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Presented by : Djamila Boussebsi

Maroua Troub Benhorma

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Modeling of CO_2 Storage in Aquifers Under Geo-Mechanical Risks Using MRST

Defense Committee

Name and Lastname	Academic Rank	Role
Ahmed Abdelmoiz	MCB	President
Asma Hadjadj	MCB	Examiner
Mohamed Riad Youcefi	MCA	Supervisor

Promotion : 2024/2025

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Introduction

1. Background of the study

Climate change is a topical environmental issue which has been linked to the rise in global average temperatures because of increase in greenhouse gases (GHG) such as carbon dioxide (CO_2) and methane in the atmosphere [1]. The level of carbon dioxide in the atmosphere rose by 40% during the 20th and 21st centuries and is now over 400 ppm (parts per million). In 2019, the level of carbon dioxide in the atmosphere was higher than at any time in at least 2 million years [2].

One effective approach to address this issue is by reducing anthropogenic emissions released into the atmosphere. A promising strategy is carbon capture and storage (CCS), which involves capturing CO2 from industrial sources such as coal-fired power plants, transporting it, and injecting it into subsurface geologic formations for permanent storage [3], including saline aquifers, depleted oil and gas reservoirs, unmineable coal seams, and other geological media.

The effectiveness of geological storage depends on a combination of physical and geochemical trapping mechanisms. Injected CO_2 is retained in deep saline aquifers through several mechanisms, including physical trapping, residual trapping, adsorption, solubility trapping, and mineral trapping [4].

However, the CCS process is accompanied by geomechanical risks due to the unavoidable pore pressure buildup, such as caprock failure, reactivation of existing faults, poroelastic response of rock, and well integrity loss. These risks lead to undesirable environmental concerns such as CO_2 leakage to the surface, induced seismicity, and surface uplift [5].

2. Literature Review

A lot of studies have examined the geomechanical properties of subsurface formations responsive to the injection of CO2. Experiences from major CCS demonstration projects such as Sleipner (Norway), In Salah (Algeria), and Weyburn (Canada) have provided significant evidence for the subsurface sensitivity to CO_2 injection. The Utsira Formation is a highly permeable and high-porosity sandstone aquifer overlain by a thick shale caprock, which has enabled efficient pressure dissipation and low geomechanical deformation. For almost 20 years of operation, no significant surface deformation or fault activation has occurred, suggesting stable storage conditions in favourable geological conditions [6]. In addition, monitoring data from Sleipner, including seismic surveys and plume imaging, confirmed the integrity of the caprock and that there were no leakage scenarios, supporting the conclusion that geomechanical risks were negligible under these conditions.

In contrast, the In Salah project in Algeria, which operated from 2004 to 2011, has often been cited as a leading example of CO_2-induced geomechanical change. CO_2 was injected into the water leg of the Krechba gas reservoir (a relatively low permeability sandstone formation), and the pressure buildup under the caprock resulted in a significant elevation of surface uplift. Satellite interferometry identified surface uplift of up to 5 mm/year or more localised above the injection wells [7]. Coupled hydro-mechanical models proposed that this deformation resulted from poroelastic expansion of the reservoir rock, driven by a high porous pressure, as pore pressures are weakly dissipated. Further modelling work showed the potential for fault reactivation under this pressure and that microseismic activity conformed to those stress changes predicted by geomechanical simulations [8]. Published studies reported that In Salah was a key case where site-specific geology, particularly low permeability and compartmentalised pressure zones, increased the need for active monitoring and geomechanical analysis to prevent caprock compromise.

Another case study is the Weyburn project in Canada, where CO_2 injection was done into a mature oil reservoir that had been subjected to decades of pressure depletion due to hydrocarbon production. The depressurization from CO_2 injection alters the in-situ stress field, causing concern for fault movement or caprock fracturing. Geomechanical modelling was used to evaluate the evolution of stress paths and to ensure injection operations did not cross thresholds. The Weyburn site was supported by full baseline characteriszation, including 3D seismic, well logs, and rock mechanics testing, all of which helped a good knowledge of the geomechanical environment and risk reduction [6].

The previous published studies show the range of geomechanical reactions to CO_2 injection, mostly driven by site-specific geologic features, past reservoir conditions, and injection technique. While Sleipner shows that under favorable conditions geomechanical hazards can be low, In Salah and Weyburn show how conditions such as low permeability and past pressure depletion can greatly affect stress fields and need careful modelling and monitoring techniques.

3. Motivation and Contribution (Thesis Objectives)

Using the MATLAB Reservoir Simulation Toolbox (MRST), this thesis presents a comprehensive framework for modelling and optimizing CO_2 storage in deep saline aquifers while accounting for geomechanical risks. The primary objective is to develop a custom MRST-based code that allows the user to input key reservoir and operational parameters, such as permeability, porosity, well locations, well flow rates, and well perforation zones, to simulate pore pressure evolution during CO_2 injection. The resulting pore pressure profiles will be validated against results from CMG (Computer Modelling Group) simulations to ensure consistency and accuracy.

Following validation, the code will compute effective stress and simulate the mechanical response of fractures during injection period by employing the Barton-Bandis model. This coupling provides critical insights into caprock integrity and fracture stability.

A further contribution of this thesis lies in the implementation of an optimization workflow using the Particle Swarm Optimisation (PSO) algorithm. The goal is to maximize CO_2 storage capacity while reducing geomechanical risks by ensuring compliance with criteria such as allowable reservoir pressure, fault and fracture stability thresholds, and safe stress paths. Compared to existing studies, which often oversimplify mechanical coupling or neglect sensitivity analysis, this work provides a more rigorous and flexible simulation-optimisation platform. The thesis concludes with a detailed discussion of results, highlighting the interplay between storage efficiency and geomechanical safety under various reservoir and injection scenarios.

Chapter I. Geological carbon storage: principles and foundations

1. Introduction

In this chapter, we aim to provide a summary of Carbon Capture Storage (CCS), outlining its importance as a strategy for mitigating climate change and its contribution to the reduction of greenhouse gas emissions; a synopsis of the CCS process chain, including capture, transport, and storage; and the importance of geological storage in maintaining long-term CO_2 containment. We will also comprehend how CO_2 is safely stored underground; the chapter then examines the mechanisms of CO_2 trapping in geological formations. This includes the discussions on structural and stratigraphic trapping, residual or capillary trapping, solubility trapping, and long-term mineral trapping, each contributing to the stability and permanence of storage. Then we will introduce the main types of geological storage, such as depleted oil and gas reservoirs and unmineable coal seams, but we will focus on deep saline aquifers since they are the primary focus of this study, as they serve as the target formation of CO2 storage modelling developed in this thesis, highlighting their physical characteristics, storage potential, and associated technical challenges.

Finally, we will present a review of global CO_2 storage projects and the lessons learned from practical applications. all of which have contributed valuable insights into storage performance, monitoring techniques, Through this comprehensive review, the chapter establishes a solid conceptual basis for understanding geological CO_2 storage.

2. Carbon Capture and Storage (CCS)

2.1. Climate Change and the Role of CCS

Greenhouse gases from human activities are the most significant driver of observed climate change since the mid-20th century [9]. Since the Industrial Revolution, humans have been releasing larger quantities of greenhouse gases into the atmosphere. In the past century, that amount has increased dramatically, with the knock-on effect of global warming. Global temperatures have accelerated in the past 30 years and are now the highest since records began [10]. One of the main greenhouse gases is carbon dioxide (CO_2), which is released through natural processes, such as volcanic eruptions, plant respiration, and animals and humans breathing. But the atmospheric CO_2 concentration has increased by 50% since the Industrial Revolution began in the 1800s due to human activities like the burning of fossil fuels and large-scale deforestation. Due to its abundance, CO_2 is the main contributor to climate change.

Carbon capture and storage (CCS) is an important part of the lowest-cost greenhouse gas

(GHG) mitigation portfolio. It is estimated that CCS alone can contribute almost a 20% reduction in emissions by 2050, and the exclusion of CCS can cause up to a 70% increase in the global cost of achieving emission reduction targets [11].

2.2. Overview of the CCS Process Chain

CCS is defined as a system of technologies that integrates three stages: CO_2 capture, transport, and geologic storage (see **Figure I.1**). Each stage of CCS is technically available and has been used commercially for many years.

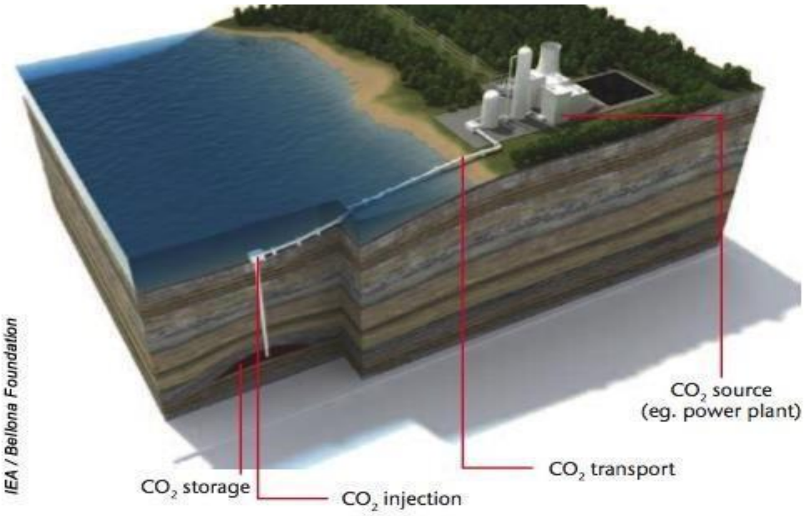


Figure I.1 . The CCS process

CO_2 capture technologies have long been used by industry to remove CO2 from gas streams where it is not wanted or to separate CO_2 as a product gas. There are currently three primary methods for CO_2 capture are post-combustion, pre-combustion, and oxyfuel. Post-combustion involves scrubbing the CO_2 out of flue gases from the combustion process. Oxyfuel involves combusting fuel in recycled flue gas enriched with oxygen to produce a CO_2-rich gas. Pre-combustion uses a gasification process followed by CO2 separation to yield a hydrogen fuel gas. Of these methods, post- combustion CO2 capture using solvent scrubbing is one of the more established for CO2 capture, and there are currently several facilities at which amine solvents are used to capture significant flows of CO2 from flue gas streams. Oxy-fuel combustion has been demonstrated in the steel manufacturing industry at plants up to 250 MW in capacity, and the related oxy- coal combustion method is currently being demonstrated. Pre-combustion CO2 capture from an integrated gasification combined cycle (IGCC) power plant has yet to be demonstrated; however, elements of the pre-combustion capture technology have already been proven in other industrial processes [12].

CO_2 transport has been utilised for over 30 years in North America; over 30 metric tonnes (Mt) of CO2 from natural and anthropogenic sources are transported per year through 6,200 km of CO2 pipelines in the USA and Canada. CO2 is transported predominantly via high-pressure pipeline networks, which present a few regulatory, access, public acceptance, and planning challenges for different regions. Ships, trucks, and trains have also been used for CO2 transport in early demonstration projects and in regions with inadequate storage.

CO_2 storage involves the injection of CO2 into a geologic formation to enhance carbon recovery. The three options for geological CO2 storage are saline formations, oil and gas reservoirs, and deep unminable coal seams [13]. It is expected that saline formations will provide the opportunity to store the greatest quantities of CO2, followed by oil and gas reservoirs. Monitoring data from projects involving injection into depleted oil and gas fields and saline formations has shown that the CO2 performs as anticipated after injection with no observable leakage [4]. Several other projects involving the injection of CO2 into oil reservoirs have also been conducted, primarily in the USA and Canada. Most of these projects use the CO2 for enhanced oil recovery (EOR), but some also intentionally store and monitor CO2 concurrently with EOR operations. The practices in respect to CO2 injection are well-known; however, more experience is needed to improve predictions of CO_2 behaviour at commercial scale. Exploration programmes are also needed to locate and characterise suitable storage sites, particularly deep saline formations.

2.3. Importance of Geological Storage

One of the primary advantages of geological storage is its capacity to handle large volumes of CO_2, making it a scalable solution for emissions from industrial sources and power plants. The process relies on natural trapping mechanisms, including structural, capillary, solubility, and mineral trapping, which collectively prevent CO_2 from migrating to the surface [14]. For instance, CO_2 can react with minerals in basalt formations to form stable carbonates, a process known as carbon mineralisation [15].

3. Types of Geological Storage Sites

There are many sedimentary regions in the world variously suited for CO2 storage. In general, geological storage sites should have **(1)** adequate capacity, **(2)** injectivity**, (3)** containment, a satisfactory sealing caprock or confining unit, and **(4)** a sufficiently stable geological environment to avoid compromising the integrity of the storage site. Criteria for assessing basin suitability [16–18] include basin characteristics (tectonic activity, sediment type, geothermal and hydrodynamic regimes); basin resources (hydrocarbons, coal, salt); industry maturity; infrastructure; and societal issues such as level of development, economy, environmental concerns, public education, and attitudes [19]. The efficiency of CO2 storage in geological media, defined as the amount of CO2 stored per unit volume [20], increases with increasing CO2 density. Storage safety also increases with increasing density, because buoyancy, which drives upward migration, is stronger for a lighter fluid. Density increases significantly with depth while CO2 is in the gaseous phase, increases only slightly or levels off after passing from the gaseous phase into the dense phase, and may even decrease with a further increase in depth, depending on the temperature gradient [21]. The depth of the storage formation (leading to increased drilling and compression costs for deeper formations) may also influence the selection of storage sites.

The pressure and flow regimes of formation waters in a sedimentary basin are important factors in selecting sites for CO2 storage [22]. Injection of CO2 into formations overpressured by compaction and/or hydrocarbon generation may raise technological and safety issues that make them unsuitable. The capacity of a reservoir will be limited by the need to avoid exceeding pressures that damage the caprock [19]. Reservoirs should have limited sensitivity to reductions in permeability caused by plugging of the near-injector region and by reservoir stress fluctuations [23]. Storage in reservoirs at depths less than approximately 800 m may be technically and economically feasible, but the low storage capacity of shallow reservoirs, where CO2 may be in the gas phase, could be problematic [19]. **Figure I.2** shows the options for

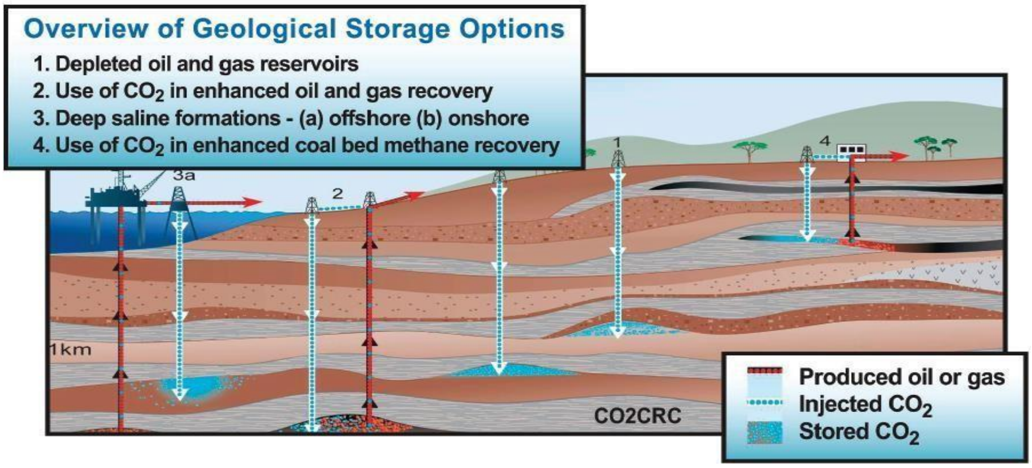


Figure I.2. Options for geological storage in sedimentary rocks [24].

3.1. Depleted Oil and Gas Reservoirs

CO2 storage in depleted oil and gas reservoirs is considered one of the most effective storage options because of several advantages, including that (i) depleted oil and gas reservoirs have been extensively studied before and during the hydrocarbon exploration stage, including the storage capacity. (ii) Surface and underground infrastructure, e.g., injection wells and pipelines, already exists and can be utilised for the storage process either without or with only minor modifications; and (iii) the injection of gases such as CO2 as an EOR technique has been widely known and employed within the oil and gas industry, and, therefore, such experience can be used for the storage process. In addition, oil and gas reservoirs are valuable hydrocarbon-containing analogues that can be used to demonstrate the effectiveness of caprock or seal over geological periods.

3.2. Deep Saline Aquifers

Saline aquifers are defined as porous and permeable reservoir rocks that contain saline fluid in the pore spaces between the rock grains. They generally occur at depths greater than aquifers that contain potable water. Usually, due to its high saline proportion and its depth, the water contained cannot be technically and economically exploited for surface uses. There is currently only one CO2 storage site worldwide in a saline aquifer. This is at Sleipner in the North Sea, where CO2 is being injected into the Utsira Sandstone Formation. The amount of CO2 that could potentially be stored in saline aquifers for a reasonable amount of time is very large. The basic criteria for all potential storage sites are as follows. Potential storage sites should be in a geologically stable area, as tectonic activity could create pathways for the CO_2 to migrate out of the reservoir through the cap rock (low permeability seal) into the overburden and potentially to the surface. Saline aquifers can be sandstones or limestones, but to be a potential storage reservoir for CO_2, they must have the following properties:

Size: The reservoir must be large enough to be able to store the quantities of CO_2 planned, e.g., the lifetime emissions of one power plant. The capacity of the storage site is the volume of pore spaces in the aquifer that could be occupied by CO2

Porosity and permeability: These parameters must be sufficiently high to both provide sufficient volume for the CO_2 and to allow injection of the CO2. As CO2 is injected into the pore spaces of the reservoir rock, it displaces much of the in-situ pore fluid. If the permeability of the rock is low or there are barriers to fluid flow, such as faults, injection will cause a progressive increase in the fluid pressure centred on the injection point. This will limit the rate at which CO2 can be injected and may ultimately limit the amount of CO2 that can be practically stored. Highly structurally compartmentalised reservoirs are likely, therefore, to be less suited to CO2 storage than large unfaulted or high-permeability reservoirs.

Depth: Usually only aquifers below 800 m below sea level are considered for CO2 storage. At temperatures and pressures in the subsurface of around 600 to 800 m, CO_2 exists in its dense phase as a liquid and occupies much less pore volume than in its gaseous phase. 1 t of CO2 occupies 509 m^3 at surface conditions of 0°C and 1 bar. The same amount of CO2 occupies only 1.39 m^3 at 1000 m subsurface conditions of 35°C and 102 bar. (see **Figure I.3**) CO2 density at a geothermal gradient of 30oC/km. In addition to a reservoir rock, an overlying “cap rock” that is impermeable to the passage of CO2 is required. When CO2 is injected into a reservoir, it is more buoyant than the reservoir fluid in the pore spaces and will rise to the top of the reservoir.

The cap rock, an impermeable, low-porosity layer, will prevent the CO_2 from migrating vertically, and so the CO_2 becomes trapped at the top of the reservoir underneath the cap rock. The cap rock provides the main trapping mechanism for the long- term security of storage. Cap rocks are usually shales, mudstones, or evaporite layers. The cap rock should ideally be unfaulted, as unsealed faults would provide migration pathways for the CO_2 out of the reservoir. In some situations, for example in faulted salt layers, faults can become resealed and therefore do not present a leakage/seepage pathway. However, their sealing nature would need to be confirmed by detailed analysis of the storage age site to ensure the integrity of the storage site.

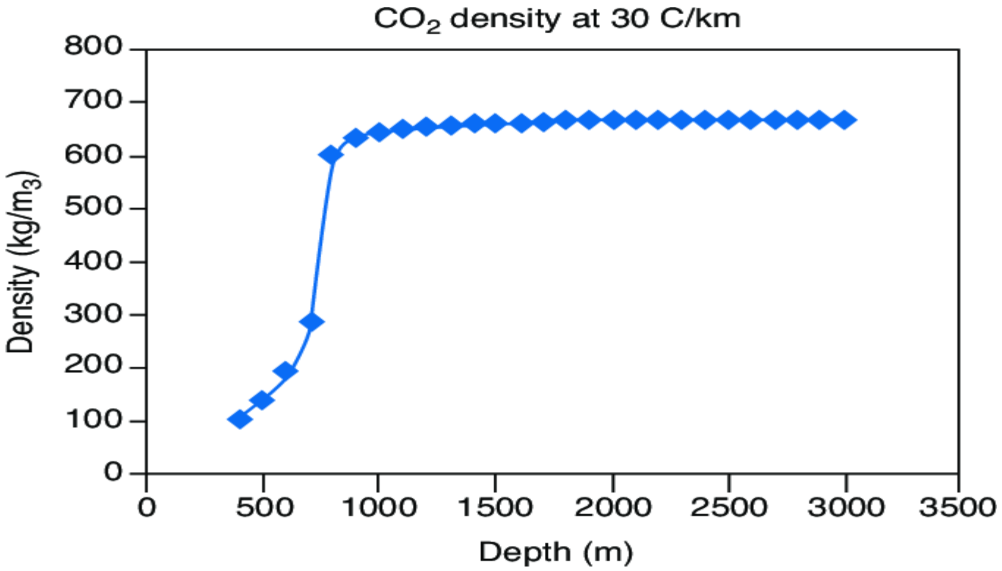


Figure I.3. CO_2 density at a geothermal gradient of 30°C/km

Storage of CO2 in saline aquifers can be in both “confined” and “unconfined” aquifers (see **Figure I.4**). Storage in confined aquifers relies on trapping of the buoyant CO_2 by structural (e.g., anticlines) and/or stratigraphic (e.g., sandstone pinchout) features and is closely analogous to gas storage schemes in hydrocarbon fields, or indeed, to natural gas storage in subsurface aquifers. In simple structural traps, volumes and migration pathways of the injected CO_2 can be predicted, and reservoir models constructed with a higher degree of certainty than in an unconfined aquifer, where the lateral boundaries are not well known. The potential storage volume in such structural traps can be very large, e.g., in the closed structures of Triassic rocks in the Southern North Sea. Here the Bunter Sandstone Formation has four-way dip closed anticlines formed by movement of the underlying Zechstein Salt into pillows and diapirs. In such cases it may not be necessary to utilise the entire capacity of the regional aquifer but only use the structural closures, therefore retaining large volumes ume of CO_2 in defined areas. This may aid the monitoring of the CO_2 over large time scales. The estimated storage capacity of the Bunter Sandstone Formation (regional extent) is 620,000 Mt. Of that total storage capacity, it is estimated 89,404 Mt of CO_2 could be stored in the closures alone. Storage in unconfined aquifers involves the injection of CO2 into large regional aquifers with no specific large structural or stratigraphic closures as a target. Once the CO_2 has been injected, it migrates upwards along the most permeable pathway until it encounters the impermeable cap rock. This provides a barrier to further vertical movement; the then migrates largely laterally, being driven by buoyancy to structurally higher levels along the cap rockreservoir boundary [24].

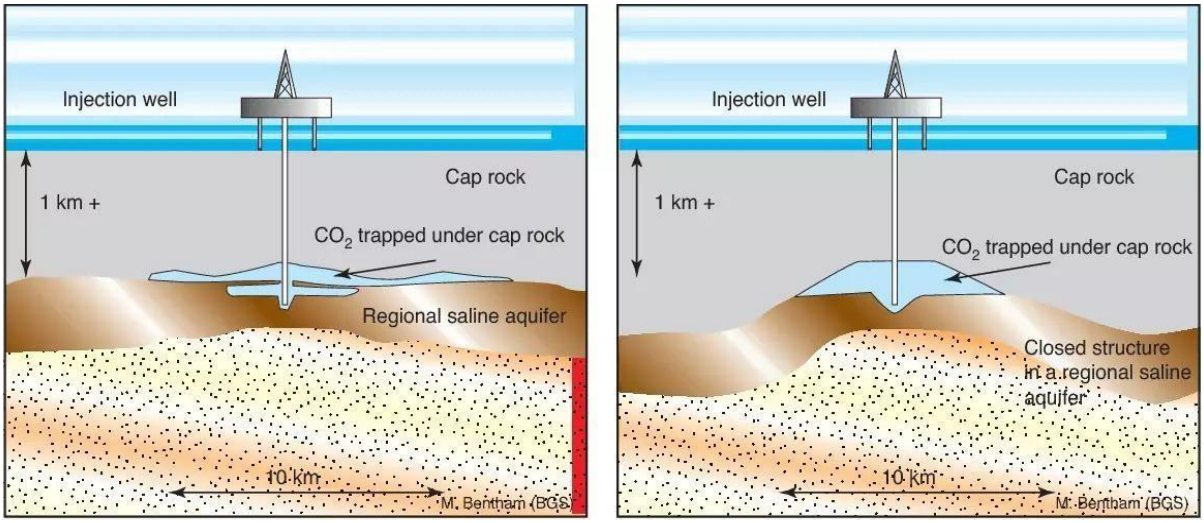


Figure I.4. Conceptual diagrams of storage in unconfined and confined aquifers

4. Mechanisms of CO_2 Trapping in Geological Formations

4.1. Geochemical trapping

When carbon dioxide (CO_2) is injected into a deep saline aquifer, it tends to migrate upward due to buoyant forces arising from the density difference between CO_2 and the brine. This migration continues until the CO_2 reaches the caprock, where it accumulates and forms a plume that spreads laterally due to the impermeability of the caprock [25].

During this process, a portion of the CO_2 dissolves into the formation brine, a mechanism referred to as solubility trapping. Solubility trapping is significant because once CO_2 is dissolved in the brine, it no longer exists as a separate buoyant phase, which eliminates its upward mobility [25, 26].

The dissolved CO_2 undergoes a sequence of geochemical reactions with both the formation water and the host rock. Initially, CO_2 dissolves in water, forming carbonic acid, which dissociates into bicarbonate and carbonate ions, as represented by the chemical reactions

$$CO_2(g) + H_2O \leftrightarrow H_2CO_3 \leftrightarrow HCO_3^{-} + H^{+} \leftrightarrow CO_3^{2-} + 2H^{+}.$$

These reactions can lead to a rise in pH and the formation of ionic species as the surrounding rock begins to dissolve. Over time, this may result in the precipitation of stable carbonate minerals, a process known as mineral trapping—the most permanent and desirable form of geological CO_2 storage. Although mineral trapping is relatively slow, potentially taking thousands of years, its long-term permanence and the large potential storage capacity in some geologic formations make it an important mechanism for sustainable CO_2 sequestration [26].

4.2. Hydrogeological trapping

There are four main trapping mechanisms that can securely store CO2, namely, structural/stratigraphic, residual, solubility, and mineral trapping [27].

a. Structural and Stratigraphic Trapping

Initially, physical trapping of CO2 below low-permeability seals (caprocks), such as very-low-permeability shale or salt beds, is the principal means to store CO2 in geological formations. In some high-latitude areas, shallow gas hydrates may conceivably act as a seal. Sedimentary basins have such closed, physically bound traps or structures, which are occupied mainly by saline water, oil, and gas. Structural traps include those formed by folded or fractured rocks. Faults can act as permeability barriers in some circumstances and as preferential pathways for fluid flow in other circumstances [28].

Stratigraphic traps are formed by changes in rock type caused by variation in the setting where the rocks were deposited. Both types of traps are suitable for CO_2 storage.

b. Residual or Capillary Trapping

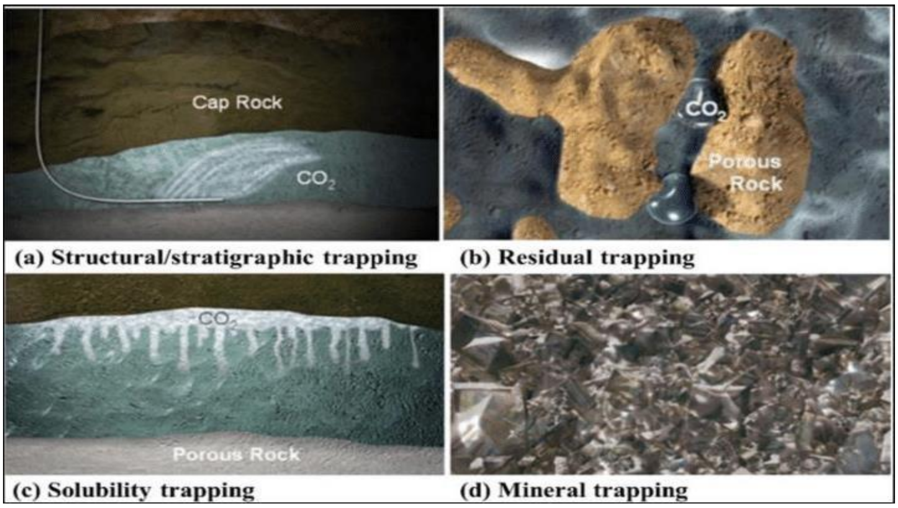
In this mechanism, the injected CO2 initially displaces the fluid as it progresses through the porous rock. As CO2 continues to move, the displaced fluid returns and disconnects and traps the remaining CO2 within pore spaces (**Figure I.5**). It is reported that the phenomenon does not happen within structural and stratigraphic traps but only where water drainage occurs during CO_2 injection.

4.3. Solubility Trapping

In this mechanism, CO2 dissolves in brine, reducing the volume of free-phase CO_2 (**Figure I.5**). CO_2 dissolution increases the brine density and can induce a gravitational instability, which accelerates the transfer of injected CO2 to CO_2-lean brine.

4.4. Mineral Trapping

In this mechanism, CO2 is involved in geochemical reactions with saline water and minerals in host rock, leading to the precipitation of carbonate phases that effectively lock up the CO2 in immobile secondary phases for geological timescales.



(a) Structural/stratigraphic trapping (b) Residual trapping
(c) Solubility trapping (d) Mineral trapping

Figure I.5.This process is slower than solubility trapping and takes place over a longer geologic timescale [29].

5. Global CO_2 Storage Projects and Lessons Learned

5.1. Sleipner Project (North Sea, Norway)

The Sleipner Project, operated by Statoil in the North Sea about 250 km off the coast of Norway, is the first commercial-scale project dedicated to geological CO2 storage in a saline formation. The CO2 (about 9%) from the Sleipner West Gas Field is separated and then injected into a large, deep, saline formation 800 m below the seabed of the North Sea. The Saline Aquifer CO2 Storage (SACS) project was established to monitor and research the storage of CO2. From 1995, the IEA Greenhouse Gas R&D Programme has worked with Statoil, which will arrange the monitoring and research activities. Approximately 1 MtCO2 is removed from the produced natural gas and injected underground annually in the field. The

CO2 injection operation started in October 1996, and by early 2005, more than 7 MtCO2 had been injected at a rate of approximately 2700 t day–1. Over the lifetime of the project, a total of 20 $MtCO_2$ is expected to be stored. A simplified diagram of the Sleipner scheme is given in **Figure I.6**. The saline formation into which the CO2 is injected is a brine-saturated unconsolidated sandstone about 800–1000 m below the sea floor The formation also contains secondary thin shale layers, which influence the internal movement of injected CO2. The saline formation has a very large storage capacity, on the order of 1–10 $GtCO_2$. 2. The top of the formation is flat on a regional scale, although it contains numerous small, low-amplitude closures. The overlying primary seal is an extensive, thick shale layer. This project is being carried out in three phases. Phase 0 involved baseline data gathering and evaluation, which was completed in November 1998

Phase 1 involved the establishment of project status after three years of CO2 injection. Five main project areas involve descriptions of reservoir geology, reservoir simulation, geochemistry, assessment of need and cost for monitoring wells, and geophysical modelling.

Phase 2, involving data interpretation and model verification, began in April 2000. The fate and transport of the CO2 plume in the storage formation has been monitored successfully by seismic time-lapse survey.

The surveys also show that the caprock is an effective seal that prevents CO2 migration out of the storage formation. Today, the footprint of the plume at Sleipner extends over an area of approximately 5 km^2. Reservoir studies and simulations covering hundreds to thousands of years have shown that CO2 will eventually dissolve in the pore water, which will become heavier and sink, thus minimising the potential for long-term leakage [30].

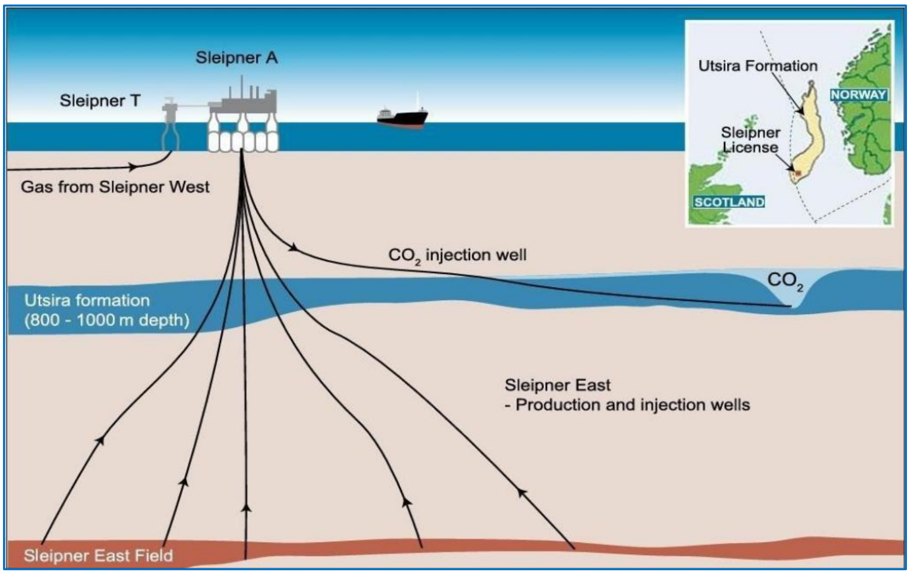


Figure I.6. Simplified diagram of the Sleipner CO2 Storage Project. Inset: location and extent of the Utsira formation.

5.2. In Salah Project (Algeria)

The In Salah Gas Project, a joint venture among Sonatrach, BP, and Statoil located in the central Saharan region of Algeria, is the world’s first large-scale CO2 storage project in a gas reservoir [31]. The Krechba Field at In Salah produces natural gas containing up to 10% CO2 from several geological reservoirs and delivers it to markets in Europe after processing and stripping the CO2 to meet commercial specifications. The project involves re-injecting the CO2 into a sandstone reservoir at a depth of 1800 m and storing up to 1.2 $MtCO_2\ yr^{-1}$. Carbon dioxide injection started in April 2004, and over the life of the project, it is estimated that 17 MtCO2 will be geologically stored. Long-reach (up to 1.5 km) horizontal wells are used to inject CO2 into the 5- mD permeability reservoir. The Krechba Field is a relatively simple anticline. Carbon dioxide injection takes place down-dip from the gas/water contact in the gas-bearing reservoir. The injected CO2 is expected to eventually migrate into the area of the current gas field after depletion of the gas zone. The field has been mapped with three- dimensional seismic and well data from the field. Deep faults have been mapped, but at shallower levels, the structure is unfaulted. The storage target in the reservoir interval therefore carries minimal structural uncertainty or risk. The top seal is a thick succession of mudstones up to 950 m thick. A preliminary risk assessment of CO2 storage integrity has been carried out, and baseline data acquired. Processes that could result in CO2 migration from the injection interval have been quantified, and a monitoring programme is planned to involve a range of technologies, including noble gas tracers, pressure surveys, tomography, gravity baseline studies, microbiological studies, four-dimensional seismic and geomechanical monitoring.

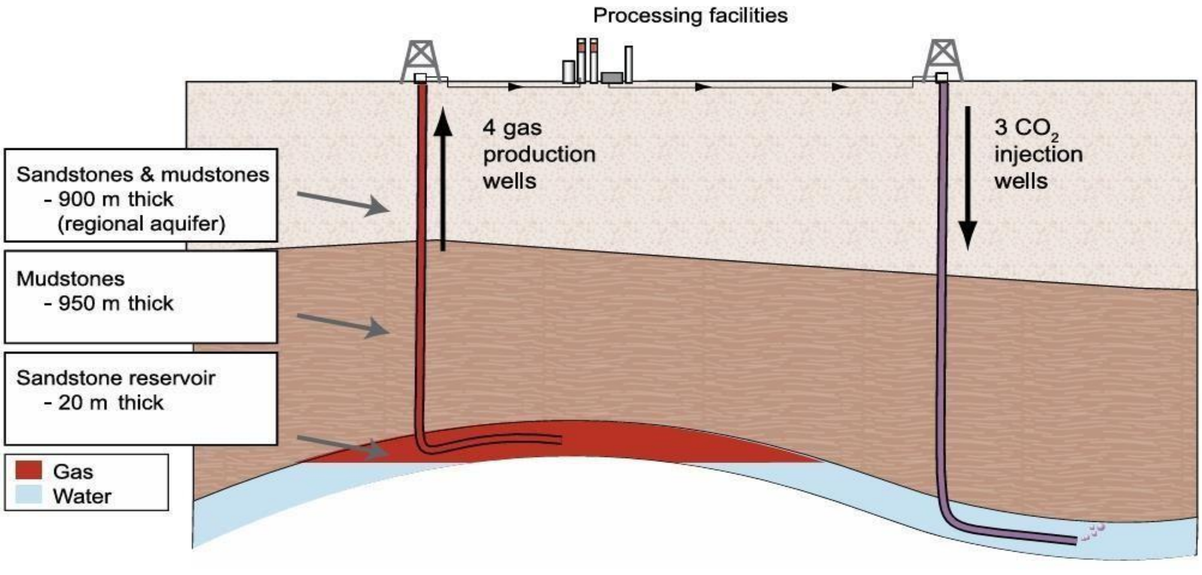


Figure I.7. Schematic of the In Salah Gas Project, Algeria. One MtCO2 will be stored annually in the gas reservoir. Long- reach horizontal wells with slotted intervals of up to 1.5 km are used to inject CO2 into the water-filled parts of the gas reservoir

Chapter II. Geomechanical risks associated with CO_2 storage

1. Introduction

When CO2 is injected and stored into an underground geological structure, the pore pressure buildup is unavoidable. The change of the pore pressure redistributes the stress status and induces the poroelastic responses at the caprock and target formation. If severe, it may lead to geomechanical hazards such as leakage of the injected CO2, surface uplift, and induced seismicity, which are major environmental concerns during the CCS project. In addition, the well integrity should be considered because the injected CO2 could be leaked through any component of the well that was designed to be used as the flowing path. Uncontrolled release of injected fluid can shorten the life cycle of the well, and it may lead to CO2 leakage. Therefore, establishment of the optimal CCS design considering the geomechanical risks is important to perform the environmentally safe project and to achieve public acceptance. There are geomechanical risks during a CCS process, but in-vestigations of causes, mechanisms, and post-analysis methods have not yet been conducted.

2. What is a geomechanical risk ?

Structural instabilities in subsurface formations are triggered by changes in pore pressure and stress conditions resulting from CO_2 injection. As CO_2 is injected, the pore pressure in the target reservoir increases, which can exceed the formation's fracture pressure, potentially causing tensile fracturing near the wellbore. Enhanced permeability techniques like hydraulic fracturing or acidizing are often employed to mitigate this risk.

Fault reactivation is another major geomechanical risk. The increase in pore pressure can reduce effective normal stress on pre-existing faults, potentially triggering slip events and induced seismicity.

3. Cap rock collapse

Since a caprock is an impermeable formation that isolates the target formation, its stability takes a major role in securing the geological structure by preventing leakage of the injected CO2. The most vulnerable portion for the shear failure during the CO2 injection is the interface of the caprock-reservoir where the largest pore pressure buildup is expected. If there is an existing fault in the target reservoir, it can be reactivated once the friction at the fault plane is reduced by the pore pressure.

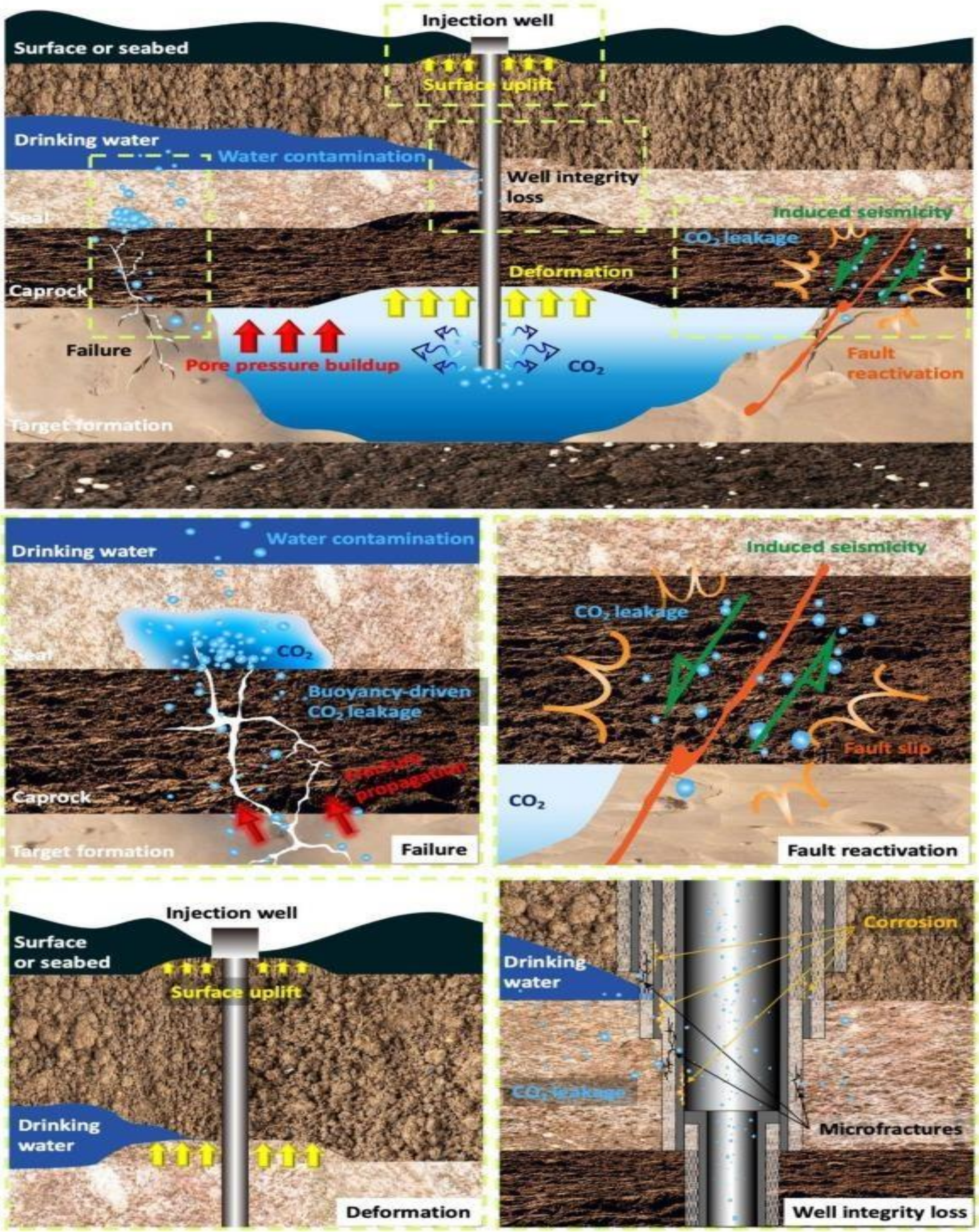


Figure II.1. Mechanisms of the potential geomechanical risks during CCS process

When the failure is occurred, the failure plane can be propagated to the caprock, which may induce the CO_2 leakage. To avoid the undesirable consequence, the geomechanical analysis needs to be performed to identify the potential instability of the caprock when the CCS project is designed. In this section, the rock effective stress principle and possible failure types are addressed with the Mohr-Coulomb failure criterion for the caprock failure and fault reactivation analysis.

3.1. Effective stress principle of the rock

The effective stress principle of rock is a fundamental concept in rock mechanics that describes how the stress within a rock mass is partitioned between the solid rock skeleton and the pore fluids contained within its pores. It was first introduced by Terzaghi in the 1920s and remains central to understanding rock deformation, strength, and failure.

a. Definition and Basic Concept

Effective stress (σ') in rock is defined as the difference between the total stress (σ) applied to the rock and the pore fluid pressure (P_f) within the rock's void spaces:

$$\sigma' = \sigma - P_f$$

This means the effective stress is the net stress that actually acts on the rock grains or solid matrix, controlling how the rock deforms and fails. The pore fluid pressure counteracts some of the applied stress, effectively reducing the stress borne by the rock skeleton.

b. Meaning and Implications

- The total stress (σ) includes all forces acting on the rock, such as overburden pressure or tectonic stresses.
- Pore fluid pressure (P_f) acts isotropically within the pores and tends to push the grains apart, reducing the load carried by the rock framework.
- Effective stress governs the mechanical behavior of the rock, including volumetric strain, shear strength, and failure mechanisms.
- Changes in pore pressure can significantly influence rock stability, for example, increasing pore pressure reduces effective stress and can lead to rock fracturing or failure [32].

c. Applications

- Effective stress is crucial in predicting rock behavior in subsurface engineering, such as reservoir geomechanics, hydraulic fracturing, tunneling, and slope stability.

- It explains how fluid injection or withdrawal changes pore pressure, thereby affecting rock strength and deformation.
- It is used to calculate the stress state that controls fracture initiation and propagation in rocks [33].

4. Fault reactivation

A fault can function as a seal or a conductive channel that needs to be taken into account when a CCS process is designed. In a geomechanical point of view, faults can be reactivated which consequently leads to unexpected CO2 leakage and undesirable seismicity [8]. During the CCS process, the CO2 plume migrates out fromthe place of injection and the region affected by the reservoir pore pressure change is enlarged. If the plume reaches the pre-existing discontinuities such as fault and fracture zone, they experience an effective normal stress decrease. When the stress drops under a specific level, the friction of the fault plane, the fault will destabilize and slip. Many studies adopted numerical approaches to predict the fault slip during pore pressure buildup. Commercial simulators such as GEM, COMSOL, and ECLIPSE are widely used to model the reservoir geometry and to characterize the flow behaviors. The geomechanical properties are added with simulators like TOUGH, FLAC3D, and the geomechanical tools of CMG and PETREL to couple the flow behaviors with the geomechanical responses of the formation developed and demonstrated a flow-geomechanical coupled modeling framework to evaluate the stability of the faults during CO2 storage enhanced oil recovery in the Farnsworth Unit (FWU) oil field in Texas, United States. Through this method, they founded out that the pressure buildup caused by water and CO2 injection causes volumetric contraction and expansion of the reservoir and changes in the total and effective stresses in the overburden-reservoir-underburden structures. They also analyzed that these changes lead to alter in shear and effective normal stress for the three major faults in the FWU. The CO2 injection rate and pore pressure should constantly be monitored at all stages of the CCS project especially when there is an adjacent fault. Rutqvist et al. [34] described procedures to determine the maximum sustainable injection pressure by a shear-slip analysis. A numerical analysis was also performed using TOUGH FLAC, which determined the maximum sustainable CO2 injection pressure.

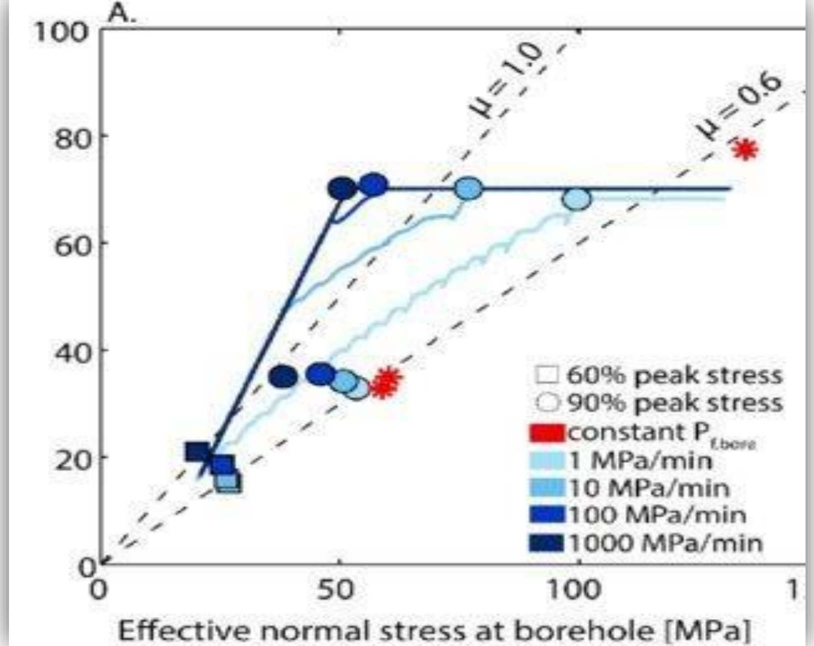


Figure II.2. Experimental results of static fault reactivation with different injection speeds. (Square: onset of fault slip while the initial stress is 60% of the peak. Circle: onset of fault slip while the initial stress is 90% of the peak.)

5. Induced Seismicity

5.1. Mechanisms and Triggers

Induced seismicity occurs when a failure plane is created in the formation or when an existing fault is reactivated, often due to excessive pore pressure buildup during a Carbon Capture and Storage (CCS) process. This pore pressure increase can lead to rock failure or fault reactivation, resulting in seismic activity. If severe, induced seismicity can be significant and perceivable by humans, threatening both the environment and public acceptance of CCS projects [35, 36]. A renowned example of induced seismicity due to fluid injection occurred in Oklahoma in 2011 and 2012, where a seismic event of magnitude 5.6 destroyed buildings and injured people [37]. Keranen et al. [35] analyzed the relationship between wastewater injection and induced earthquakes in Oklahoma, finding that a large time gap between injection and seismic events is possible. The study also emphasized that adjusting the volume of injected fluids is essential to prevent reaching critical reservoir pressures that could trigger fault slips. Weingarten et al. [61] further analyzed the relationship between induced seismicity and injection well types, identifying a higher occurrence of seismic activity in saltwater disposal (SWD) wells than in enhanced oil recovery (EOR) wells. The study concluded that higher maximum injection rates corresponded to higher seismicity in SWD wells and recommended analyzing a range of geological, hydrogeological, and operational conditions associated with induced seismicity.

5.2. Risk Assessment and Monitoring

To manage induced seismicity risks, it is crucial to control the pore pressure by managing the injection rate during the design stage of CCS processes. Verdon et al. [38] developed a geomechanical model for the Weyburn CO2 storage site to depict pore pressure changes and fracture potential, helping assess the risk of injection-induced seismicity. Zoback [39] proposed minimizing pore pressure buildup as a key strategy to reduce induced seismicity risks and recommended joint efforts from operators and regulators to establish operating protocols in areas at risk, commonly referred to as the traffic-light system. This system limits injection rates based on seismic activity levels and can stop injection processes if seismic activity becomes severe. Sites in Basel, Switzerland, and Ohio, United States, have adopted such systems to mitigate induced seismicity [40]. Yeo et al. [41] investigated the 2017 Pohang Mw 5.5 earthquake, linking pore pressure changes to seismic events and emphasizing the need for monitoring and controlling CO2 injection rates and pressure during CCS projects to avoid seismicity. Additionally, Alghannam and Juanes [42] reported that injection-induced earthquakes are more strongly influenced by the injection rate than by the total injection volume. Using a poroelastic model based on rate-and-state friction theory, the study concluded that induced earthquake risk is higher when the injection period is shorter for a fixed injection volume.

6. Reservoir deformation

Reservoir deformation during carbon dioxide (CO2) capture and storage (CCS) is a critical geomechanical concern arising primarily from changes in pore pressure and chemical interactions within the reservoir rock. When large volumes of CO2 are injected into deep geological formations such as depleted oil and gas fields or saline aquifers, the increased pore pressure induces a poroelastic response in the rock, often causing deformation of the reservoir and surrounding formations.

Key aspects of reservoir deformation during CO2 injection include:

- **Poroelastic deformation:** Injection increases pore pressure, reducing effective stress and causing the reservoir rock to expand or deform elastically. This can lead to ground surface uplift or subsidence depending on the reservoir and caprock properties.
- **Visco-plastic and creep deformation:** In depleted reservoirs like chalk formations, CO2 injection can trigger both expansion due to pressure build-up and continued compaction from viscous deformation processes initiated during prior hydrocarbon production. These

competing effects influence the vertical movement of the reservoir top and long-term stability.

- **Chemo-hydro-mechanical effects:** Injected CO2 acidifies formation brine, triggering mineral dissolution and precipitation reactions that alter rock porosity, permeability, stiffness, and strength. These chemical changes can exacerbate deformation by weakening the rock matrix or, conversely, improve sealing through mineral precipitation. Such coupled processes affect reservoir injectivity, integrity, and caprock sealing capacity over time and space.
- **Fault and fracture interaction:** Deformation can influence fault zones, potentially creating leakage pathways for CO2 if faults are reactivated or if fractures propagate due to stress changes.
- **Monitoring deformation:** Satellite-based geodetic techniques like InSAR have been successfully applied to monitor ground surface deformation related to CO2 injection at various sites. These methods provide centimeter to sub-centimeter resolution of uplift or subsidence patterns, enabling assessment of reservoir behavior and storage safety.

In summary, reservoir deformation during CO2 capture involves complex mechanical and chemical interactions that can lead to expansion, compaction, and changes in rock properties. Understanding and monitoring these processes is essential to ensure the long-term integrity and safety of geological CO2 storage.

7. Well Integrity Loss

During the process of capturing and injecting carbon dioxide (CO2) into deep geological formations via wells (Class VI wells), well integrity loss is a critical concern that can lead to the unintended migration or leakage of CO2. This leakage poses risks to underground sources of drinking water and the environment.

7.1. Causes of Well Integrity Loss During CO2 Injection

a. Mechanical Stress and Pressure Variations

- Pressure increases in the storage reservoir due to CO2 injection can cause mechanical stress on well components, potentially leading to fractures or failures in casing and cement.
- variations during injection can also induce mechanical stresses affecting well integrity.

b. Legacy Wells and Incomplete Plugging

- Old or abandoned wells penetrating the CO2 storage formation, especially those drilled before current standards, may lack proper cement plugs or have deteriorated plugs, serving as potential leakage pathways for CO2.
- Improper plugging or incomplete cementing during well abandonment increases the risk of CO2 migration along the wellbore.

7.2. Consequences of Well Integrity Loss

- Leakage of CO2 into overlying aquifers can contaminate underground drinking water sources either by direct CO2 migration or by forcing brine into these aquifers under pressure.
- Environmental damage, regulatory penalties, loss of public trust, and financial losses for operators can result from containment failure.

In summary, well integrity loss during CO2 capture and injection in water wells arises mainly from chemical corrosion, mechanical stresses, and legacy well issues. Preventing integrity loss requires rigorous engineering, monitoring, and management to ensure long-term containment and protection of drinking water resources.

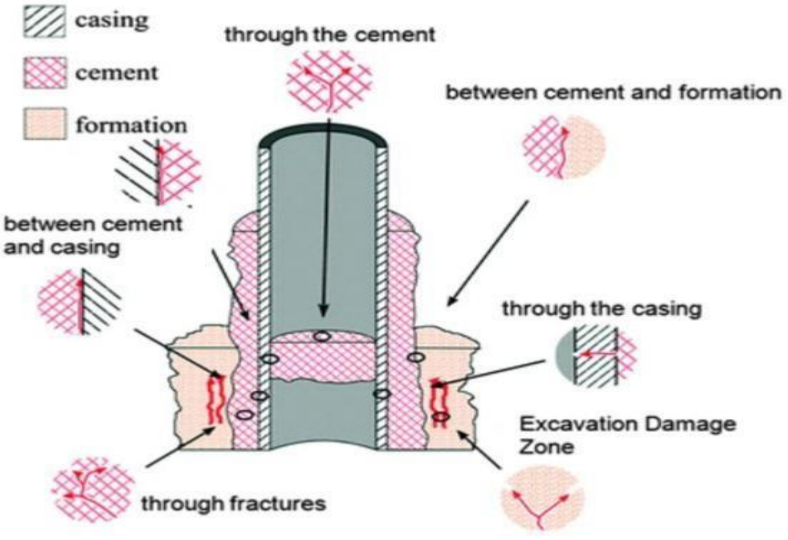


Figure II.3. Possible leakage pathways around the well.

8. Solutions to geomechanical risks

Solutions to geomechanical risks associated with co2 injection involve a combination of careful assessment, monitoring, and engineering strategies to ensure safe and effective containment. Key approaches include:

8.1. Comprehensive Geomechanical Risk Assessment and Modeling

Conduct coupled geomechanics-dynamic-thermal modeling to evaluate changes in stresses, rock mechanical properties, and deformation due to CO2 injection. This modeling integrates reservoir pressure, CO2 concentration, water saturation, and temperature data to predict risks such as fault reactivation, caprock failure, and well integrity breaches.

Use flow-geomechanical coupled simulations to analyze the impact of pressure buildup on reservoir and caprock stability, fault behavior, and surface deformation, enabling optimization of injection schemes to avoid exceeding fracture pressures.

8.2. Injection Management

- Control injection rates to prevent excessive pore pressure buildup that could induce tensile fractures or fault slip. Maintaining pressure below fracture and fault reactivation thresholds is critical.
- Employ well stimulation methods such as hydraulic fracturing or acidizing near the wellbore to enhance permeability and reduce injection pressures when necessary.

8.3. Well Integrity Protection

- Monitor and maintain well integrity to prevent CO2 leakage through damaged casing or cement. Address chemical corrosion risks by selecting materials resistant to CO2-induced degradation and by regular inspection and remediation of well components.
- Design completions to withstand axial loading and reservoir compaction stresses to avoid buckling or cement failure.

8.4. Fault and Caprock Stability Management

- Identify and characterize faults and caprock seals to ensure they can maintain integrity under injection-induced stress changes. Use Mohr-Coulomb failure criteria and geomechanical models to predict fault reactivation and caprock failure risks.
- Implement pressure relief strategies such as relief wells to control pore pressure distribution and reduce fault slip risk.

8.5. Monitoring and Adaptive Management

- Continuously monitor surface uplift, induced seismicity, and subsurface pressure changes to detect early signs of geomechanical issues.

- Adapt injection operations based on monitoring data and model predictions to mitigate emerging risks and ensure long-term containment.

These solutions are part of an integrated workflow for carbon capture and storage (CCS) projects, which is essential for safe CO2 containment and to mitigate leakage risks in hydrocarbon fields, saline aquifers, and other geological formations worldwide.

Chapter III. Numerical simulation of modeling of CO_2 storage in saline aquifers under geomechanical risks

1. CO_2 injection simulation using MRST

1.1. Workflow

This section presents the simulation framework and results of CO2 injection into deep saline aquifers, with a specific focus on assessing geomechanical risks such as caprock failure and leakage. The numerical modelling was carried out using the MATLAB Reservoir Simulation Toolbox (MRST), an open-source and extensible platform developed by SINTEF for reservoir flow simulation [43]. The model represents a vertical cross-section of a layered aquifer- caprock system and includes detailed petrophysical, fluid, and structural characteristics relevant to CO_2 storage.

Two simulation scenarios are investigated: a base case with no leakage, in which the caprock remains intact, and a second case where elevated pore pressures induce geomechanical failure, resulting in increased permeability and CO_2 migration beyond the storage formation. The injection schedule in both scenarios is controlled using MRST's rampup Timesteps function to simulate gradual changes in injection rate, thereby mimicking real-world operational practices. Pressure and saturation distributions are analyzed to understand plume migration, storage efficiency, and seal integrity over a 10-year period (5 years of injection followed by 5 years of monitoring).

Although MRST does not include fully coupled geomechanical modelling, this study employs Barton and Bandis model to dynamically alter permeability in response to effective stress in the caprock layer. This allows the simulation to capture key fracture- triggering mechanisms without the need for external coupling.

1.2. Model parameters used in simulation

In this study, a comprehensive 2D reservoir model was constructed to simulate CO_2 storage behavior using MRST. The reservoir model consists of multiple layers with varying geological properties, including permeability, porosity, and rock mechanics parameters. Boundary conditions were applied to mimic real-world reservoir conditions, with injection well strategically placed within the reservoir. **Table I.1** presents full description of the 2D model created for simulating the CO_2 injection. As shown in this table, 33 layers were defined to represent the subsurface structure, with particular emphasis on layer 12 as sealing shale cap rocks. This layer was designated to undergo cap rock failure modeling using the Barton/Bandis model to simulate their mechanical integrity under stress.

In the rock properties section, the porosity of the layers was uniformly defined as 0.13 across the entire reservoir model to represent the pore volume fraction within the rock matrix. Additionally, the permeability the permeability was set to 15 milliDarcies (mD) for all layers except for the cap rock layer, which is layer 12, where lower permeability values of 10^{-6} mD, reflecting their impermeable nature and limited fluid flow capacity.

One vertical injector well has been strategically placed for the injection of CO_2 into the central cell of the created reservoir, precisely located within grid cell 13 1. This injector well serves as the only well of CO_2 injection in the model. To regulate reservoir pressure and prevent excessive pressure buildup, the maximum flow rate injection was set at 0.1 million tonnes per year, which is equivalent to 375.2 m^3/day, for case one, and 1.5 million tonnes per year, which is equivalent to 5,627.9 m^3/day, for case 2. Interval perforations were defined for CO_2 injection into specific reservoir intervals. The perforations were defined for cells 13 1 30:33.

The simulation scenario starts from January 1, 2000, to January 1, 2010. To assess the long-term effectiveness of CO_2 injection and its impact on reservoir behavior, the injector well is scheduled to be shut-in after 5 years of continuous injection. Subsequently, the simulation will continue until 2010, allowing for the observation of post-injection reservoir response and the evaluation of reservoir performance over an extended timeframe.

1.3. Caprock fracturing simulation based on the Barton–Bandis model

The implementation of the Barton and Bandis model in sealing rock layer 12 serves a crucial role in simulating the mechanical behavior of these cap rock formations within the CO_2 storage reservoir model. In our case, the Barton and Bandis model is utilized to simulate the failure behavior of the sealing rock layers, which are essential for maintaining reservoir integrity and preventing CO_2 leakage. This model was coded and coupled with MRST CO2 injection simulation. The fracture opening stress parameter, set at 2000 kPa in our simulation, represents the critical stress threshold at which fractures within the rock mass begin to open, allowing for fluid migration and potential leakage pathways. By incorporating this parameter into the model, we can accurately simulate the response of the cap rock layers to stress changes induced by CO_2 injection, thereby assessing the risk of fracturing and its implications

Section	Parameter	Value
GRID	Dimensions (nx × ny nz)	25 × 1 × 33
	Domain size (X Y × Z) [m]	2000 × 1500 100
	Depth interval [m]	500–600
	Grid type	Cartesian tensor grid
Rock	Porosity	0.13 (uniform)
	Aquifer permeability	15 md
	Caprock permeability (layer 12)	1e-6 md (initial)
Fluid	Phases	CO_2 (gas) and brine (water)
	Brine viscosity	0.8 mPa·s
	CO_2 viscosity	Calculated via CO2props() (MRST)
	Brine density	1000 kg/m³
	CO_2 density	Computed from EOS at 15 MPa, 70°C
	Capillary pressure model	Inverse square-root ($pc \propto 1/\sqrt{Sw}$)
Well	Location	Central cell, bottom 4 layers (30–33)
	Type	Rate-controlled injection
	Injection rate (Case 1)	0.1 million tonnes/year
	Injection rate (Case 2)	1.5 million tonnes/year
Simulation	Injection duration	5 years
	Post-injection monitoring	5 years
	Timestep control	rampupTimesteps() with monthly/biweekly
	Gravity	Enabled
Geomechanics	Caprock tensile strength (σ_tensile)	100 × 6894.76 Pa
	Caprock failure permeability	233 mD (after fracture)
	Permeability update logic	Based on effective stress at Layer 12

Table III.1. Description of the employed 2D model

1.4. Simulation results

As mentioned early, two primary cases were analyzed :

- A base case where CO_2 is injected under conservative operational conditions without inducing caprock failure. (this was ensured by reducing the injection flow)
- A geomechanically active case, where increased injection rates and finer timestep resolution result in caprock permeability changes and leakage.

This modelling effort incorporates pressure- and stress-based permeability updates within the caprock, simulating fracture onset using simplified geomechanical rules.

1.4.1. Case study 1: CO_2 injection without caprock failure

Table III.2 presents the setting parameters used for simulating the first case. In this scenario, a low injection rate and moderate timestep resolution were selected to ensure a stable pressure profile during CO_2 injection. The goal was to evaluate the storage capacity and flow behaviour under ideal containment conditions.

Parameter	Value
Injection rate	0.1 million m^3/year (normalized)
Injection period	5 years
Post-injection monitoring	5 years
Time steps	Monthly (rampupTimesteps(5*year, year/12, 2))
Caprock permeability	Fixed at 1e-6 mD (no failure allowed)

Table III.2. Setting parameters of case study 1

Figure III.1 depicts the permeability distribution in the reservoir after simulating 5 years of CO2 injection and 5 years of post-injection periods for case 1. The visualization confirms that Layer 12, at approximately 540 m depth, acts as a low-permeability caprock, with values near 1e-6 mD (dark blue), while the surrounding aquifer layers exhibit much higher permeability (~15 mD, yellow). This contrast ensures lateral CO_2 migration beneath the caprock, effectively preventing vertical flow unless pressure buildup or structural failure occurs. The distribution validates the model's representation of a safe containment system for CO_2 storage.

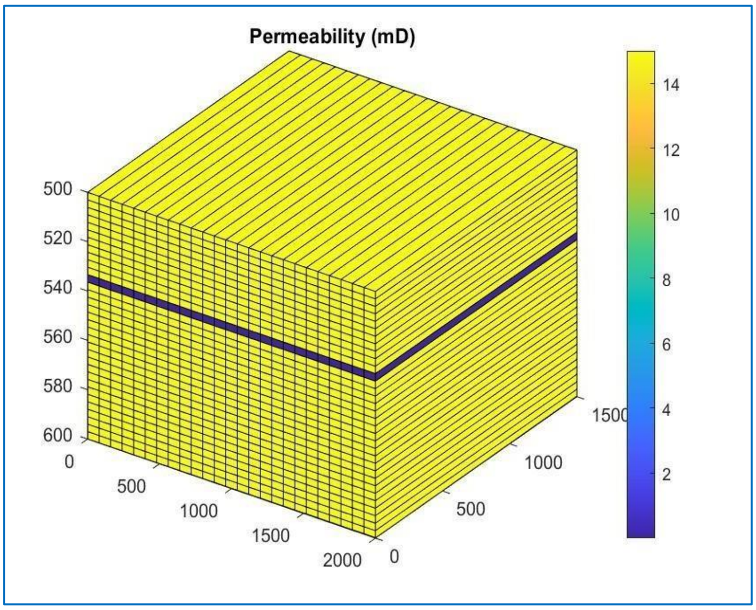


Figure III.1. Case 1: 3D Permeability visualization after simulating 5 years of CO2 injection and 5 years of post-injection periods

The sequence of four saturation profiles captures the temporal evolution of CO_2 plume migration during injection into a reservoir with an intact caprock are depicted in **Figure III.2**. As shown, at Timestep 1, CO_2 is concentrated near the injection point, appearing as a localized yellow zone indicating high saturation, while surrounding blue regions represent low or zero CO_2 saturation. By Timestep 31, the plume rises under buoyant forces and encounters the low-permeability barrier at layer 12, causing it to spread laterally and form a distinctive mushroom-shaped yellow front. At Timestep 93, lateral migration intensifies, with the high-saturation (yellow) region expanding beneath the caprock and pushing outward. By Timestep 124, the plume stabilises, forming a broad, well-confined yellow zone under the seal, while blue areas persist in zones untouched by CO_2. A narrow light-blue vertical tail beneath the injector may reflect numerical diffusion or minor grid leakage. Overall, the plume remains structurally trapped below the caprock, confirming its sealing integrity and effective containment of the injected CO_2.

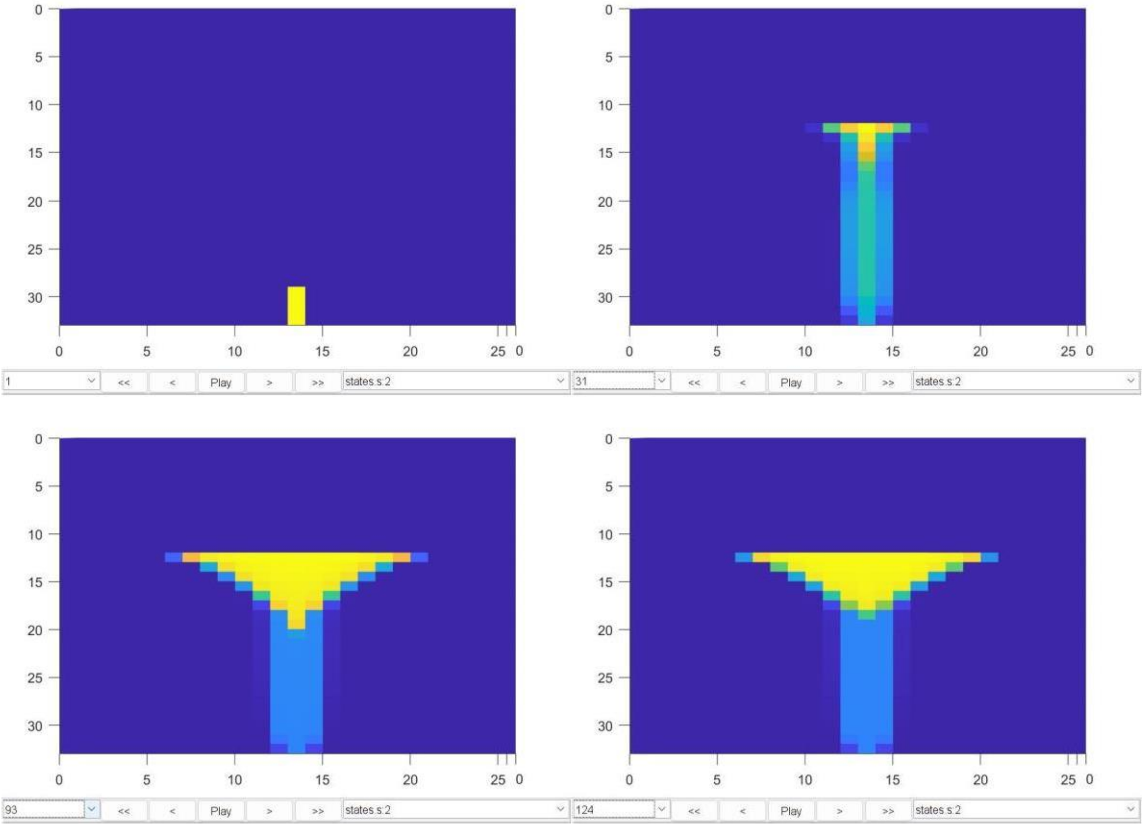


Figure III.2. Cas 1: 2D plots depicting the CO2 saturation distribution during the injection and post injection periods.

1.4.2. Case Study 2: Geomechanical failure and CO_2 leakage

Table III.3 reports the setting parameters used for simulating the second scenario. In this case, operational parameters were adjusted to promote rapid pressure buildup, enabling the evaluation of fracture-triggered leakage through the caprock.

Parameter	Value
Injection rate	1.78 million m^3/year (normalized)
Injection period	5 years
Post-injection monitoring	5 years
Time steps	Bi-weekly (rampupTimesteps(5*year, year/24,1))
Caprock failure criterion	Effective stress < $-\sigma_t$ (tensile threshold)
Caprock permeability post-failure	Increased to 233 mD

Table III.3. Setting parameters of case study 2.

Figure III.3 depicts the permeability distribution in the reservoir after simulating 5 years of CO2 injection and 5 years of post-injection periods for case 2. This 3D visualization illustrates the permeability distribution (in mD) within the reservoir, with a color-coded block model revealing a predominantly low-permeability matrix (below20 mD, shown in blue) and a distinct high-permeability anomaly exceeding 220 mD (highlighted in yellow). As evident from the figure, the permeability in the caprock (layer 12) significantly increased after CO_2 injection, indicating possible induced fracturing due to high pressure buildup. This development represents a critical risk, as it provides a potential leakage conduit for CO_2 migration beyond the intended storage zone.

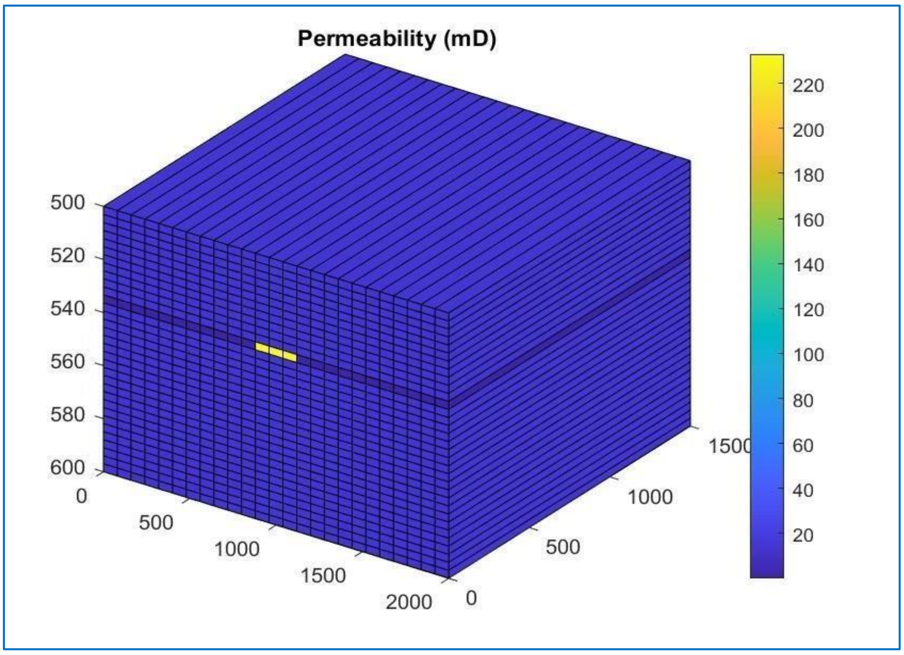
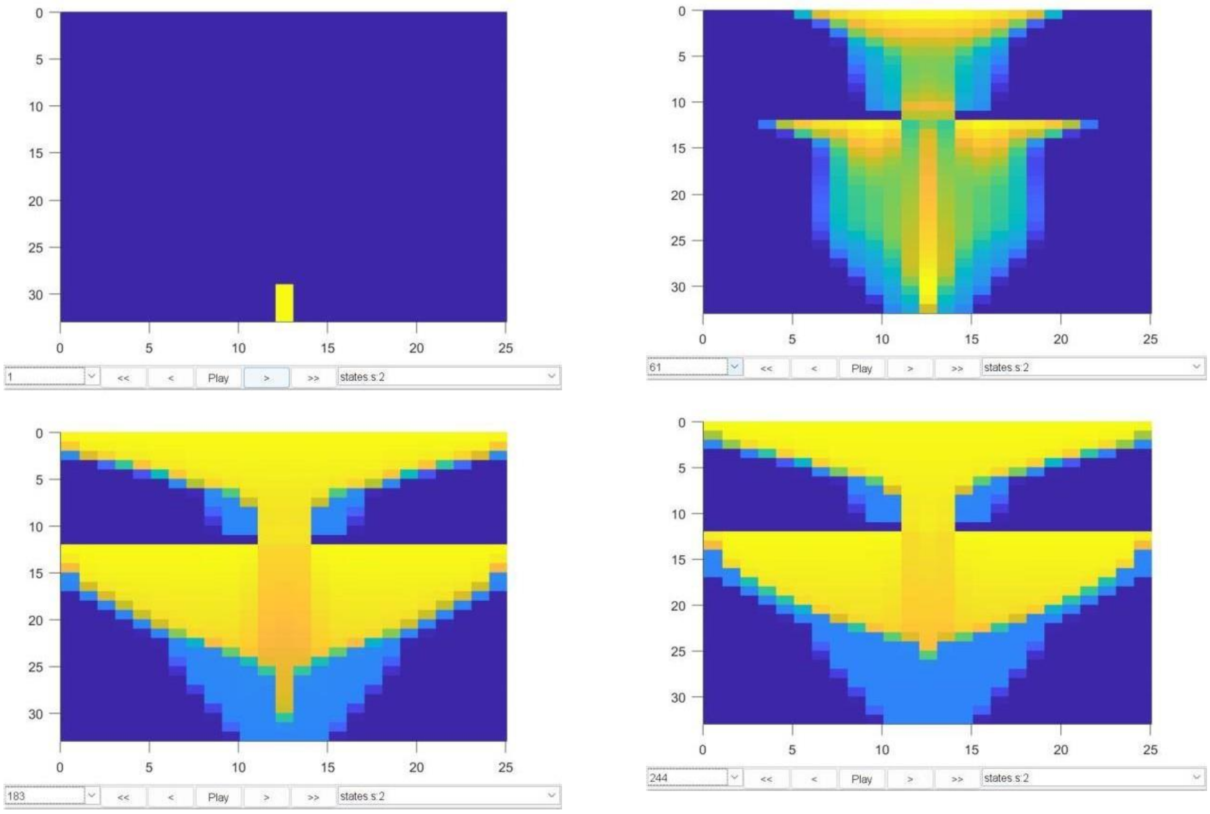


Figure III.3. Case 2: 3D Permeability visualization after simulating 5 years of CO2 injection and 5 years of post-injection periods

The sequence of four saturation profiles illustrates the dynamic progression of CO_2 migration under conditions of geomechanical failure and leakage is illustrated in **Figure III.4**. At Timestep 1, CO_2 appears as a localised, high-saturation zone (yellow) directly above the injection point, confined within a narrow vertical region, indicating early-stage injection into an undisturbed domain. By Timestep 61, the plume expands significantly both vertically and laterally, revealing the onset of leakage through a compromised caprock, as indicated by the upward and outward spread of saturation into overlying layers. At Timestep 183, the leakage pathway becomes more pronounced, forming a V-shaped high-saturation zone that extends into upper formations, suggesting continued CO_2 migration along mechanically altered pathways. By Timestep 244, the plume achieves a broader distribution, with saturation fully penetrating the upper domain and spreading horizontally, confirming the failure of the sealing integrity and the establishment of a dominant leakage conduit. This progression highlights the critical influence of mechanical damage on CO_2 containment, emphasising the need for integrated geomechanical-reservoir monitoring in storage projects.

Figure III.4. Cas 2: 2D plots depicting the CO2 saturation distribution during the injection



and post injection periods.

2. Optimization of CO_2 Injection Using Particle Swarm Optimization

2.1. Formulation of the optimization problem

In the present section, the simulation workflow was coupled with a metaheuristic algorithm, namely Particle Swarm Optimization (PSO) to enable the optimization of the controllable parameters and factors such as the injection rate and the well positions, during the CO_2 injection process. To do this end, an objective function was set as maximizing the CO_2 injection with constraint of minimizing the geomechanical risk. The idea was to identify the best well positions for well-1 and well-2 along with the optimum CO_2 injection rate to maximize the amount of the injected CO_2 with inducing failure in the cap rock (layer12), which can result in leakage of CO_2 plume. Using the simulation workflow model described in the previous section, it is possible to assess different candidate solution of the PSO algorithm while converging toward the optimum solution. The search space for this optimization problem is constrained by operational limitations and reservoir dimension. The injection flow rate specify maximum limit to avoid collapse of the surface equipment's while the well positions range between the first and the lest cell in the x-direction of the reservoir model. **Table III.4** summarizes the formulation of the investigated optimization problem. This mono-objective optimization approach enables the development of the best solution that simultaneously improves CO_2 injection and minimizes the risk associated with for the cap-rock failure, implying a more efficient CO_2 injection process.

	Parameter/Function	Objective/Constraint Formulation
Objective Function	$CO2\ injection\ simulation$ $(well\ positions, flowrate)$	Maximize $CO2$ injection
Constraints	$Cap\ rock\ faillure$ $(well\ positions, flowrate)$	$first\ cell < well\ position < last\ cell$
		$0.1 * 10^6\ \frac{Tonnes}{year} < flowrate < 4\ * 10^6\ \frac{Tonnes}{year}r$

Table III.4. Formulation of the Optimization Problem Studied.

2.2. Model Construction

To ensure that every optimization trial starts from the same baseline, we build and save a fully defined MRST reservoir model before executing the PSO routine. This model includes the grid, heterogeneous rock properties, initial conditions, and fluid definitions. Similar grid dimensions used in the previous section were employed in the optimization study. We we create a 25 × 1 × 33 Cartesian grid over a 500–600 m depth interval. The top of the caprock layer at about 540 meters. However, both porosity and permeability were defined with heterogenous distribution to investigate its effect on well position through the optimization study. The permeability heterogeneity was produced by a Gaussian Random Field (GRF) with a given mean, variance, nugget, and correlation range, reflecting realistic subsurface variability. Within reasonable bounds, porosity was randomly selected (0.13–0.27 for aquifer; 0.12–0.22 for caprock). To maintain an initial seal, caprock permeability is maintained in the ultra-low range (10^{-7}–10^{-5} D). The accurate assignment of the low-perm caprock and heterogeneous aquifer is confirmed by a brief 3D plot as depicted in **Figure III.5**. Heterogeneous permeability field showing aquifer zones with 15–45 mD (yellow, red) and an ultra-low-permeability caprock layer (~10^{-7}–10^{-5} D, blue). As shown in this figure, the pronounced contrast confirms lateral CO_2 migration within the high- permeability aquifer, while the caprock provides an effective vertical seal. Aquifer heterogeneity suggests preferential flow paths that will influence plume shape and must be considered in optimization.

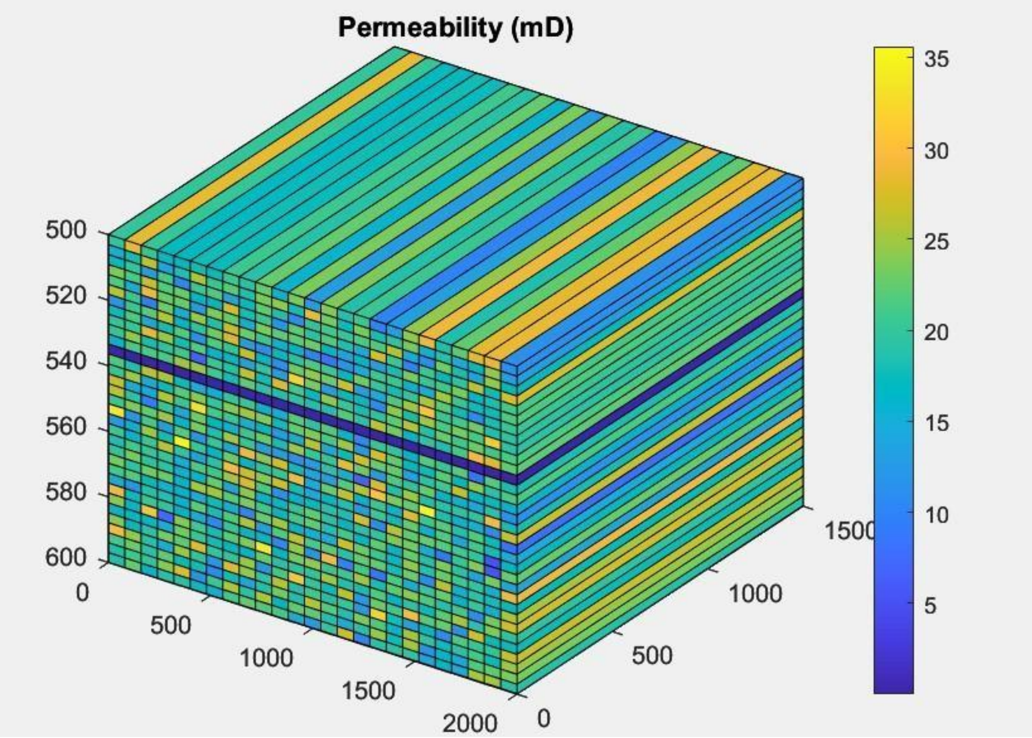


Figure III.5. Permeability distribution in heterogeneous reservoir

2.3. Particle Swarm Optimization

The steps for implementing PSO for the optimization of the CO2 injection opertaion are summarized as follows:

- For the first iteration:

– Representation: The optimization problem variables (injection rate, well-1 and well-2 positions) are organized in input vector form using the following representation:

Well-1 pos	Well-1 pos	$Injection\ rate$

where i represents the size of the population of possible solutions.

– Initialization: The initial population, denoted as P_t is generated randomly. The individuals in P_t are the candidate solution that would be enhanced at each iteration.

– Evaluation : PSO tracks, for each particle: its fitness, measured by running simulation for each particle to and asses its impact on the overall CO2 injection and the caprock state.

– At each iteration, the particles update their positions in the search space based on their own experience as well as the experience of other particles in the population, as described below :

$$V_i^{t+1} = \omega V_i^t + C_1 r_1^t (pbest_i^t - X_i^t) + C_2 r_2^t (gbest_i^t - X_i^t) \quad \text{(III. 1)}$$

$$X_i^{t+1} = X_i^t + V_l^{t+1} \quad \text{(III. 2)}$$

where $r1$ and $r2$ are random numbers uniformly chosen in the interval [0; 1], $C1$ and $C2$ are constants known as acceleration coefficients, which determine the relative influence of the cognitive and social components on particle movement, and ω is the inertia weight, introduced by Shi and Eberhart in 1998 [44]**,** to control the balance between exploration and exploitation of the search space. Typically, better control over these mechanisms can be achieved by initially setting the inertia weight ω to a relatively high value (to encourage exploration at the beginning), and then gradually decreasing it to a lower value towards the end (to favor exploitation) [45]. The following formula is used to linearly decrease the inertia weight over time:

$$\omega_t = \omega_{max} - \left(\frac{\omega_{max} - \omega_{min}}{t_{max}}\right) t \quad \text{(III. 3)}$$

where t is the current iteration, t_{max} is the maximum number of iterations, ω_{max} and ω_{min} are the initial and final values of the inertia weight, respectively. **Table III. 5** reports the PSO setting parameters used in this study.

Parameter	Value / Setting
Swarm size	30
Maximum number of iterations	15
C1	2
C2	2
ω	0.729

Table III.5.. PSO setting parameters.

2.4. Optimization results

Table III.6 reports the optimal well locations along with the optimum CO2 injection rate identified after running an extensive optimization process using the PSO algorithm.

Well-1 position	First cell

Well-2 position	Last cell
CO2 injection rate	$4 \times 10^6 \frac{tonnes}{year}$

Table III.6. the optimum values of the investigated factors

According to this table, the wells are positioned at the reservoir boundaries. With this well configuration, the injection flow can be maximized at 4 million tonnes per year, which is equivalent to 10 958.9 tonnes per day, without inducing fractures in the cap rock. **Figure III.6** depicts the convergence iterations using the PSO algorithm. As illustrated, the PSO reached the optimum solution by iteration 6. This fast convergence can be attributed to the large population size used (population of 30 individuals).

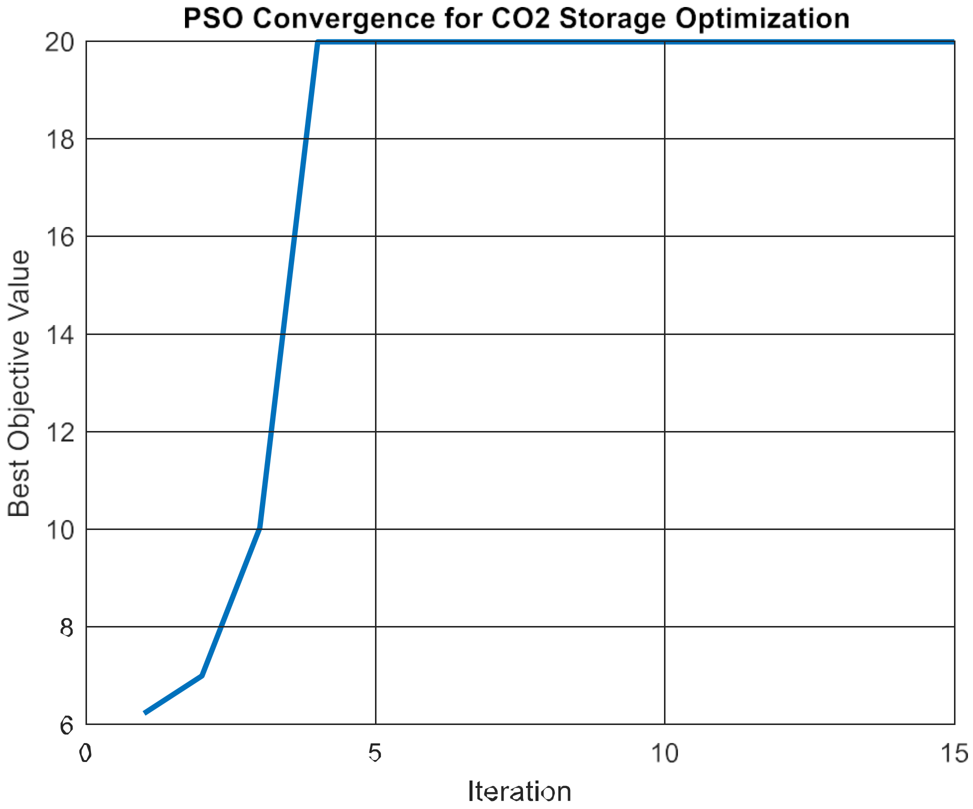


Figure III.6. PSO convergence iterating during the CO2 storage optimization

General Conclusion

This thesis explored how CO_2 can be safely stored in deep saline aquifers, with a strong focus on avoiding geomechanical issues like caprock failure. To do this, we combined theoretical research, numerical modelling using MRST (MATLAB Reservoir Simulation Toolbox), and an optimisation method based on Particle Swarm Optimisation (PSO).

The work started by looking at carbon capture and storage (CCS) as a strategy for reducing emissions, with particular attention to deep aquifers because of their large storage potential. we reviewed the main storage mechanisms and some well-known case studies to better understand both the opportunities and the difficulties involved in geological CO_2 storage.

One of the main achievements of this project was building a simulation model that updates the caprock's permeability depending on stress changes, using the Barton–Bandis fracture model. We tested this model in two different scenarios: one with safe, low-rate injection and another with higher injection rates that risked causing fractures and leaks. These results made it clear that how and where we inject CO_2 has a big impact on both storage success and rock stability.

To improve decision-making, we applied PSO to find the best combination of well locations and injection rate that would store the most CO_2 without breaking the caprock. The optimisation process worked well and showed that even small changes in setup can make a big difference in safety and efficiency.

Overall, this study shows the value of using simulation and optimisation together when planning CO_2 storage projects. The framework we developed using MRST and PSO can help guide future research and practical applications, especially in cases where uncertainty and risk need to be carefully managed.

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عنوان المذكرة: **نمذجة تخزين ثاني أكسيد الكربون في الخزانات الجوفية تحت المخاطر الجيوميكانيكية باستخدامMRST**

اللقب: بن حرمة , بوسبسي **الاسم:** مروة طروب , جميلة **المؤطر:** محمد رياض يوسفي

ملخص

يتناول البحث التحدي المتمثل في تخزين ثاني أكسيد الكربون بشكل آمن في الخزانات المالحة العميقة مع مراعاة المخاطر الجيوميكانيكية، لا سيما فشل السقف الصخري بسبب الضغوط العالية الناتجة عن الحقن. إن ضمان كفاءة التخزين وسلامة التكوين أمر أساسي لنجاح احتجاز الكربون على المدى الطويل.

تم تنفيذ نهج قائم على المحاكاة باستخدام أداة محاكاة الخزانات .MATLAB (MRST) تضمن النموذج تدفقًا ذا مرحلتين من ثاني أكسيد الكربون والمحلول الملحي، وشمل تقييم خطر حدوث شقوق في السقف الصخري باستخدام نموذج بارسون-بانديس الجيوميكانيكي. ولتحسين ترتيب الآبار ومعدل الحقن، تم دمج خوارزمية تحسين السرب الجزيئي (PSO) مع إطار المحاكاة.

تم إجراء دراستين حالتين: الأولى مع معلمات حقن محافظة تحافظ على سلامة السقف الصخري، والأخرى مع معدلات حقن أعلى أدت إلى حدوث شقوق واحتمال حدوث تسرب. نجح تحسين PSO في تحديد استراتيجية حقن تعظم تخزين ثاني أكسيد الكربون مع تجنب الفشل الميكانيكي.

يوفر هذا العمل إطارًا قويًا ومرنًا لتحسين حقن ثاني أكسيد الكربون تحت القيود الجيوميكانيكية. ويظهر أهمية ربط محاكاة الخزانات مع نمذجة مخاطر الشقوق والتفكير الأمثل باستخدام خوارزميات ميتاهيرستية لدعم تخزين الكربون الجيولوجي بشكل آمن وفعال وموثوق.

كلمات مفتاحية: احتجاز وتخزين الكربون ,(CCS) المخاطر الجيوميكانيكية ,المحاكاة العددية باستخدام(MRST) خوارزمية تحسين السرب الجزيئي(PSO) .

Memory title : Modeling of CO_2 Storage in Aquifers Under Geo-Mechanical Risks Using MRST

Name: BENHORMA ; Boussebsi **First name:** Maroua Troub ; Djamila **Directed by:** Mohamed Riad Youcefi

Abstract

The thesis addresses the challenge of securely storing CO_2 in deep saline aquifers while accounting for geomechanical risks, particularly caprock failure due to high injection pressures. Ensuring both storage efficiency and formation integrity is essential for long-term carbon sequestration success.

A simulation-based approach was implemented using the MATLAB Reservoir Simulation Toolbox (MRST). The model incorporated two-phase flow of CO_2 and brine and included a caprock fracture risk assessment using the Barton–Bandis geomechanical model. To optimize well placement and injection rate, a Particle Swarm Optimization (PSO) algorithm was integrated with the simulation framework.

Two case studies were performed: one with conservative injection parameters that maintained caprock integrity, and another with higher injection rates that led to fracture and potential leakage. The PSO optimization successfully identified an injection strategy that maximized CO_2 storage while preventing mechanical failure.

This work provides a robust and flexible framework for optimizing CO_2 injection under geomechanical constraints. It demonstrates the importance of coupling reservoir simulation with fracture risk modeling and metaheuristic optimization to support safe, efficient, and reliable geological CO_2 storage.

Le résumé doit être rédigé en deux langues différentes au moins

Key words: Carbon Capture And Storage , Geomechanical Risks , Numericl Simulation (MRST), Particle Swarm Optimization (PSO).

Titre du mémoire : Modélisation du stockage du CO_2 dans les aquifères sous risques géomécaniques à l’aide de MRST

Nom : Benhorma ; Boussebsi **Prénom :** Maroua Troub ; Djamila **Encadreur :** Mohamed Riad Youcefi

Résumé

La thèse aborde le défi du stockage sécurisé du CO_2 dans les aquifères salins profonds tout en tenant compte des risques géomécaniques, en particulier de l'échec du caprock en raison des fortes pressions d'injection. Assurer à la fois l'efficacité du stockage et l'intégrité de la formation est essentiel pour le succès à long terme de la séquestration du carbone.

Une approche basée sur la simulation a été mise en œuvre à l'aide de l'outil MATLAB Reservoir Simulation Toolbox (MRST). Le modèle a intégré un écoulement biphasique de CO_2 et de saumure, et a inclus une évaluation du risque de fracturation du caprock en utilisant le modèle géomécanique Barton–Bandis. Pour optimiser le placement des puits et le taux d'injection, un algorithme d'optimisation par essaim de particules (PSO) a été intégré au cadre de simulation.

Deux études de cas ont été réalisées : l'une avec des paramètres d'injection conservateurs maintenant l'intégrité du caprock, et l'autre avec des taux d'injection plus élevés entraînant des fractures et un risque de fuite. L'optimisation PSO a permis d'identifier une stratégie d'injection maximisant le stockage du CO_2 tout en prévenant les défaillances mécaniques.

Ce travail fournit un cadre robuste et flexible pour l'optimisation de l'injection de CO_2 sous des contraintes géomécaniques. Il démontre l'importance de coupler la simulation de réservoir avec la modélisation du risque de fracture et l'optimisation métaheuristique pour soutenir un stockage géologique du CO_2 sûr, efficace et fiable.

Mots clés : Captage et stockage du carbone (CSC) ,Risques géomécaniques , Simulation numérique (avec MRST) , Optimisation par essaim de particules (PSO)

Le résumé doit être rédigé en deux langues différentes au moins