservoir primarily comprises high-purity limestone (>95% calcite) with occasional occurrences of dolomitic limestone. Consequently, the initial response following CO₂ injection is expected to involve dissolution processes near the wellbore, given that the reaction rate constant of calcite is approximately 17 times higher than that of dolomite (Smith et al., 2013).

We identified three proximity areas for the CCS Rock-Type clustering, which is based on porosity and permeability thresholds (Fig. 43). Existing literature suggests that the desired criteria for CO₂ site storage for reservoir typically include a depth greater than 2500 ft to achieve the supercritical phase of CO₂, porosity greater than 10%, permeability greater than 100 mD, and gross thickness greater than 20m (Chadwick, 2008). However, these criteria may differ for carbonate reservoirs compared to siliciclastic reservoirs. Therefore, in this study, we conducted preliminary screening for the Upper Kharaib member carbonate reservoir, taking into consideration additional factors such as the vertical and lateral distribution of each Facies Association, its thickness, and the potential CO₂ trapping mechanism. Despite the proven oil accumulation in the study area, irrespective of the Facies Association, there are no issues with the capacity or capability for CO₂ storage sites in general. The upcoming intriguing subject for discussion revolves around the potential behavioral model of CO₂ injection within each facies association, which in turn has significant implications on determining the optimal placement of injection wells both for CCS or CCUS projects.

In the context of reservoir characterization, the facies denoted as FA1 and FA2, which display high porosity and permeability values, exhibit a well-developed internal pore fabric geometry with a high degree of pore connectivity. This favorable internal pore structure facilitates efficient fluid flow within the rock, indicating that structural trapping is the likely mechanism for potential carbon dioxide (CO₂) trapping in these rock types. According to this mechanism, CO₂ would migrate vertically, eventually reaching the top of the reservoir and contacting the Hawar seal, where it would be effectively trapped.

Conversely, the middle ramp facies display moderate reservoir quality with relatively good porosity but lower permeability values. Despite their less-than-ideal permeability, these facies possess a silver lining in their smaller pore networks, which can be advantageous for the residual trapping mechanism. The limited permeability may hinder the rapid movement of CO₂, but the intricate network of pores can enhance the process of residual trapping, where CO₂ becomes immobilized within the pore spaces due to capillary forces. Thus, while these reservoirs may not be the primary candidates for conventional CO₂ storage, their unique characteristics make them promising contenders for effective carbon capture and storage strategies, particularly through residual trapping mechanisms.

The outer ramp FA or basinal lithofacies exhibit the lowest quality in terms of porosity and permeability. These facies are known to be a dense or tight zone, as evidenced by previous research. It is predominantly located in the lowermost interval of the Upper Kharaib reservoir and is not considered a viable candidate or target for carbon storage. Additionally, scattered data points with high permeability but low porosity may indicate later diagenetic overprint as well as influenced by structural features such as fractures or faults and a restricted or isolated environment, making predictions about its distribution challenging.

There is a significant positive correlation between core plug porosity and permeability, suggesting effective interconnection between interparticle macropores and micropores. This connectivity is primarily attributed to the preservation of porosity by grain-rimming calcite cement. This cementation process has contributed to enhanced resistance of the limestones against mechanical compaction (Morad et al., 2019b).

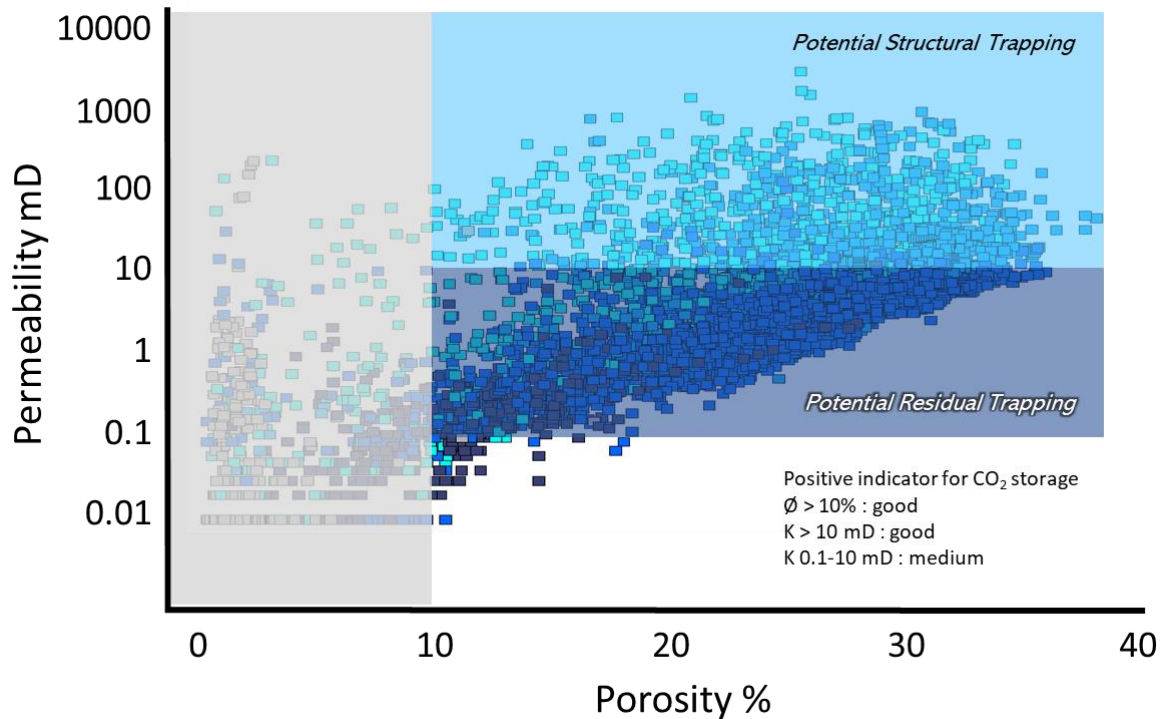


Figure 5. 1 The initial screening for carbon storage based on physical properties threshold identifies three regions of rock types that are in close proximity to each other. (After Chadwick, 2008).

Furthermore, the data obtained from the study area does not encompass information regarding the seal rock characteristics, regional study by Leuven et al. published in 2010 display the isopach map of Hawar shale Member nearby study area range between 30-40 ft or 9-12 m thickness proven to be an effective seal for Upper Kharaib reservoir. Similarly,

the proximity of Hawar seal around the study area exhibits a thickness that varies between 25 to 50 ft, as reported by Vahrenkamp et al. (2015). It referred as the Lower Aptian Dense zone of marly facies and has been established as a reliable sealing formation for the Upper Kharaib reservoir in the study area, which has been proven to retain an impressive oil column of up to 148 m or 485 ft shown by the log data. This fact is addressing Hawar shale integrity and containment to hold any type of fluid even the CO₂.

5.3 Conceptual CO₂ Trapping Mechanism in Upper Kharaib Reservoir

Porosity refers to the proportion of void space in a rock or sediment, while permeability is the ability of the rock to permit fluid flow (Guo, 2019). Both properties are crucial for CO₂ storage, as they determine the capacity of the reservoir to store CO₂ and the ability of CO₂ to move through the rock formation.

A reservoir with high porosity but low permeability may be capable of accommodating a significant volume of CO₂, but the movement of CO₂ through the rock to fill the available pore space may be challenging. On the other hand, a reservoir with high permeability but low porosity may facilitate easy CO₂ injection but have a limited storage capacity.

Therefore, to ensure efficient and effective CO₂ storage, it is necessary to strike a balance between porosity and permeability. The specific cutoff values for porosity and permeability will be determined by the geological properties of the storage formation and the desired storage objectives.

The trapping mechanism of CO₂ injection refers to the physical and chemical processes that prevent the CO₂ from escaping back into the atmosphere. There are three main types of trapping mechanisms: structural, residual, and solubility (IPCC, 2005). Structural trapping involves the physical entrapment of CO₂ in the pore spaces of rocks, while residual trapping occurs when CO₂ is trapped as a liquid phase after the injection pressure is reduced. Local capillary trapping refers to the process by which buoyant free-phase carbon dioxide (CO₂) becomes trapped underneath capillary pressure barriers induced by heterogeneities in the subsurface rock formations (Saadatpoor et al., 2009). Residual trapping, also known as capillary trapping, occurs when CO₂ is immobilized in bubbles or ganglia within pores through the process of capillary snap-off at low saturations (Ide et al., 2007). Solubility trapping is the chemical reaction between CO₂ and the formation water, resulting in the formation of carbonate minerals. While all three trapping mechanisms are important, residual and solubility trapping is considered the most reliable and long-lasting, as it results in the permanent mineralization of CO₂. Therefore, it is the preferred mechanism for CO₂ injection and storage.

In carbonate reservoirs, other than porosity and permeability, capillary pressure plays an important role in CO₂ storage by influencing the trapping mechanism. Capillary pressure in carbonate rocks is generally higher than in sandstone rocks due to their smaller pore sizes and complex pore networks. This means that CO₂ injected into carbonate reservoirs is more likely to be trapped by residual trapping, where it reacts with the formation water to form stable carbonate minerals in longer processes.

Overall, the effectiveness of CO₂ storage in carbonate reservoirs depends on a range of factors, including the pore structure, mineralogy, and presence of fractures and faults. By

carefully considering these factors, suitable sites for CO₂ injection can be selected to maximize long-term storage through the most effective trapping mechanisms. These hypotheses should be examined by the reservoir Modelling and also through lab experimental in which to see the geochemical reaction as well as the dominant trapping mechanism in carbonate reservoir for each Facies Association.

The implementation of a facies association model for CO₂ injection screening may not fully encompass the intricacies of the Upper Kharaib reservoir. Its purpose would be to identify general trends during the early screening stage, and further detailed research would be necessary. The presence of small-scale facies heterogeneity in the reservoir drives variations in permeability. These variations, combined with factors such as capillary pressures, relative permeabilities, and wettability, significantly impact fluid flow and hydrocarbon production (e.g., Namba and Hiraoka, 1995; Chilingarian et al., 1992; Cunningham and Chaliha, 2002; Masalmeh et al., 2003; Gomes et al., 2008; Carvalho et al., 2011). Moreover, smaller layers may not exhibit direct correlation between wells, suggesting moderate to intricate depositional configurations influencing lateral facies diversity (e.g., Ehrenberg et al., 2018). Further understanding the influence of small-scale facies variations on fluid movement is crucial for enhancing reservoir sweep efficiency. It's essential to retain the most notable small-scale heterogeneities in the framework model to prevent their loss during upscaling.

The diagram in Figure 5.2 presents a schematic representation of potential mechanisms for trapping CO₂ in the Upper Kharaib reservoir. The concept involves injecting CO₂ into a deep saline aquifer in order to simplify the models. The schematic model is designed to align with the vertical succession of the Upper Kharaib profile for each Facies Association.

To validate the accuracy of the schematic model, it needs to be tested using numerical reservoir simulation models for CO₂ plume profile and geochemical reaction along the wellbore as well as laboratory experiments utilizing outcrop or core data that represent the lithofacies of each Facies Association. A thorough understanding of the geological complexity of the reservoir and its characterization is essential for accurately predicting the outcome of post-CO₂ injection and for determining the optimal location and depth of the injector well perforation. The selection of such a strategy is heavily dependent on the objective, whether it is solely for permanent CO₂ storage or an engineering attempt for enhanced oil recovery in a depleted reservoir.

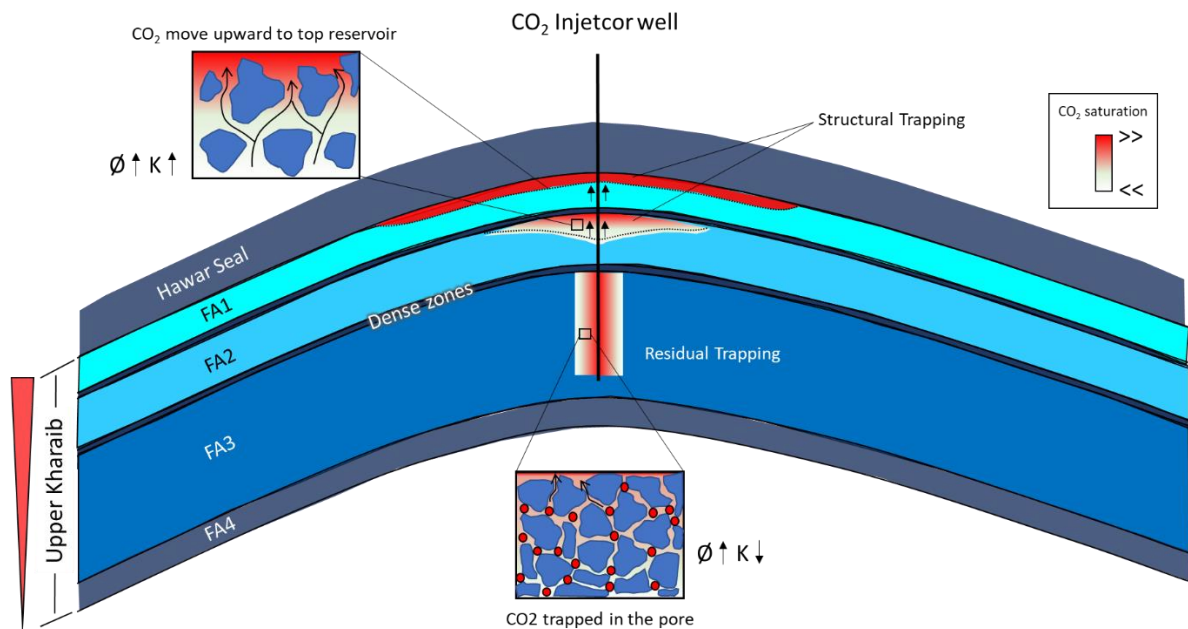


Figure 5. 2 A schematic diagram depicting the possible CO₂ trapping mechanisms for each Facies Association in a saline formation. The residual trapping is commonly related to capillary pressure resulted from internal fabric of the reservoir, and usually happened in the low permeability facies.

The Upper Kharaib reservoir is a hydrocarbon-bearing formation that has been established in the study area. It is capable of efficiently storing a range of fluids, including CO₂, without being constrained by facies associations. However, the optimal lithofacies for effective sweep efficiency and enhanced oil recovery are the inner shoal-shoal FA or rudist-grainstone lithofacies due to their superior pore connectivity. The middle ramp FA, which is dominated by wackestone-packstone facies, has poor-medium pore connectivity and is likely to result in residual trapping. These facies are ideal due to the longer time needed to reach the ultimate cap rock of the top reservoir. The selection of the appropriate facies should be based on their individual advantages and linked to the overall industrial strategy and mitigation measures during and after the CO₂ injection process.

The primary objective of any carbon capture project is to ensure the permanent sequestration of CO₂ in the subsurface, thereby mitigating the release of greenhouse gases into the atmosphere. Achieving this objective requires a thorough understanding of various interrelated processes in the subsurface, including fluid-rock interaction, maximum flowrate-pressure related to geomechanics, plume profile modelling, and monitoring, as well as the integrity of the seal rocks. A comprehensive understanding of these processes is essential for effective implementation of carbon capture projects. It is important to note that the success of carbon capture projects depends on the ability to accurately model and monitor the behaviour of CO₂ in the subsurface, which requires the integration of multiple disciplines, including geology, geophysics, and reservoir engineering. Therefore, it is imperative to conduct further research on these subjects to ensure the successful implementation of carbon capture projects.

5.4 Model Grid Size and Complexity

Based on the results of the three cases modelled above, it can be concluded that the grid cell size determines the level of detail with which the model represents real geology. This can be observed from the comparison of histograms between raw well logs, upscaled logs, and the overall model, where differences arise due to averaging value compensation in certain areas. The extent of the grid model area has minimal impact on overall plume migration monitoring since the distribution of CO₂ migration is concentrated primarily around the injection well area. Across all three cases during the 200-year monitoring period, simulated CO₂ plume movement only reaches a maximum of 2-4 km away from the wellbore.

Furthermore, the grid cell size generally affects simulation performance and the magnitude of injection rates. Based on the simulation exercise applied in this study, high-resolution grid model increases simulation runtime significantly and requires smaller injection rates. This is because applying a high injection rate to small cells often triggers simulation warnings due to exceeding tolerance limits and significant pressure differences between cells.

In CO₂ injection schemes, field-scale areas may be deemed excessively large for observing CO₂ migration, especially over monitoring periods spanning hundreds of years. In several similar exercises, there are examples of grid modelling with relatively small coverage areas to observe CO₂ migration patterns, as seen in studies by Liner et al in 2011. Several studies have been conducted on a subfield level near the wellbore, as it is crucial to observe the

thermodynamic reactions at the pore scale and their correlation with studies on wellbore stability.

5.5 Vertical vs Lateral CO₂ plume migration

Naturally, injection of CO₂ at first will propagate radially away from the wellbore and replace the brine (Figure 5.3). Considering this process alongside the observations from the simulations conducted, both theoretical considerations and simulation results indicate that the primary migration of supercritical CO₂ is predominantly influenced by buoyancy forces or density differences, leading to vertical migration. Whether employing a layer cake model or a 3D geological model, the migration of the CO₂ plume tends to exhibit a vertical trajectory, irrespective of variations in both the vertical and lateral dimensions. It is noteworthy that differential density and pressure plays a crucial role in facilitating vertical migration, thereby causing buoyancy forces to exert significant dominance over the movement of supercritical CO₂. The upward movement of CO₂ is explained by the balance between capillary forces, which retain CO₂ within the pore structure, and buoyancy forces, facilitating its upward migration (Zhang and Song, 2014, Urych et al., 2022). This upward motion of CO₂ occurs independently of gravity forces and displaces fluids with lower density than brine beneath the seal rock (Mackay, 2013), thus structurally trapping itself. This structural or physical trapping necessitates both lateral and vertical seals (Iglauer et al., 2015a) and is referred to as structural, stratigraphic, or hydrodynamic trapping. This process is critical for any storage site to prevent CO₂ leakage through the seal rock during

the initial decade, and then the other trapping mechanisms begin to take effect (Bachu et al., 1994).

However, lateral migration is also evident in the simulation results. This occurs when the supercritical CO₂ encounters impermeable layers, such as seal rocks or internal baffle layers, and follows the dip of the reservoir beds (Fig. 5.3). For instance, in the case where the injection well is positioned on the flank of an anticline, lateral migration is observed. From the injection point to the uppermost section of the reservoir, lateral dispersion patterns are apparent, albeit with varying degrees of extent. This phenomenon is also observed in studies like the Sleipner case, especially in reservoirs containing internal baffling layers that naturally hinder the vertical movement of CO₂.

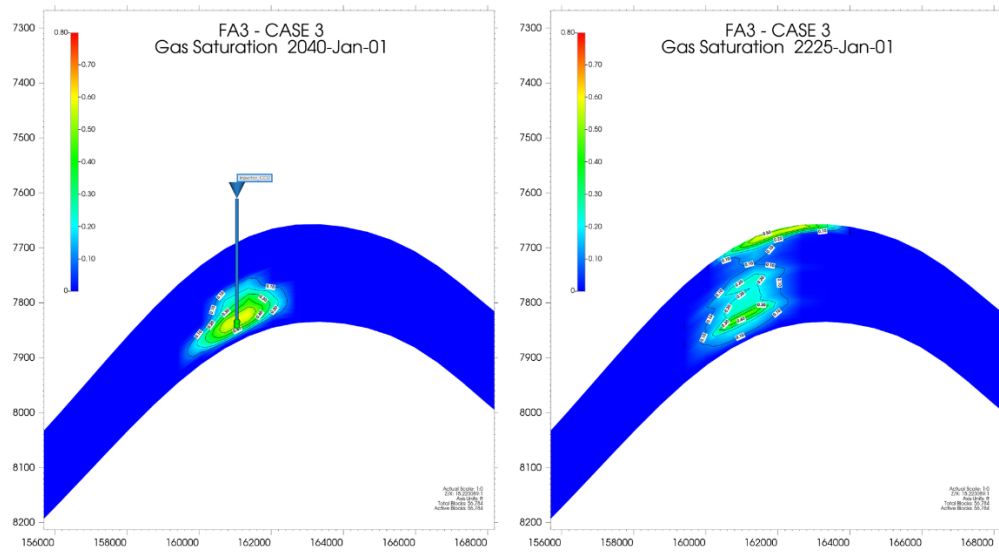


Figure 5. 3 The gas saturation profile in the years 2040 (during injection) and 2220 (post-injection) for Case 3, demonstrating that the primary migration for Supercritical CO₂ is characterized by vertical migration.

Expanding upon this discussion, it is essential to consider the complex interplay between buoyancy-driven vertical migration and lateral dispersion mechanisms in CO₂ plume behavior. While buoyancy forces primarily dictate the overall movement patterns, lateral migration can occur due to factors such as reservoir heterogeneity and the presence of internal baffling structures. Understanding these migration dynamics is critical for accurately predicting CO₂ plume behavior and informing the design of effective carbon capture and storage strategies.

5.6 Relationship between pH changes and CO₂ dissolved in brine post the injection

During and after CO₂ injection, significant changes occur in the pH levels of the surrounding environment. This is primarily due to the dissolution of CO₂ in water, which forms carbonic acid (H₂CO₃), leading to a reduction in pH. In subsurface environments like saline aquifers, where CO₂ injection for storage is common, this pH decrease can have diverse implications. The acidification resulting from CO₂ injection can potentially influence mineral dissolution and precipitation reactions especially in carbonate reservoir, thereby altering the overall geochemical composition of reservoir fluids (Xu et al., 2016).

Additionally, the injection of CO₂ into saline aquifers can trigger reactions with minerals present in the formation rock, resulting in mineral dissolution or precipitation. These reactions can further impact pH levels within the reservoir. For instance, the dissolution of carbonate minerals in aquifer rock can serve as a buffer, partially offsetting the pH decrease caused by CO₂ dissolution (Li et al., 2017). However, the effectiveness of mineral

dissolution in buffering pH changes depends on several factors, including mineral composition, fluid-rock interactions, and injection conditions.

The simulation results also demonstrate a correlation between the distribution of CO₂ dissolved in brine and changes in pH. The distribution patterns of both during and post-injection are similar. Another interesting observation is that during the post-injection monitoring phase, CO₂ dissolved in brine will migrate downward following density-driven convection, resulting in a decrease in pH as the brine saturated with CO₂ moves towards the down flank area (Fig. 5.4).

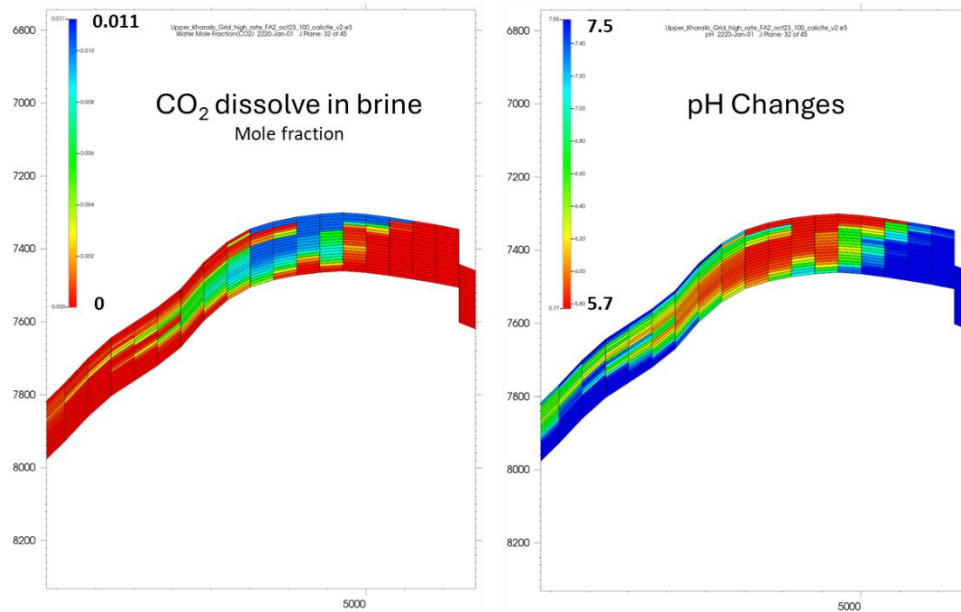


Figure 5. 4 The distribution pattern of CO₂ dissolution and pH changes post injection in the year 2220 – Case 1.

The process of CO₂ dissolving in formation fluid is commonly known as solubility trapping (Li et al., 2020a). After injection, the supercritical CO₂ rises to the interface between the caprock and reservoir, spreading laterally beneath the caprock as a separate phase. Upon

contact with hydrocarbons (in depleted oil reservoirs) or formation brine (in deep saline aquifers), CO₂ dissolves into the fluids, facilitating mass transfer until equilibrium is reached, thereby enhancing residual and structural trapping capacities (Ali, 2018; Gutiérrez and Lizaga, 2016). The solubility of CO₂ in formation fluid is influenced by factors like temperature, pressure, and brine salinity (Chang et al., 1996), with the dissolution driven by molecular diffusion at the fluid interface.

However, the slow molecular diffusion coefficient lengthens the CO₂ dissolution process, which could span thousands of years (Lindeberg and Wessel-Berg, 1997). Upon dissolution, CO₂ slightly increases the density of the formation water, typically by around 1%, compared to normal formation water (Bachu and Adams, 2003; Kumar et al., 2004), prompting a downward flow of the formation brine due to gravitational forces. This flow enhances the mixing of formation brine and CO₂, accelerating the diffusion mechanism and leading to increased CO₂ dissolution. Consequently, this process reduces the upward movement of CO₂ and augments the storage capacity of the geological formation (Ajayi et al., 2019; Zhang et al., 2009; Zheng et al., 2020).

5.7 Residual Trapping in Upper Kharaib Reservoir

Based on Rebelle et al.'s 2012 study on reservoir characterization of the Upper Kharaib reservoir, an attempt was made to correlate rock types of petrophysical groups with geological facies. The findings revealed a 60-75% correlation between good reservoir quality and grainstone dominated facies. The study also presented data on mercury injection capillary pressure (MICP) and pore throat size distribution, demonstrating that

grainstone-dominated facies have larger pore throat sizes and exhibit the lowest water saturation profiles.

According to the study conducted by Alabere et al. in 2023, they presented data from mercury injection capillary pressure (MICP) analysis of Lower Cretaceous carbonate reservoirs in Abu Dhabi. The findings revealed a wide variation in pore throat size, ranging from micropores to mesopores and macropores, associated with different lithofacies (Fig. 5.5). They also observed that grain-dominated facies could exhibit a bimodal pore network consisting of both micropores and macropores, whereas mixed grain-dominated facies typically fall within the mesopore range. In contrast, mud-dominated facies, characterized by low porosity and permeability, are predominantly associated with micropores in terms of pore-throat size.

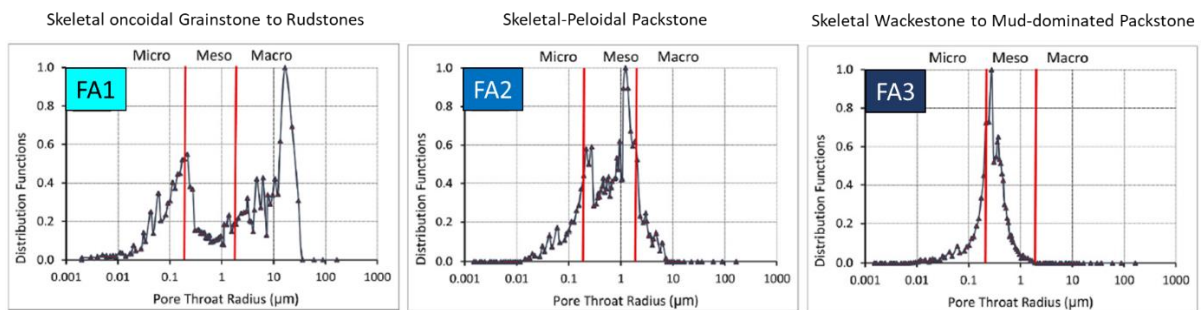


Figure 5. 5 Example of Mercury injection capillary pressure analysis conducted on various limestone textures associated with the Facies Association scheme identified within Lower Cretaceous carbonate formations (Modified after Alabere et al., 2023)

Residual trapping, often referred to as capillary trapping, is closely linked to capillary pressure. CO₂ injection in low to moderate-quality reservoirs or mix grain texture facies, such as FA3 in Upper Kharaib carbonate, or in this case, coincidentally located at the

bottom of the reservoir, results in the highest values of residual trapping and dissolution compared to CO₂ injection in the middle (FA2) or upper part (FA1) of the reservoir (Table 8, 9, 10). Studying injection into deeper sections of saline aquifers has been explored as a strategy to enhance trapping efficiency. Due to CO₂'s buoyancy compared to formation brine, it naturally ascends within the aquifer, with residual trapping occurring along its migration route, immobilizing a significant portion of the injected CO₂ (van der Meer and van Wees, 2006). Although the buoyant plume is inherently unstable and could potentially lead to fingering, fine-scale simulations suggest that CO₂ tends to follow preferential flow paths dictated by geological heterogeneity (Bryant et al., 2006).

5.8 Implications of Reservoir Heterogeneity in the simulation

In this study, it's important to note that the analysis is limited to considering only stratigraphic and facies heterogeneity. The presence of faults and fractures, which can significantly influence fluid flow pathways and CO₂ migration, were not included in the analysis. Therefore, the results of this study may not fully capture the complexities introduced by faults and fractures in real-world CO₂ storage scenarios.

The simulation demonstrates the significant impact of facies and stratigraphic heterogeneity within a reservoir on the distribution patterns of CO₂ and its effects on various reservoir parameters. The results of the three simulations show considerable differences in terms of gas saturation distribution profiles, mineral reactions, pH changes, and CO₂ dissolution in brine. Overall, heterogeneity plays a crucial role in restricting the migration of CO₂ to the top reservoir area, as depicted in Figure 5.6. Furthermore,

heterogeneity also affects the concentration profiles of residual trapping, where a more heterogeneous reservoir provides a larger volume of residual trapping compared to a homogeneous reservoir.

In the case of saline aquifer storage, residual trapping and reservoir heterogeneity can be advantageous when CO₂ injection is aimed at trapping the CO₂, provided that there is sufficient storage capacity available. Initially, Sleipner stood out as the prime model for CO₂ storage, leading to the assumption that optimal storage locations would boast high permeability and relatively uniform properties. However, it's crucial to acknowledge that higher permeability could lead to accelerated migration rates and injection challenges. The focus has now shifted, especially with the rise of projects like In Salah in Algeria (Riddiford et al., 2005), towards evaluating the feasibility of utilizing low-quality, heterogeneous saline formations as suitable storage sites (Flett et al., 2005; 2007).

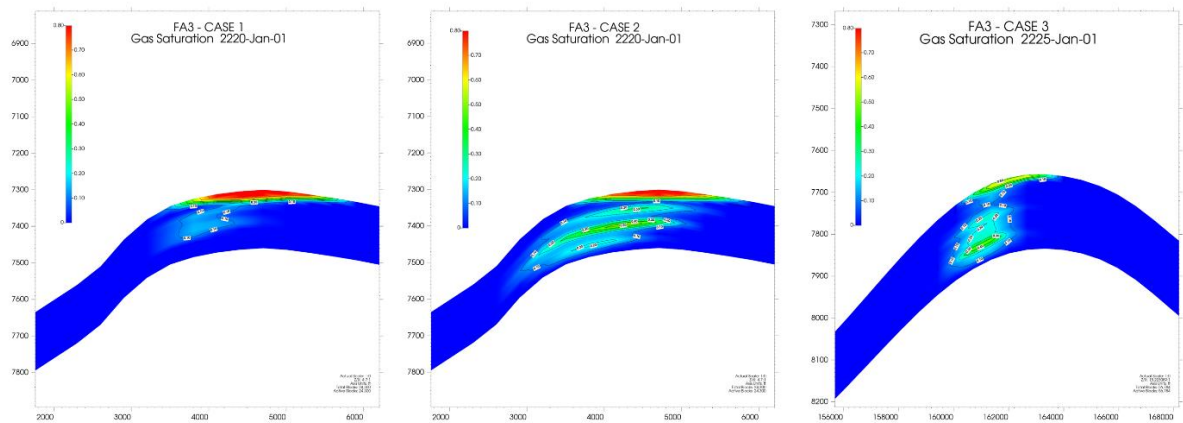


Figure 5. 6 The comparison of gas saturation after 200 years of monitoring post CO₂ injection in FA3 between layer cake model (case1), layer cake with low permeable baffle layers model (Case 2), and 3D geological model (Case 3)

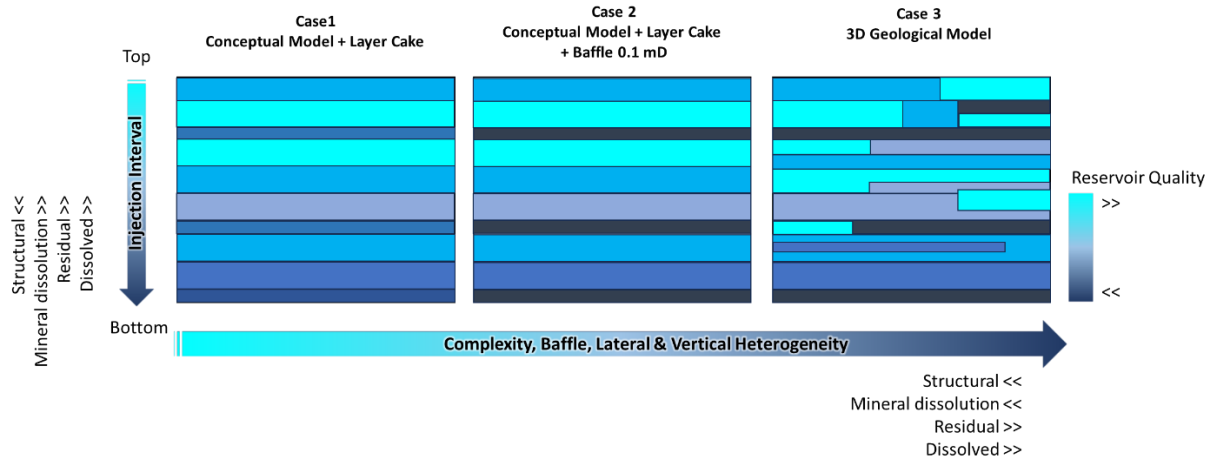


Figure 5. 7 Summary illustration of the effect on the overall trapping mechanism: injection interval in the upper part vs bottom part of reservoir and the comparison between UKM model grid Case1, Case2, and Case3.

The summarized impact of reservoir heterogeneity is depicted in Figure 5.7. Generally, injecting into the bottom interval of the reservoir results in reduced structural trapping and increased mineral dissolution, leading to higher percentages of residual and dissolution trapping. Moreover, greater model complexity and heterogeneity correlate with decreased structural trapping and mineral dissolution, while exhibiting higher percentages of residual and dissolution trapping after 200 years of monitoring.

5.9 The role and impact of internal baffle layers for CO₂ plume profile and migration process

Typically, impermeable rocks act as barriers, impeding vertical movement of gases upwards and hindering downward vertical movement of CO₂-saturated water. As a result, lateral movement becomes more prominent. The extent of this lateral movement varies

depending on the impermeable rocks content, distribution and continuity (Ghanbari et al., 2006). In the simulation results, particularly evident in Case 3 with injection at the reservoir's bottom (FA3), the well bottom hole pressure (BHP) exhibits a distinctive profile over time, as illustrated in Figure 50 below.

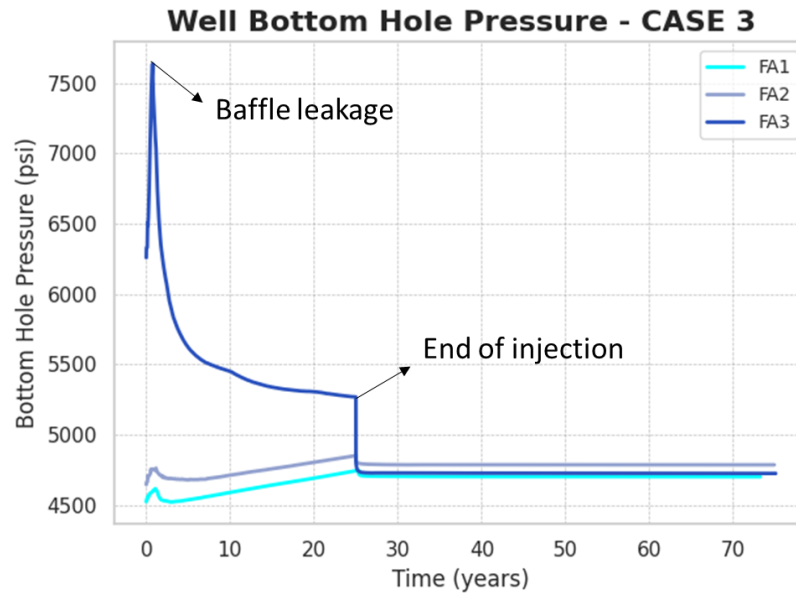


Figure 5. 8 The well bottom hole pressure profile between FA1 and FA3 location.

The well bottom hole pressure at the FA3 location exhibits a markedly distinct profile compared to that at the FA1 and FA2 location. Initially, during the early years of injection, there is a notable spike in the pressure profile, which could potentially indicate localized pressure buildup near the injection interval, likely due to the presence of baffle layers. Subsequently, a decrease in pressure occurs, signalling pressure release resulting from exceeding the pressure tolerance limit and subsequent leakage of the baffle layers. This leakage persists until the end of injection, gradually decreasing until reaching equilibrium with the system. In contrast, the FA1 and FA2 profile displays a smoother pressure buildup throughout the injection period, with minor pressure drops occurring at the onset and the

end of injection. Additionally, the post-injection pressure increments for all three cases are similar, approximately around 150-200 psi.

The existence of an internal baffle zone, particularly with a permeability value of less than or equal to 0.1 mD, significantly affects the overall migration of the CO₂ plume and the profiles of thermodynamic and geochemical reactions, as depicted in Figure 5.9 below.

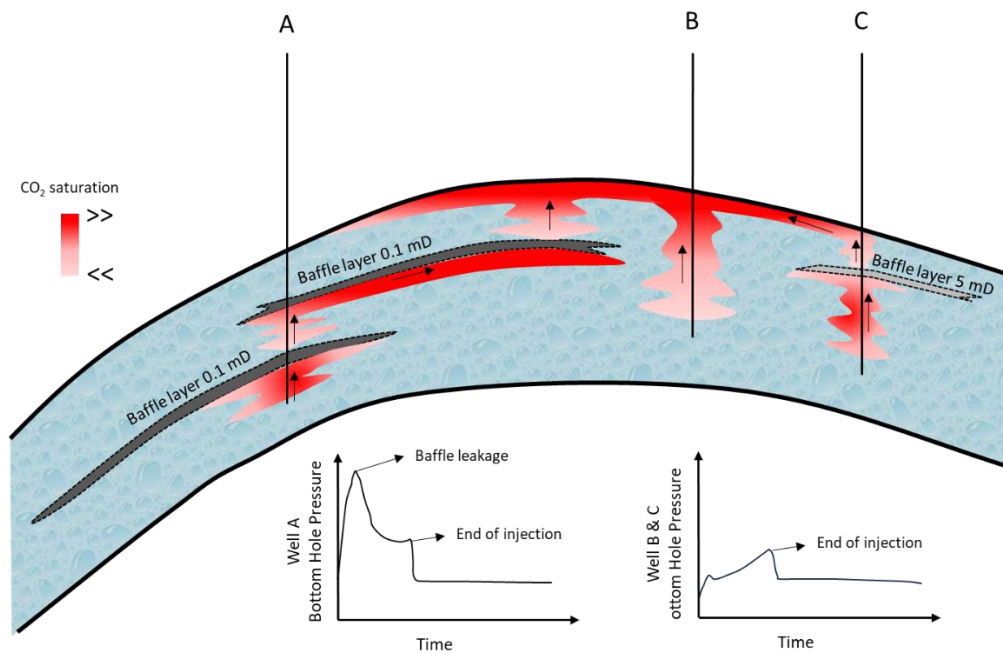


Figure 5. 9 The illustration on impact of internal baffle zones for CO₂ plume migration, saturation profile and bottom hole pressure signature.

CHAPTER 6

CONCLUSIONS AND RECOMMENDATIONS

6.1 Conclusions

There are several conclusions that can be drawn from the results of this study, as follows:

- In conclusion, the Upper Kharaib Member, which is part of the Thamama Group, is widely distributed across the Middle East, particularly in the Eastern region, and serves as a prolific reservoir in countries such as Qatar, Oman, Saudi Arabia, and Kuwait. The overall succession of the Upper Kharaib Member demonstrates a trend of shallowing and coarsening upward of platform carbonate facies deposition.
- The Upper part of the Upper Kharaib Member is characterized by Shoal-Inner Ramp Facies Association, which exhibits good to very good reservoir quality with porosity ranging from 10-30% and permeability ranging from 100-2000 mD. On the other hand, the Lower-Middle part of the Upper Kharaib Member is dominated by Middle Ramp Facies Association, which displays low to medium reservoir quality with porosity ranging from 10-30% and permeability ranging from 0.1-100 mD. The Middle Ramp Facies Association has an average thickness of 100 ft, accounting for 60% of the total gross thickness of the Upper Kharaib reservoir.
- Reservoir Quality: Reservoir quality is influenced by both depositional characteristics and diagenetic processes. Typically, grain dominated facies exhibit superior reservoir quality compared to mud dominated facies.

- CCS Cluster I or FA1 & FA2 cluster exhibits the best reservoir properties and is considered a desirable candidate for carbon storage, while Rock Type/Cluster II (FA3) shows moderate potential based on its porosity. The Shoal-Inner Ramp Facies Association is identified as the best candidate for carbon storage, considering its properties and potential for structural trapping mechanisms. The Middle Ramp Facies Association presents the second-best option for carbon storage due to its thick portion within the Upper Kharaib reservoir and potential for residual trapping mechanisms. Permeability enhancement, particularly in FA3 rocks, is likely to occur during the CO₂ injection dissolution phase.
- Overall, the Upper Kharaib reservoir represents a capable and ideal candidate for carbon storage and/or CO₂-enhanced oil recovery (CO₂-EOR) purposes in the Middle East. The combination of enhanced oil recovery with carbon capture and storage (CO₂-EOR) presents a promising opportunity in the Middle East region, considering the potential of utilizing the Upper Kharaib reservoir for such purposes.
- Primary CO₂ Migration: Generally, involves vertical or upward movement until encountering low permeability zones, facilitating lateral migration; highly sensitive to low permeability zones (~0.1 mD), potentially impeding upward migration.
- Impact of Baffle Zones: Baffle zones or low permeability zones presence, might could be recognized by well bottom hole pressure breakdown profiles (e.g., FA3 example), enhance storage efficiency by impeding CO₂ upward movement, leading to increased residual and dissolution trapping and broader entrapment.
- Reservoir Complexity and Heterogeneity: Complex lateral variations can limit lateral migration, underscoring the importance of identifying and modelling low permeability

zones for selecting optimal injection/perforation sites. Overall trapping mechanism profile or percentage very impacted by the heterogeneity of the reservoir, lowering the percentage of structural trapping while increasing the percentage of residual and dissolution trapping.

- **Injection Well Placement:** Flank placements prove more efficient for CO₂ storage, slowing down migration compared to crestal placements. The crestal well placement primarily only allow vertical upward migration.

6.2 Recommendations

We acknowledge that there are multiple significant opportunities for improvement in this study, and the following recommendations are provided for further research:

- **Improve Data Quality:** If applicable, obtain additional data such as capillary pressure to enhance the accuracy and reliability of the model. Consider acquiring more comprehensive datasets to reduce reliance on assumptions in modelling parameters.
- **Seal Integrity study:** A detailed seal integrity study will help identify and mitigate potential risks associated with CO₂ leakage, thereby enhancing the overall safety and reliability of the storage site.
- **Study Geomechanics:** Conduct thorough investigations into geomechanically parameters for each rock type or lithofacies. Understanding these parameters is crucial for ensuring storage security and wellbore stability during CO₂ injection.

- **Determine Maximum Injection Rate:** Investigate the maximum injection rates feasible for each rock type or lithofacies. This information is essential for optimizing injection strategies and minimizing risks associated with CO₂ injection.
- **Faults and Fracture within the reservoir:** the presence of faults and fractures were not included in the analysis due to the limited data. Therefore, the results of this study may not fully capture the complexities introduced by faults and fractures in real-world CO₂ storage scenarios. Future studies should aim to incorporate these structural heterogeneities to provide a more comprehensive understanding of their impact on CO₂ storage dynamics and reservoir performance.

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Vitae

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Sani commenced his journey at KFUPM as a graduate student within the Geoscience Department in 2022. His research is centered on measurement and monitoring techniques for CCS projects, specifically in modelling the potential migration routes of CO₂ plumes and investigating the impact of reservoir heterogeneity on plume patterns and trapping mechanism. He is an experienced Professional with a background in Petroleum Geology and has 11 years of experience in a complete cycle upstream oil and gas business, from exploration, development, and well delivery stage of projects (Basin screening, ILX, prospect maturation, Geological Static Modeling, and Well Planning). During his master's program, he published a conference paper presented at the 2023 EAGE 84th Annual Meeting in Vienna, Austria, and gave two technical presentations at the IPTC 2024 international conference in Dhahran, Saudi Arabia.

List of Publications and Presentation Generated from this Thesis

Conference Paper

Yusmananto, S., Fahmi, B., Ferreira, I., Ibrhim, S., & Koeshidayatullah, A. (2023). CO₂ storage and utilization potential in the Middle East: Lessons learned from the Cretaceous carbonate reservoirs. 84th EAGE Annual Conference & Exhibition. Extended abstract available at: <https://doi.org/10.3997/2214-4609.202310207>

Conference Presentation

Yusmananto, S., and Koeshidayatullah, A. (2024). Unveiling The Hidden Dance: Modelling the Impacts of CO₂ Injection on Subsurface Dynamics and Potential Trapping Mechanisms in The Upper Kharaib Carbonate Reservoirs. IPTC-23850