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NUMERICAL SIMULATION OF CO₂ FLOW IN POROUS ROCK CORES USING ANSYS

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DECLARATION

I declare that this document is an original work of my own authorship and that it fulfils all the requirements of the Code of Conduct and Good Practices of the Universidade de Lisboa.

ABSTRACT

In the context of the Anthropocene era, characterized by significant human influence on the environment, the Earth's temperature has risen by 2 degrees Celsius, primarily due to the emission of greenhouse gases, with carbon dioxide (CO₂) standing out as one of the main contributors. In response to this alarming trend and in an effort to address climate change, the international community has set goals through agreements and treaties, including the Paris Agreement and the Kyoto Protocol, with the intention of mitigating emissions and limiting global warming.

This manuscript focuses on a specific strategy to address CO₂ emissions: carbon capture and storage (CCS) technology. Through the implementation of various techniques, this technology aims to reduce the amount of CO₂ released into the atmosphere, thereby contributing to the mitigation of the impacts of climate change.

The study's focus expands to address critical parameters that must be considered to understand how CO₂ behaves in porous media. These include aspects such as porosity, permeability, and forces influencing fluid flow, such as capillarity and gravity. A detailed understanding of these factors is essential for assessing the effectiveness of CCS techniques in specific contexts.

Portugal emerges as a particular case study, and its situation is examined in terms of suitability for CO₂ storage. Considering its geological characteristics and potential storage sites, the potential for Portugal to contribute to global mitigation efforts is evaluated.

As an integral part of this work, an initial simulation is presented that analyses the behaviour of CO₂ at the beginning of the injection process.

In summary, this project addresses not only CCS technology and its associated techniques but also the fundamental parameters and specific considerations of Portugal in the context of climate change mitigation.

Keywords: Carbon Capture and Storage (CCS), Porous Media, CO₂ Injection, Geological Parameters, Simulation, Portugal, Sustainability.

RESUMO

No contexto da era antropogênica, caracterizada pela significativa influência humana no meio ambiente, a temperatura da Terra aumentou em 2 graus Celsius, principalmente devido à emissão de gases de efeito estufa, com o dióxido de carbono (CO₂) destacando-se como um dos principais contribuintes. Em resposta a essa tendência alarmante e num esforço para enfrentar as mudanças climáticas, a comunidade internacional estabeleceu metas por meio de acordos e tratados, incluindo o Acordo de Paris e o Protocolo de Kyoto, com a intenção de mitigar as emissões e limitar o aquecimento global.

Este manuscrito se concentra em uma estratégia específica para lidar com a emissão de CO₂: a tecnologia de captura e armazenamento de carbono (CCS). Por meio da implementação de diversas técnicas, essa tecnologia visa reduzir a quantidade de CO₂ liberada na atmosfera, contribuindo assim para a mitigação dos impactos das mudanças climáticas.

O foco do estudo se expande para abordar parâmetros críticos que devem ser considerados para entender como o CO₂ se comporta em meios porosos. Isso inclui aspectos como porosidade, permeabilidade e forças que influenciam o fluxo de fluidos, como capilaridade e gravidade. Uma compreensão detalhada desses fatores é essencial para avaliar a eficácia das técnicas de CCS em contextos específicos.

Portugal surge como um estudo de caso particular, e sua situação é examinada em termos de adequação para o armazenamento de CO₂. Considerando suas características geológicas e possíveis locais de armazenamento, avalia-se o potencial de Portugal para contribuir para os esforços globais de mitigação.

Como parte integrante deste trabalho, é apresentada uma simulação inicial que analisa o comportamento do CO₂ no início do processo de injeção.

Em resumo, este projeto aborda não apenas a tecnologia CCS e suas técnicas associadas, mas também os parâmetros fundamentais e considerações específicas de Portugal no contexto da mitigação das mudanças climáticas.

Palavras chave: Captura e Armazenamento de Carbono (CCS), Meios Porosos, Injeção de CO₂, Parâmetros Geológicos, Simulação, Portugal, Sustentabilidade

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Abbreviations List

CO₂: Carbon Dioxide

CAC: Carbon Capture and Storage

pH: Potential of Hydrogen

CCS: Carbon Capture and Storage

YAC: Yacimiento (Reservoir)

T&D: Temperature and Pressure

HSE: Health, Safety, and Environment

RO: Reverse Osmosis

PM: Porous Medium

SCAL: Special Core Analysis Laboratory

TOC: Total Organic Carbon

SOR: Saturation Oil Ratio

WAG: Water Alternating Gas

EOR: Enhanced Oil Recovery

EGR: Exhaust Gas Recirculation

SC-CO₂: Supercritical CO₂

PVT: Pressure-Volume-Temperature

SWT: Simulated Well Test

R&D: Research and Development

E&P: Exploration and Production

DTU: Downhole Temperature and Pressure

1. Introduction

1.1. Motivation

Greenhouse gases have triggered significant climate changes since the Anthropocene era, with an increase of almost 2°C in the Earth's temperature. This phenomenon, known as climate change, is primarily attributed to the uncontrolled emission of gases such as carbon dioxide, methane, nitrous oxide, and industrial gases. These atmospheric pollutants act as a thermal blanket, trapping heat and generating a greenhouse effect that disrupts climatic balances.

This rise in global temperature has substantial environmental and health consequences. On the one hand, it contributes to the increase in extreme weather events such as hurricanes, droughts, and floods. On the other hand, human health is directly affected, not only by climate change itself but also by the presence of smog and air pollution largely generated by these greenhouse gases.

Carbon dioxide, mainly from fossil fuel combustion, leads the list of contributors to global warming. Methane, released during food production and fossil fuel exploitation, also plays a crucial role. Nitrous oxide, derived from agriculture and industrial activities, as well as specific industrial gases, add complexity to the picture.

In addition to altering weather patterns and increasing the frequency of extreme weather events, climate change induced by these greenhouse gases also threatens biodiversity. Animal and plant species face challenges in adapting to a rapidly changing environment, with possible migrations, extinctions, and ecosystem changes.

In summary, the influence of greenhouse gases on climate change not only raises temperatures but also triggers a series of environmental and health impacts that require urgent measures to mitigate and adapt to this new climate reality.

Carbon dioxide is the primary greenhouse gas, responsible for approximately three-quarters of emissions. It has the capacity to linger in the atmosphere for thousands of years. In 2018, carbon dioxide levels reached 411 parts per million at the Mauna Loa Atmospheric Baseline Observatory in Hawaii, marking the highest monthly average ever recorded. Carbon dioxide emissions primarily stem from the combustion of organic materials, including coal, oil, gas, wood, and solid waste.[1]

To address this, we must mention and explain the Paris Agreement, adopted in December 2015, is a binding international treaty that seeks to comprehensively address climate change. It sets the goal of limiting the global temperature increase to below 2°C, with additional efforts to achieve 1.5°C. All countries commit to submitting nationally determined contributions with specific measures to reduce emissions, and a global transparency system is implemented. A global assessment is conducted every five years, starting from 2023, to enhance climate ambition. The agreement also includes objectives to strengthen adaptation capacity, reduce vulnerability, and

address losses and damages associated with climate change. The significance of technological, financial, and capacity-building support to developing countries for fostering actions in adaptation and mitigation is emphasized. [2] Close 2019, 28 countries had issued declarations for climate change mitigation, with many incorporating strategies to transition to renewable energy sources. However, several societal, economic, and technological barriers need to be overcome to achieve net-zero emissions. The International Energy Agency (IEA) emphasizes that advancing clean energy technologies is pivotal for reaching the net-zero emissions target by 2050.[3]

To mitigate climate change, the possibility of storing CO₂ to prevent its release into the atmosphere has been under consideration. Consequently, projects known as Carbon Capture and Storage (CCS) are already underway.

1.2. Objectives

The project sets forth a series of interconnected and fundamental objectives for its execution. Firstly, it aims to conduct a comprehensive analysis of the global environmental situation. This analysis will provide insights into current challenges related to climate change and environmental degradation. Additionally, the project seeks to acquire in-depth knowledge about Carbon Capture and Storage (CCS) technologies and explore projects related to these technologies worldwide. This exploration of existing projects will enrich our understanding of the practices and solutions implemented to mitigate carbon dioxide (CO₂) emissions.

Another objective of the project is the simulation and study of CO₂ behaviour when injected into a porous medium. This entails creating models and conducting simulations to analyse how CO₂ interacts with the porous medium, its mobility, and the resulting changes in the system. Understanding these processes is crucial for assessing the feasibility and efficiency of CO₂ injection in this specific context.

In summary, the objectives of this project are to promote the carbon storage technique, identify crucial parameters that need to be understood to comprehend CO₂ behaviour in porous media, and conduct a simple simulation of CO₂ injection into a porous medium using ANSYS.

1.3. Structure.

The initial phase of the project comprises an introductory section that explores the current environmental scenario, the challenges associated with climate change, and the relevance of carbon dioxide (CO₂) storage. Specific objectives are established to be achieved within the project.

Subsequently, we delve into the literature review section, drawing insights from previous projects, scientific journals, and relevant literature. Various aspects of CO₂ capture and storage methods,

different storage formations, and crucial parameters such as permeability, wettability, and CO₂ behaviour in its various states are explored.

Following this comprehensive literature review, the project seamlessly transitions to subsequent sections. These sections focus on understanding the geological aspects of Portugal and their relevance to the project's objectives. This includes an in-depth examination of geological parameters crucial in shaping the simulation process. Additionally, key definitions are introduced to ensure clarity in the project's terminology. The groundwork laid in these sections paves the way for a detailed description of the mathematical model and the numerical methods that will be employed in the simulation, ultimately contributing to a well-rounded and informed study.

During the simulation phase, the project centres on replicating and understanding supercritical CO₂ injection into a porous material. This involves the meticulous design of simulation models, the creation of intricate meshes, and the use of ANSYS CFX for numerical analysis. Although simulation is a straightforward part of the project, the primary goal is to predict outcomes, optimize strategies, and provide valuable insights into the viability and efficiency of this environmentally significant process. The results and analysis of the simulation are integrated with the abundant information gathered throughout the research.

2. Bibliographic Review

2.1. CCS Technology

Carbon capture and storage (CCS) is widely acknowledged as a vital tool in meeting climate change targets [4], it is therefore essential to explain what it consists of

CCS can be divided into three steps:

Capture Stage: Carbon capture is essential for mitigating greenhouse gas emissions and is achieved through various methods, notably pre-combustion, post-combustion, and oxy-combustion. In pre-combustion, carbon is captured before combustion using technologies such as Integrated Gasification Combined Cycle (IGCC) and Integrated Reformed Combined Cycle (IRCC). These processes, utilized in "blue hydrogen" production, contribute significantly to carbon emission reduction.

Post-combustion involves capturing carbon from the exhaust gases of plants burning fossil fuels. This widely employed industrial process utilizes technologies like solvent-based absorption, membrane separation, mineralization, adsorption, and cryogenic capture. Each method has distinct advantages and drawbacks.

Oxy-combustion, on the other hand, entails burning fuel in an oxygen-rich environment, facilitating cleaner combustion, and significantly reducing CO and SO₂ contents in the exhaust gases. This method proves cost-effective for new plants, with the advantage of producing nearly pure CO₂ directly compressible and storable without extensive purification. The Chemical Looping Combustion (CLC) technique provides a cost-effective alternative. It utilizes a metal oxide as an oxygen source, reducing the need for intensive CO₂ purification. However, challenges such as metal degradation and energy consumption during metal cycling exist.

In summary, carbon capture involves a range of complex and diverse technologies, each with its own set of advantages and challenges. The choice of a particular method depends on factors like efficiency, economic viability, and the specific characteristics of the industrial plant or process. [4]

Transport Stage: Carbon capture is followed by its transportation from the capture point to its final storage location. Generally, CO₂ is compressed to a pressure above 8 MPa to facilitate and reduce the cost of its transportation through pipelines, the most used method in mature market technologies. However, it can also be transported in liquid form, either by trucks or tanker ships, although this option is occasional and of limited utility on a large scale.

The first long-distance CO₂ pipeline was implemented in the 1970s in the United States, with over 2500 km currently in operation. These pipelines operate in a condensation phase, with flow driven by compressors at the initial end and intermediate compression booster stations. Although pipeline transport is the predominant method, maritime transport is also considered, with costs in

both cases dependent on distance and the quantity of product transported. Estimated costs for pipeline transport, according to the IPCC, range from 1 to 8 dollars per ton of CO₂ for a nominal distance of 250 km. In comparison, maritime transport is determined by the tank volume and the characteristics of loading and unloading systems. Figure 2.20 establishes a cost comparison between pipeline and maritime transport based on distance. [4,5]

In summary, CO₂ transport involves significant cost considerations depending on distance, quantity transported, and the selected method, whether by pipeline or by sea. Despite advances in transport technology, small quantities still pose economic feasibility challenges on a large scale.

Sequestration Stage: The last step is the storage of CO₂, this is the most studied step, because although all three are necessary to combat global warming, it is this step that is being studied in various projects, because it is the one that allows the pollutant gas to be stored and not sent to the atmosphere. The manuscript will delve into more detailed explanations of the most feasible storage methods, including depleted oil and gas reservoirs, deep saline aquifers, coal layers, and formations. The common approach in all cases involves injecting CO₂ into underground rock formations. Formations that have historically held fluids such as natural gas, oil, or brine are ideal for secure carbon dioxide storage, although potential issues may arise with gas leakage through old boreholes. Additionally, coal seams can serve as CO₂ storage sites, provided the coal is unlikely to be mined in the future and exhibits sufficient permeability. [6]

Every facet of society and the economic sector will contribute to achieving carbon neutrality. While complete emission reduction is presently unattainable, it remains achievable soon. Strategies for the energy transition encompass embracing low-carbon transportation options, government incentives for public transport over individual vehicles, adopting clean energy sources, decreasing CO₂ production intensity, and focusing on efficient technologies like green hydrogen and carbon capture and sequestration. Several major companies around the world have been involved in carbon capture and storage (CCS) projects as part of their efforts to reduce greenhouse gas emissions.

ExxonMobil, Shell, Chevron, BP, Total Energies, Adani Group, Equinor, Occidental Petroleum, Air Liquide, are just a few of the many companies that have been exploring and applying carbon capture and storage technologies as part of their climate change mitigation strategies. It is curious that all of them are oil companies, using this technology as one of the so-called CO₂ offsets that companies must make to reduce pollution. The participation of large companies in these projects is crucial to advance the technology and contribute to the reduction of greenhouse gas emissions.

Apart from CCS, there is another technique known as CCU (Carbon Capture and Utilisation). Carbon capture, use and storage (CCUS) technology addresses the reduction of atmospheric CO₂ through safe capture and storage for future uses, such as hydrocarbon recovery. It is essential to meet the goal of limiting global temperature rise and significantly reduces greenhouse gas emissions in carbon-intensive sectors such as electricity and industry. It also plays a crucial

role in decarbonising sectors such as steel, cement, and chemicals, where there are no current alternatives.

This technology is more novel and is still under study, but there are already companies such as Repsol that are interested in this technology to be able to use the captured CO₂ efficiently. [7]

Having explained this technology, to understand which parameters are important to understand how CO₂ will behave when stored in a porous medium, we must first define the most important parameters to be taken into account in laboratory experiments, simulations and real projects, so the following sections will try to explain these important practices and we will take up the various storage options available.

2.2. Fluid/Gas flow in porous media

It is essential to establish a set of parameters or criteria to optimize the project. For a geological site to be designated as a potential storage location, a key condition must be met—ensuring CO₂ containment through a geological framework.

Hence, a favourable criterion involves the presence, confirmed, or projected, of reservoir formations within the basin. These formations should possess suitable porosity and permeability, surpassing a specified threshold value. They should also exhibit extensive lithological strength and uniformity, while being capable of confining free CO₂ within an acceptable permeability threshold and ensuring sufficient vertical and lateral continuity. [8]

The term 'strategic trap' refers to various sealed geological containers with the capacity to trap and hold oil, natural gas, or other subsurface fluids, including aquifers. These traps are formed by changes in rock types, pinch-offs, unconformities, or sedimentary features such as reefs. Structural traps, on the other hand, are formed by deformed rock layers, such as faults and folds, which provide geometries conducive to hydrocarbon and groundwater retention in aquifers. [9].

Identifying storage formations is crucial, particularly ones capped by impermeable seals or integrated into traps that prevent CO₂ from escaping into the atmosphere. When assessing the long-term performance of the storage system, meticulous characterization ranks among the most pivotal aspects.

To qualify as suitable, a seal should not disregard the potential presence of faults or fractures, which could serve as primary pathways for CO₂ leakage. Consequently, it is imperative to demonstrate its aptness by considering potential fracture zones that could impact CO₂ release, ensuring its effective functionality during injection operations. In Figure 1, we can observe the potential formations that rocks can have.

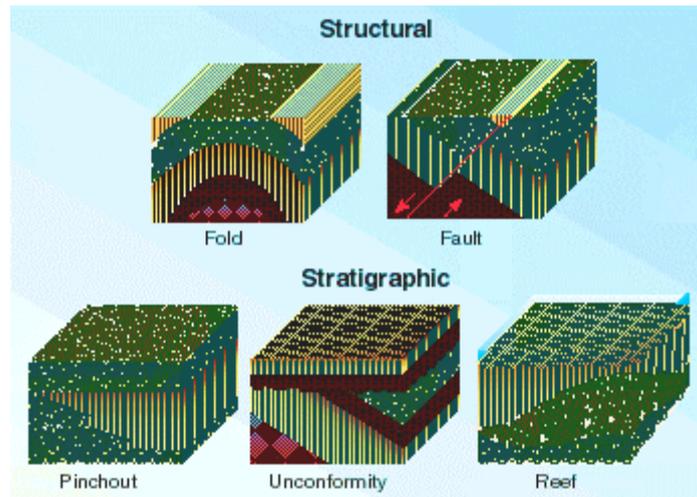


Figure 1:Block diagrams of structural and stratigraphic traps.[9]

Rock masses containing voids (porosity) can be categorized as reservoirs, provided that these rocks are cohesive (permeable) and possess the ability to both retain and facilitate the flow of fluids. Consequently, there are two fundamental properties that rocks need to exhibit:

- **Porosity:** Porosity is a critical factor that directly influences the storage capacity of the reservoir. It refers to the amount of empty space within the rocks that can hold fluids, such as water or hydrocarbons.
- **Permeability:** Permeability is equally vital as it dictates the fluid displacement inside the rock. It determines the injection flow rate and, consequently, the extent to which the reservoir can be exploited. [10]

2.1.1 Porosity

The porosity of a rock is defined as the percentage of void volume in relation to its total volume and, gives an idea of the formation's ability to store fluids, Figure 2 shows a schematic representation of different types of porosities, and within the image, we have a brief explanation of each of the types shown.[11]

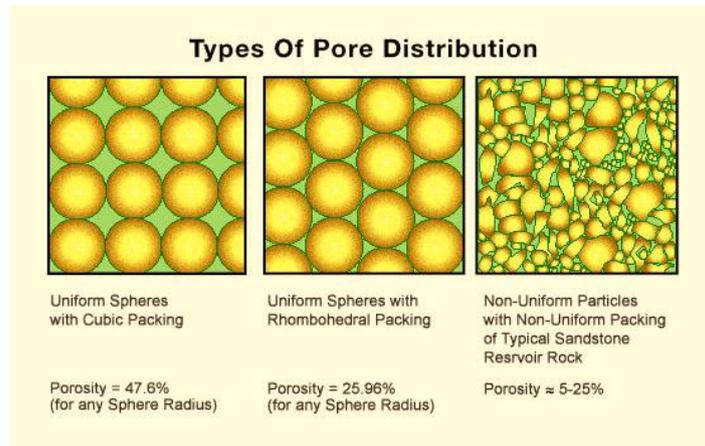


Figure 2: Types of pore distribution [11]

When discussing porosity, it is essential to make a distinction between total porosity and effective porosity. Total porosity refers to the complete volume of all void spaces present in a material or porous medium. This porosity encompasses all pores, regardless of their connectivity or accessibility. On the other hand, effective porosity specifically refers to the volume of pores that are interconnected and, therefore, allow the flow of fluids through them. In other words, effective porosity represents the fraction of the total porosity that is available for a fluid, such as CO₂, to occupy and flow through.

This distinction is fundamental in the study of permeability and fluid storage capacity in porous media because effective porosity is what truly contributes to a material's ability to retain or transport fluids, as in the case of CO₂ storage in porous geological formations.

Different rock types exhibit varying porosity ranges, as porosity is influenced by factors like grain shape, arrangement, and size. For carbonate rocks dominated by limestone and dolomite, primary porosity changes stem mainly from compression, dissolution, and precipitation. These processes can create new pore spaces, introducing secondary porosity. [12]

In contrast, sandstone typically has porosity ranging from 5-30%, determined by the classification of its constituent grains, resulting in a more uniform composition. [13]

To accommodate significant fluid volumes, the reservoir's porosity should ideally exceed 10-12%. As a result, the preferred materials typically include siliciclastic rocks and, in some cases, carbonate rocks. However, concerning CO₂ storage, certain challenges may arise due to interactions between the gas and the rock. It's worth noting that carbonates can also effectively store substantial fluid volumes. Nevertheless, when it comes to CO₂ storage, potential issues may emerge due to the interactions between the gas and the rock [12]

2.1.2 Permeability

Permeability is a property of porous materials that is an indication of the ability for fluids (gas or liquid) to flow through them. Fluids can more easily flow through a material with high permeability than one with low permeability [13].

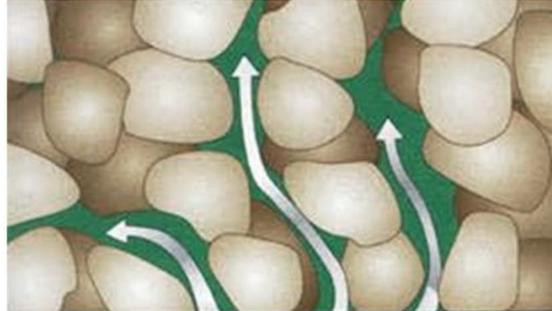


Figure 3 Permeabilities of various rocks vary according to their directional properties. In the case of anisotropic sedimentary formations, factors such as shape, size, distribution, and depositional environment play a significant role in controlling this variation [14]

Distinguishing between various types of permeability reveals the following categories:

1. Absolute Permeability is generally measured in the International System (SI) in units of "m²" (square metres). This unit represents the ease with which a single fluid can flow through a porous material, such as rock. In the SI system, neither the Darcie unit nor the "millidar" unit is used for absolute permeability, as these are obsolete or non-standard units. Therefore, absolute permeability is quantified in square metres (m²) in the international system. [15]

2. Effective Permeability: This refers to the preferential flow or transmission capacity of a specific fluid in the presence of other immiscible fluids within the reservoir. For instance, the effective permeability of gas in a gas-water reservoir. Factors like fluid saturations and reservoir characteristics impact effective permeability. Unlike absolute permeability, which applies when only one fluid phase is present, effective permeability considers multiple fluid phases. [16]

3. Relative Permeability: This dimensionless term adapts the Darcy equation to scenarios with multiphase flows. Relative permeability quantifies the ratio of a particular fluid's effective permeability at a given saturation to its absolute permeability at full saturation. When only one fluid phase is present in a rock, its relative permeability is 1.0. Calculating relative permeability enables a comparison of fluid flow capabilities in the presence of different fluids, as the existence of multiple fluid phases typically hinders fluid movement. [17].

Permeability is an inherent property of rock that, as observed, often diminishes due to fluid movement. This decline is primarily attributed to the partial breakdown of certain rock components, particularly clay minerals. These resultant tiny particles can obstruct finer pores upon displacement, leading to a deceleration in fluid movement.

A higher permeability value corresponds to a more desirable reservoir formation. Permeability's determining factor can either be extrinsic or intrinsic. Extrinsic factors are specific to the formation and hinge on pore size, while intrinsic factors are contingent on fluid characteristics like viscosity. Porosity and permeability maintain a close relationship and wield pivotal influence in the choice of CO₂ storage solutions.

2.1.3 Pressure

Pressure stands as a paramount element wielding substantial influence over fluid properties within the reservoir, governing their mobility and displacement dynamics.

Research has established that shifts in pressure within a given layer across various points in the reservoir propel the movement of water. Analysing and classifying reservoir pressures offer insights into the intricate dynamics of fluids within the sedimentary reservoir. Apart from entirely isolated formations within a fully sealed reservoir, pressure transmits through diverse fluids from one location to another within the hydrodynamic system. This gives rise to two discernible pressure categories. [18,19]

- Hydrostatic pressure: corresponding to the weight of the columns of the water that would be placed between the measuring point and the Surface of the water.

$$P_{hydrostatic} = \rho * g * Z \quad \text{Equation 1 Hydrostatic pressure. [18,19]}$$

P: hydrostatic pressure expressed in Pa

ρ : density expressed in kg·m⁻³

g: gravity expressed z:in m·s⁻².

z: Depth expressed in m².

- Hydrodynamic pressure: due to the flow of water from a high-pressure zone to a lower pressure zone. [20]

The pressure at a storage point will be the resultant of both pressures, with hydrostatic pressure usually predominating. It should also be noted that the hydrostatic pressure will increase as the salinity increases.

To summarise, temperature will also play an important role to consider, its influence is limited to reducing the viscosity of liquids, to favour the circulation of fluids, and the reaction speed of the fluids. [21].

2.3. Fluid Properties

2.2.1 Capillary forces

Liquids exhibit remarkable properties due to molecular attractive forces, which manifest themselves as cohesion and adhesion. Cohesion involves the attraction between molecules in the liquid itself, while adhesion refers to the attraction between molecules in the liquid and molecules on other surfaces. [22]

Due to cohesion, liquids could resist tensile forces at the interface with air, and this is known as surface tension. Cohesion allows the liquid to resist tensile stresses, which contributes to the formation of a stable surface at the boundary with air. On the other hand, adhesion allows the liquid to stick to the surfaces of other bodies. When liquid molecules have a significantly higher adhesion than cohesion, the liquid tends to stick to the walls of the container with which it is in contact. This phenomenon results in an increase or elevation of capillarity at the surface of the liquid. [23]

In contrast, when cohesion predominates over adhesion, a depression in capillarity is experienced. In this case, the liquid molecules show a preference for sticking together, which can lead to the liquid retracting from the walls of the container, causing a decrease in the height of capillarity at the liquid surface. [24]

In summary, the relationship between cohesion and adhesion plays a crucial role in the manifestation of phenomena such as surface tension and capillarity in liquids.

the reservoir rock, which may vary in type (oil or gas reservoir, saline aquifer, coal beds, salt formations), hosts immiscible phases such as oil, water and gas. In each of these environments, equilibrium between these phases is maintained by capillary forces.

Capillary pressure indicates the pressure difference at the interface separating two non-mixing fluids. The interfacial tension seeks to minimise the interface area, comparable to the tension in a rubber band. To maintain equilibrium at the interface, the internal pressure must exceed the external pressure.

In an oil or gas reservoir, these capillary forces play a crucial role in the behaviour of the fluids. In a saline aquifer, the salinity of the water adds additional considerations to the capillary properties. In a carbon reservoir, the interaction with the carbon layers introduces unique factors that influence the capillary forces.

The capital forces can be represented by the following formulas:

$$P_c = P_{nw} - P_w \quad \text{Equation 2: normal}$$

$$P_c = P_0 - P_w \quad \text{Equation 3: oil-water}$$

$$P_c = P_g - P_w \quad \text{Equation 4: gas-oil}$$

In first equation, P_c represents capillary pressure. P_{nw} represents the pressure of a non-wetting phase (e.g., gas) and P_w represents the pressure of the wetting phase (e.g., liquid). The capillary pressure is the difference between the pressure of the non-wetting phase and the pressure of the wetting phase.

Second equation P_c represents capillary pressure. P_0 represents the pressure of a specific fluid phase, which is often used to represent oil in the context of oil-water systems. P_w represents the pressure of the wetting phase (water). The capillary pressure is the difference between the pressure of the oil phase and the pressure of the water phase.

Third equation P_c represents capillary pressure. P_g represents the pressure of a specific fluid phase, which is often used to represent gas in the context of gas-water systems. P_w represents the pressure of the wetting phase (water). The capillary pressure is the difference between the pressure of the gas phase and the pressure of the water phase.

The following figure provides a more visual representation of capillary forces. [25,26]

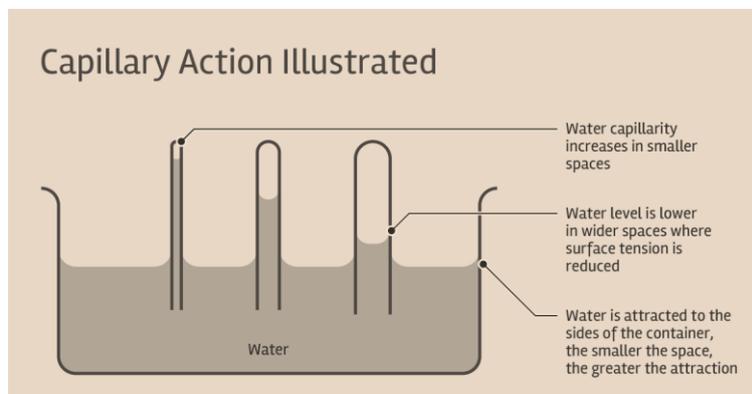


Figure 4: Capillary action causes the water [26]

2.2.2 Viscous forces

Viscous forces, as defined, pertain to the inability of a fluid to withstand shearing stress. Yet, fluids do resist shearing movements. The property quantifying a fluid's resistance to such motion is referred to as viscosity [27].

These viscous forces relate to the inherent pressure gradients within fluid flow through reservoirs, in accordance with Darcy's Law.

In the realm of fluid dynamics, viscous forces wield a critical role in shaping injection and production rates, aiming to counteract the water/gas coning effect. This effect describes the inflow of water/gas towards the production well's entrance, driven by the interplay between gravitational [28].

2.2.3 Gravity forces

Gravity forces constrain fluids to a spatial position inside a reservoir that is primarily influenced by buoyancy force. The positions of gas, oil, and water inside the pore space are determined by

their density differences. The complete distinction of the elements by density variation, known as gravity segregation, never truly ends.

The ideal in which there are no clear limits between gas, oil, and water is largely attributable to forces of capillary (Dandekar, 2006). Capillary forces are larger within the tiniest pores than they are elsewhere. Will oppose gravity and limit gravitational segregation between phases (for example, water and petroleum). When the motion caused by gravitational forces is expressed as an equation, two immiscible objects are brought together. [29]

2.2.4 Wettability

Wettability is characterized by the inclination of a fluid to adhere or disperse across a solid surface when other immiscible liquids are present [30]. In cases where multiple phases exist within the rock matrix, one is termed the wetting phase, while the other is designated as the non-wetting phase. The propensity of a liquid to spread on a solid surface indicates a solid wetting preference of the liquid phase over the solid phase. The interaction between the rock and the two phases can involve a preferential wetting by one of the phases or wetting by both phases simultaneously, denoted as a mixed-wetting rock, illustrated in figure 5. The aforementioned researcher delineates six wetting conditions, encompassing water-wet, oil-wet, neutrally-wet, intermediate-wet, fractional-wet, and mixed-wet states. Neutrally-wet signifies a system devoid of a specific wetting preference for either oil or water. In the intermediate-wet state, the system exhibits an equal wetting preference for both oil and water. Fractional wetting characterizes a system where certain minerals display a higher affinity for oil wetting, while others exhibit a higher wetting preference. [30,31].

Wettability is described as a fundamental characteristic of both rocks and fluids, with its intricacies rooted in the complexity of force interactions that govern capillary behaviour. It is widely acknowledged that the wettability of a reservoir significantly influences the spatial distribution of fluids within the pore space, thereby impacting fluid flow throughout the reservoir. Wettability measurements play a crucial role in deducing the most probable irreducible water saturation and residual oil saturation. The former represents the total hydrocarbons present in the reservoir within the pay-zone, while the latter indicates the hydrocarbons that will remain trapped in the porous media after water flooding.

Numerous studies have demonstrated the inherent dependency of wettability on both lithology and fluid properties [30]. Concerning irreducible water saturation, it has been observed that the saturation of water is consistently higher than 20-25%, particularly when water acts as the wetting phase. Conversely, when water serves as the non-wetting phase, the irreducible water saturation typically hovers around 15% [30,31,32,33].

Imbibition refers to the displacement of a non-wetting fluid by a wetting fluid, resulting in increased saturation of the wetting fluid. These investigations consistently highlight the critical role of

wettability in governing the natural imbibition process. Spontaneous imbibition is defined as the inherent adsorption of a wetting fluid on the mineral rock surface. [34,35]

Forced imbibition is a common practice in petroleum reservoirs, involving the application of external forces to promote the imbibition of the wetting phase (e.g., water injection for water-wet rocks). Imbibition dynamics are influenced by various properties, including porosity, permeability, porous structure, matrix size and shape, fluid viscosity, initial water saturation, wettability, interfacial tension, relative permeability, and gravity. The contact angle serves as a classification for the wettability of a surface with respect to a liquid, as illustrated in Figure 5. [34,35]

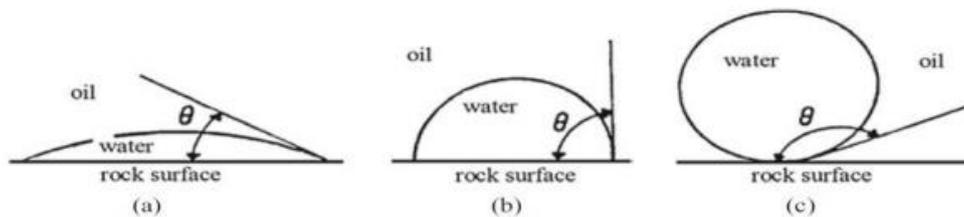


Figure 5:Wettability- type of contact angle [32]

Wettability is a dynamic property, which makes it a time-varying characteristic. It is important to note that the wettability of the rock can undergo changes even before the measurement processes are carried out, mainly due to the use of polar components as solvents (e.g. ketones, alcohols, etc.). These changes in wettability have a direct impact on capillary pressure, relative permeability, water flow behaviour, as well as irreducible water saturation and residual oil saturation. [34,35,36]

In a broader context, the importance of wettability in CO₂ storage lies in its direct influence on CO₂ injection and retention processes in geological formations. Understanding wettability is essential to anticipate and control the efficiency of CO₂ storage in subsoils, as it affects the interactions between CO₂, water, and porous rock. Proper wettability management can optimise storage capacity and reduce the risks of unwanted CO₂ mobility, thus contributing to effective carbon capture and storage strategies to address climate change.

2.4. Gas Properties

The term "gas" represents one of the three states of matter. Unlike liquids, gases do not have a fixed shape; instead, they occupy the entire space of the container that holds them. Additionally, gases are highly compressible and can readily mix with other gases. However, unlike liquids, gases are typically not soluble in water or other liquids and do not exhibit the same level of intermolecular cohesion as liquids. Figure 8 shows the three states of matter and the key points of matter change.

In our project, the relevant gas is CO₂. At room temperature and pressure, CO₂ is an odourless, colourless, slightly acidic, and non-flammable gas. However, its state varies according to changes in pressure and temperature, allowing it to be stored in geological formations as a gas, liquid, or in a supercritical state.

The point at which a substance can exist in equilibrium as both a gas and a liquid under the highest pressures and temperatures is called the triple point. [37].

The assessment of geological formations for CO₂ storage includes the crucial consideration of the behaviour and variation of free CO₂ properties in relation to temperature, pressure, and thus, depth. The phase in which CO₂ is stored in these geological formations, whether as a gas, liquid, or in a supercritical state, is determined by the specific conditions of temperature and pressure at the storage depth. [38].

Under atmospheric conditions, CO₂ is a thermodynamically stable gas and denser than air. At temperatures below its "critical point" (31.1°C and 7.38 MPa = 72.8 atm), CO₂ remains in a thermodynamically stable gaseous state. Whether in the form of a gas or liquid, at higher temperatures and pressures, CO₂ assumes a supercritical state. In this state, while it still behaves as a gas by expanding to occupy all available space, its density is akin to that of a liquid, increasing proportionally with temperature and pressure, ranging from 200 to 900 kg/m³. [39]

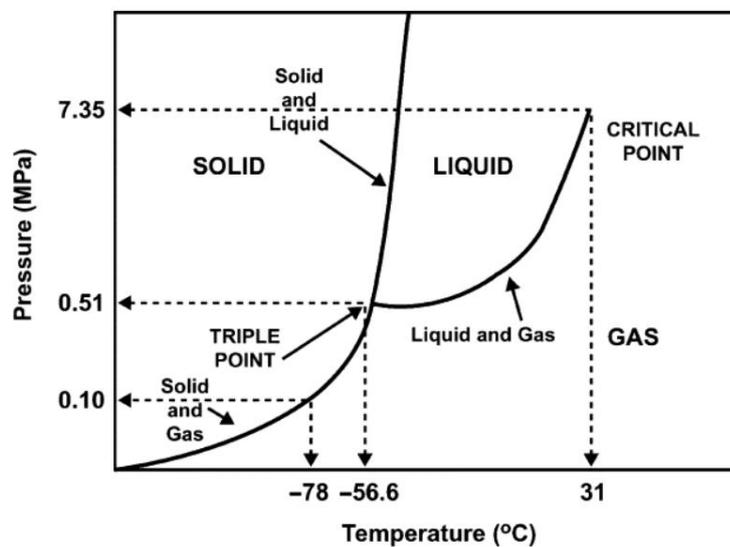


Figure 6: CO₂ Phase diagram of pressure (MPa) vs. Temperature (°C) for CO₂ [40]

Depending on the depth, CO₂ is stored in different ways. Up to a depth of 500-600 metres, CO₂ is stored as a gas with too low a density for economically significant and efficient storage volumes to be considered. Figure 9 can give another form to explain these phenomena.

At depths of 600-1000m, there is an abrupt increase in density because, at these depths, the average temperature and hydrostatic pressure are close to the CO₂ critical point. [41].

At a geothermal gradient of 25°C/km or an average hydrostatic pressure gradient of 10 MPa/km, the temperature and pressure at depths of 800-850 m are such that CO₂ will be in a supercritical state. Under normal conditions of pressure and temperature (0°C and 1 atm), one tonne of CO₂ occupies 500 m³ to 18 m³ at depths of more than 800 m. [42].

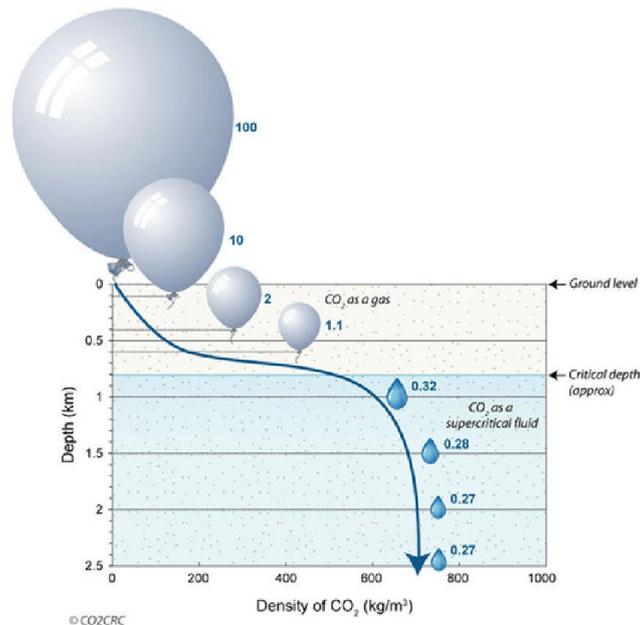


Figure 7: CHange of density and Volume of CO₂ [43]

The importance of CO₂ behaviour concerning temperature, pressure, and depth is highlighted in the assessment of sedimentary basins for their suitability for CO₂ storage. [38].

The depth required to reach supercritical CO₂ conditions varies widely, depending on factors such as surface temperature and geothermal and pressure gradients within a basin. [38].

The geothermal regime of a sedimentary basin is influenced by various heat sources, tectonics, proximity to heat sources such as magma, and the thermal conductivity of rocks. Additionally, pressure in the pores of sedimentary rocks generally approximates hydrostatic pressure, but in some cases, it may exceed it due to fluid compression or the extraction of oil or gas. [44].

The pressure in the geosphere is related to lithostatic and hydrostatic pressure, and it is essential to understand how these pressures influence the pores of sedimentary rocks.

The temperature distribution in a sedimentary basin is continuously calculated along the sedimentary sequence. In contrast, the pressure distribution must be determined individually for each sedimentary interval due to the complexity of aquitards and other factors [45].

The variation of CO₂ density with depth has significant implications for CO₂ storage and flow. In "hot" basins (geological formations where temperature increases significantly with depth), CO₂ density initially increases with depth due to pressure, but then decreases due to opposing effects of temperature. On the other hand, in "cold" basins (geological formations that show a different temperature variation with depth), the relationship between density and depth may be different, suggesting the existence of an optimal depth for storing CO₂ as a free phase [38].

In summary, depth, as well as geothermal and pressure conditions, are critical factors in assessing a basin's suitability for CO₂ storage. These factors vary by location and can have a significant impact on storage capacity and safety.

In Figure 10, a graphical representation illustrates the relationship between temperature and pressure in the context of CO₂ storage. This figure provides a visual depiction of how these two variables vary in sedimentary basins and how this variation affects optimal CO₂ storage conditions. It serves as a valuable tool for understanding the influence of temperature and pressure on the supercritical phase of CO₂ and helps identify the most favourable conditions for safe and efficient CO₂ storage. [38].

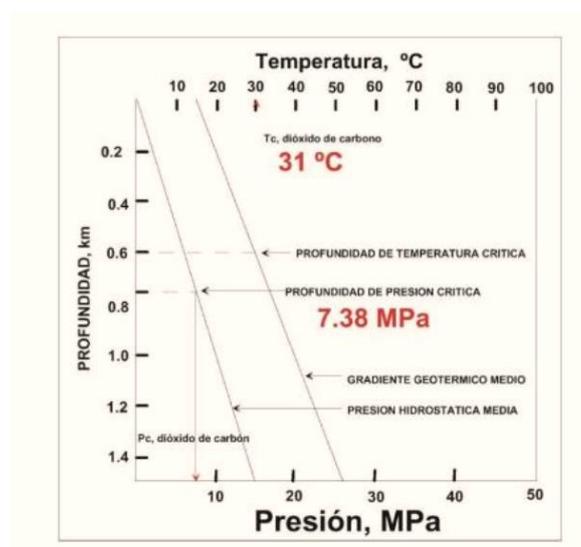


Figure 8: relationship between temperature and pressure in the context of CO₂ storage [44]

In the absence of such a connection, the actual pressure may exceed the hydrostatic pressure, resulting in an increase in pressure as the fluid may be compressed by the surrounding formations, so that this part of the weight of the upper layer is borne by the water in the system. Pressure build-up can also occur naturally or because of the extraction of fluids such as gas or oil from sediments. [38]

The optimal storage conditions for carbon dioxide in the subsurface are obtained when it is stored in a supercritical state, so it is necessary to study the pressure characteristics directly related to the depth and temperature of formation. Due to the formation of the buoyancy effect of carbon

dioxide in relation to the initial liquid, the evaluated pairs of pressure and temperature values will be in the upper part of formation. [45]

It is possible to determine the pressure P in a formation, if there is no additional pressure due to geological movement, by determining the hydrostatic pressure proportional to depth: whatever the depth of the formation.

Increasing the depth of the reservoir formation favours risk analysis as greater depth moves the fluid away from the surface, reducing the possibility of leakage and increasing the distance of the leakage path, although increased depth is related to increased drilling costs, another aspect to consider. [45]

2.5. Storage

As mentioned in the explanation of CCS technology, CO₂ is stored in various geological formations. In this section, four options for CO₂ storage are explained.

1. Hydrocarbon deposits

CO₂ can be stored in depleted or still producing hydrocarbon reservoirs, the latter being used to increase oil and gas recovery.

One of the key approaches in the oil industry is Enhanced Oil Recovery (EOR). In this process, various techniques, including the injection of carbon dioxide (CO₂), are used to improve the extraction of oil from reservoirs. Figures 11 and 12 below illustrate the EOR process and how CO₂ can improve oil mobility.

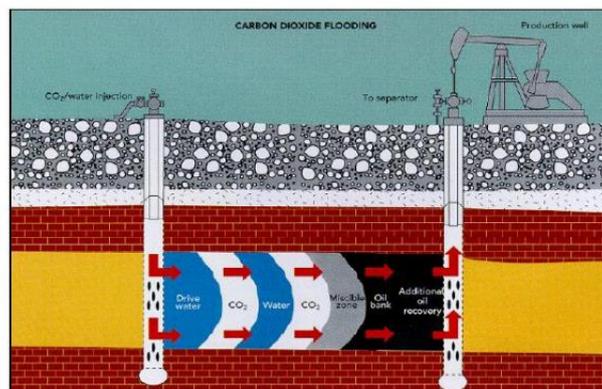


Figure 9: EOR system with CO₂ injection [46]

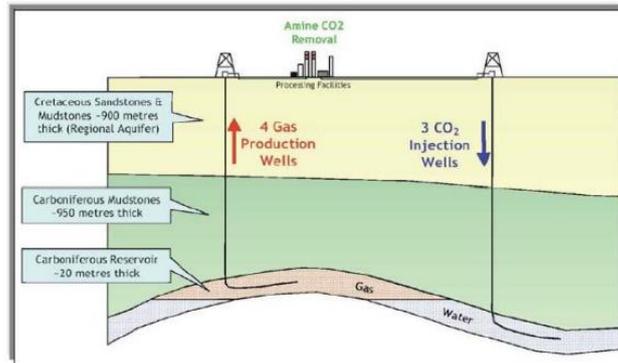


Figure 10: EOR installation with CO₂ injection [46]

In EOR operations, CO₂ improves the mobility of crude oil if miscibility is reached, as its viscosity is decreased while reservoir pressure is maintained or increased. In a situation of CO₂ immiscibility, CO₂ is used to repressurize the reservoir, pushing the oil towards the producing wells. Once depleted, oil fields offer the opportunity to be used as CO₂ storage, like storage in deep permeable formations with saline water.

These hydrocarbon fields offer an economic benefit that can offset the costs of capturing, transporting, and storing CO₂.

A similar situation applies to gas fields. In both cases, as the pressure of the hydrocarbon is reduced, a considerable volume of pores filled with gas at low pressure is formed inside the storage rock, which is not usually clogged by the flow of water and can be used to store CO₂. Once they are exhausted, there do not seem to be any technical barriers to this, and there are currently recurring experiences of natural gas storage in geological formations in different countries.

If storage in the enhanced oil recovery (EOR) or enhanced gas recovery (EGR) options is not possible, gas reservoirs will most likely be used instead of oil reservoirs, since it is usual to extract 90% of the existing reserves, leaving a large amount of free space if it has not been saturated by water.

The depth of hydrocarbon fields varies from 7000m, with an average depth of 1500m. This implies that CO₂ is stored under supercritical conditions, maximizing its storage density. On the other hand, it is common for fields to have a reduced pressure with respect to the initial pressure, which is in favour of CO₂ storage. In addition, this form of storage has the advantage that the confinement capacity of the system has been demonstrated by the retention of hydrocarbons for millions of years.

The major limitation of using hydrocarbon fields as a form of CO₂ storage is the high possibility of unsealed or poorly sealed wells, which can lead to leakage pathways. Also, this option is restricted to countries that have reservoirs with limited storage capacity due to the size of existing traps.

The possibility of reservoir collapse can be expected if there has been a significant reduction in pore pressure, which will reduce the available storage volume. Finally, the proximity to sources of CO₂ generation may be inadequate. [46].

2. Aquifers

Geological CO₂ storage emerges as an effective solution to mitigate industrial CO₂ emissions, with the preferred method for the Spanish context being storage in saline aquifers. While widely accepted, there is still a need to develop and refine various methodologies and technologies to make this concept fully viable [47].

This approach involves injecting supercritical CO₂ into deep aquifers, which are porous and permeable rocks containing highly saline water. To be an effective reservoir, these aquifers must be capped by layers of impermeable rock acting as a seal. Over time, carbon dioxide will dissolve in the aquifer water, precipitate forming minerals, and occupy the porous spaces. Although underground storage has been industrially tested, especially in oil operations, new developments and methodologies are required [47].

The injection of carbon dioxide (CO₂) into deep saline aquifers stands out as a crucial option for geological CO₂ storage, aiming to reduce anthropogenic greenhouse gas emissions. Previous studies (such as Bachu, 2003; IPCC, 2005; USDOE, 2007a; Bradshaw et al., 2007) suggest that, compared to other primary alternatives like depleted hydrocarbon reservoirs or deep coal seams, deep saline aquifers have the highest potential capacity worldwide for CO₂ storage.

Furthermore, due to their extensive occurrence, these formations are more likely to be located near sources of CO₂ emissions. In this approach, supercritical CO₂ can be efficiently stored due to the elevated density achieved under the inherently high pressures at which it is typically found. The confinement mechanisms available for CO₂ over time further enhance the volumetric storage capacity of these reservoirs [48].

However, this method of CO₂ storage could be considered more innovative because we primarily live in the era of coal and fossil fuels. Therefore, initially, more attention was given to storage in hydrocarbon deposits. For example, the fear that injecting CO₂ into these formations could cause earthquakes, as seen in the experience of the Castor project in the Gulf of Valencia, where the reuse of an old oil well generated significant seismic activity.

Nevertheless, recent studies, such as the one published in the PNAS journal by researchers from Berkeley, the Federal Institute of Technology in Lausanne, and the Institute of Environmental Diagnosis and Water Studies of the CSIC, have shed light on the feasibility and safety of this technique. Jesus Carrera, one of the authors of the study and a research professor at the CSIC, emphasizes that the choice of location is crucial. They seek formations of porous rocks filled with saltwater, abundant worldwide, where storing CO₂ would be relatively straightforward. The greater elasticity and capillarity of these formations make them less prone to tensions that could trigger earthquakes. The critical moment occurs at the beginning, during the CO₂ injection, where it is

essential to displace the water filling the rock pores. However, Carrera emphasizes that this risk can be mitigated by starting the process with a reduced flow.

A successful example of this technique is found in Norway, where in 1996 Statoil Hydro launched the first CO₂ storage project in Europe at the Sleipner gas field. This project has demonstrated the effectiveness and safety of storage in deep saline aquifers in the open sea, at considerable depths below the seafloor. To date, 10 million tons of CO₂ have been successfully stored in the Utsira well, equivalent to the emissions from two years of the entire Norwegian fleet.

Economically, the main challenge lies in separating CO₂ from other gases present, such as nitrogen. However, the proven technical feasibility and seismic safety make CO₂ storage in saline aquifers an attractive and promising option for combating climate change.[49].

3. Carbon layers

This storage consists of injecting CO₂ into the coal layers through adsorption mechanisms and releasing the CH₄ (which must also be captured) existing in the porous matrix. This is due to the greater affinity of coal for CO₂ than for CH₄, and this technique saves on injection costs.

This method has several disadvantages, such as the low permeability of the coal, especially as the depth increases, and the high cost due to the large number of boreholes [46].

4. Salt structures

This option requires prior excavation of the rock, which is carried out by dissolution, to create a cavity that can be occupied by the CO₂. Figures 13, 14 shows graphically what this formation looks like.

Properties such as low permeability and self-sealing properties of saline rocks make CO₂ storage possible. These rocks can occur in nature as saline domes, which usually have a very homogeneous mineralogical chemical composition, or in stratified saline formations, with intercalations of non-saline saline materials. In the two figures presented below the paragraph, we can visually observe examples of the salt formations mentioned earlier.

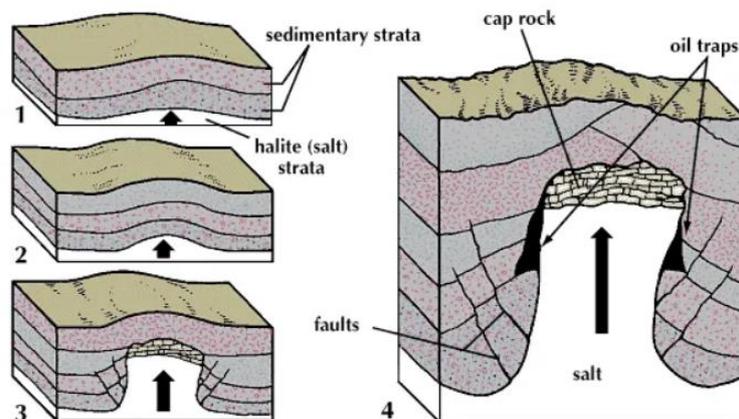


Figure 11: Example of formation of Salt dome [50]

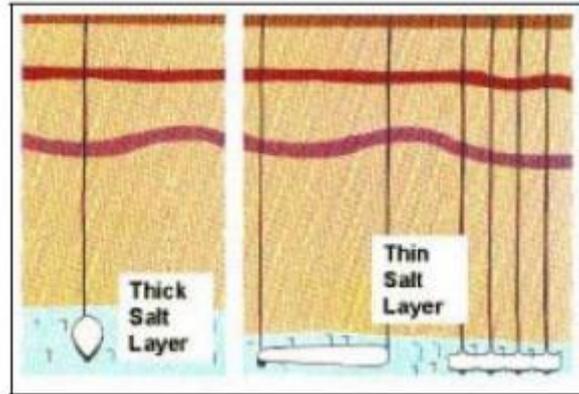


Figure 12: caverns or salt mine [51]

The main advantages of this option are its large capacity, high filling rate, the potential economic value of the resulting brine and the fact that it can be a permanent or temporary CO₂ store. Also, CO₂ storage can be done in relatively light cavities, without the need to maintain critical thermodynamic conditions. As the most expensive CO₂ storage method, it is possibly an option when no other formations are available in the area to be stored.

To guarantee the stability of the cavity, the excavation must have minimum conditions of power and extension of the salt formation, which leads to the generation of brine that will have to be managed as waste or as an industrial product.

On the other hand, there are many uncertainties about the long-term behaviour of these systems. The saline material is under stress and behaves as a viscos-plastic substance producing the creep process. Knowledge of the response of the salt cavity and the upper strata to this creep process is critical to the viability of the repository. [52,53]

The characteristics for this option to be used as geological storage are:

- Adequate porosity, permeability, and salinity.
- The existence of a top layer, impermeable to the flow of CO₂,
- Be in geologically stable areas.
- Have a size (extent), large enough to store the amount of CO₂, which allows the viability of the storage. [52,53].

Assessing the CO₂ storage potential within a geological formation isn't a straightforward calculation. The total storage capacity is contingent upon the scale of the storage facility. Larger facilities offer greater space to contain fluid or gas content.

For formations oriented horizontally, fluid storage extends further compared to structures in geological formations. Fluids would primarily occupy the shallower sections of the formation, like small domes or undulations, consequently reducing overall capacity.

Divergent outcomes emerge from estimates by different authors when calculating regional and global storage. Although capacity calculations rely on simple algorithms tailored to specific retention mechanisms, performing these calculations for a defined volume of rock mass at specific depth, temperature, and pressure within a given region or site is intricate.

The complexity of capacity assessment stems from the array of distinct traps and confinement mechanisms, their temporal effectiveness, and the various physical states in which CO₂ can be stored. Examples of envisioned confinement mechanisms include:

- Structural/stratigraphic
- Hydrodynamic
- Residual
- Solubility-based
- Mineral-based
- Adsorption-based

The evaluation of storage capacity introduces multiple levels of uncertainty. These assessment levels demand comprehensive data from diverse disciplines that must be harmonized. For precise examination of storage capacity on a local scale, the most effective approach involves constructing a geological model and employing that information in reservoir simulation. Notably, this discussion pertains to CO₂ capture and storage. [54]

2.6. CO₂ Injection

There are various types of carbon dioxide (CO₂) injection techniques used in geological storage, and these methods vary based on the nature of the geological formation and the specific objectives of the project.

In the case of miscible injection, CO₂ is introduced into the geological formation to achieve complete mixing with the existing oil or gas. This process enhances the efficiency of oil or gas recovery, significantly increasing the overall storage capacity for CO₂. On the other hand, immiscible injection involves the introduction of CO₂ into the formation without complete mixing. This results in the expansion and mechanical displacement of oil or gas toward the production well, achieving substantial recoveries but generally with less efficiency compared to miscible injection. [55]

Another noteworthy method is supercritical CO₂ injection, where CO₂ is brought into a supercritical state through elevated temperatures and pressures. This state improves solubility and mobility, enhancing the displacement of hydrocarbons. Additionally, water or polymer-assisted injection combines CO₂ with other fluids to improve displacement efficiency and enhance hydrocarbon recovery. This is achieved by controlling the mobility of fluids within the geological formation. [56]

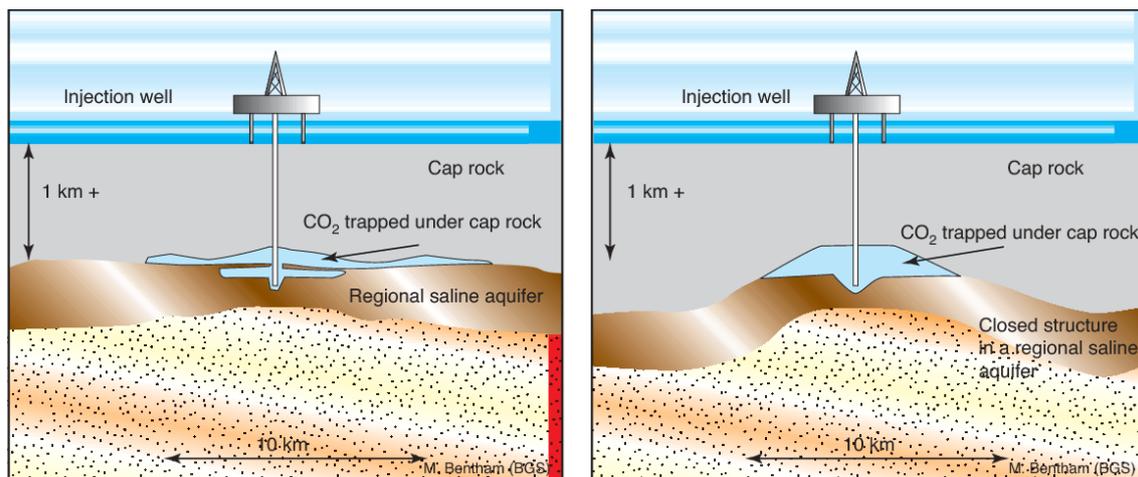


Figure 13: "Graphic example of what the injection of CO₂ into a saline aquifer would look like." [58]

Moreover, CO₂ injection in coal beds is a specific technique that not only serves the purpose of geological storage but also facilitates the release of adsorbed methane, contributing to enhanced recovery. In parallel, injecting CO₂ into deep saline aquifers, apart from depleted oil and gas reservoirs, involves a reaction with minerals in saline water, resulting in the formation of carbonates and contributing to the mineralization of CO₂. [57]

In conclusion, the selection of a particular injection method depends on the specific geological characteristics of the formation and the primary goals of the project, whether focused on

optimizing hydrocarbon recovery or achieving long-term CO₂ storage for climate change mitigation.

2.7. Portugal's Potential for CO₂ Storage

It is important to assess Portugal's climate and its options for CCS storage.

Portugal aims to reduce emissions by a range of 45% to 55% by 2030, 65% to 75% by 2040, and 85% to 90% compared to emission levels in 2005. Despite not having exploited oil and gas fields, the country possesses areas of interest for CO₂ storage, located in sedimentary basins along its coast. [59]

2.7.1 Geology of Portugal and Relevant Considerations

The geology of Portugal is diverse and presents an interesting geological history due to its location on the Iberian Peninsula and its interaction with various geological processes over time. Here's a general overview of Portugal's geology:

- 1. Coastal Oceanic Zone:** Portugal's western coast is influenced by the Eurasian Tectonic Plate and the African Tectonic Plate. This has led to the formation of a wide continental shelf and the presence of submarine canyons and steep drops on the shelf.
- 2. Azores Volcanic Chain:** The Azores is a volcanic archipelago in the middle of the Atlantic Ocean, formed by the interaction of the North American Plate, the Eurasian Plate, and the African Plate. Past and ongoing volcanic activity has resulted in island formation and rugged landscapes.
- 3. Iberian Peninsula Mountain System:** Portugal shares the Iberian Peninsula with Spain and is influenced by the Eurasian Tectonic Plate and the African Tectonic Plate. The Central Iberian Range extends north into Portugal, featuring mountains and reliefs primarily of Hercynian origin.
- 4. Sedimentary Deposits and Metamorphic Rocks:** In Portugal, there are sedimentary deposits and metamorphic rocks dating from the Palaeozoic to the Cenozoic. Marine, fluvial, and lacustrine sediments are found in various areas of the country, and metamorphic rocks result from processes related to plate collision during the Hercynian orogeny.
- 5. Minerals and Natural Resources:** Portugal is known for its mineral deposits, including tin, tungsten, copper, lead, and zinc. The Trás-os-Montes region, for example, hosts significant mineral deposits. Quarries for marble, granite, and slate have also been exploited in different parts of the country.
- 6. Volcanic Rocks:** Volcanic rocks dating from different geological periods are found in the Azores and some areas of the mainland, like the Lisbon region. These rocks are the result of volcanic activity that has affected the region over millions of years.

7. Oil and Natural Gas Deposits: Portugal has some oil and natural gas deposits in its territorial waters, especially in the Atlantic Basin off its western coast. However, the exploitation of these resources has been limited due to technical and environmental challenges. [60,61]

In summary, Portugal's geology is diverse, characterized by a combination of tectonic processes, volcanic activity, and sedimentation over different geological periods. This diversity has resulted in a wide range of landscapes and the presence of mineral and energy resources in various parts of the country. As can be seen in Figures 19 and 20, which depict the geology of Portugal.

2.7.2. National storage assessment, storage options, potential and capacity

Geological Storage of Carbon Dioxide, Decree-Law no. 60/2012, of 14 March, establishes the legal regime for the activity of geological storage of carbon dioxide (CO₂). This title results from the transposition of Directive 2009/31/EC - Geological Storage of Carbon Dioxide, of the European Parliament and of the Council, of 23 April.

In Portugal, suitable areas for CO₂ storage are located in sedimentary basins along the Atlantic coastal margin. Given that over two-thirds of the Portuguese continental territory consists of igneous and metamorphic rocks, geological storage of CO₂ is unfeasible in these areas. Offshore sedimentary basins, such as Northwest, West, and Algarve, present promising opportunities.

Geospatial and geological-geophysical studies have identified potential areas in projects funded at both national and international levels. The Northwest, West, and Algarve basins have been highlighted:

- a) Northwest Basin: 2,150 km² offshore with an estimated CO₂ storage capacity (central P50) and an uncertainty interval.
- b) West Basin: 22,000 km² on land and sea with a variable storage capacity (central P50) and an uncertainty interval.
- c) Algarve Basin: 8,500 km² on land and sea with an estimated storage capacity and an uncertainty interval.

The theoretical storage capacity in deep saline aquifers in Portugal is approximately 7.09 Gt of CO₂ (central P50), with an uncertainty interval. [62]

Figure 13 illustrates the geographical distribution of sedimentary basins with thirty-six potential storage units and storage capacity estimates (P50) for each unit. While promising units are identified, there is a recognized need for future studies to review capacities and feasibilities.

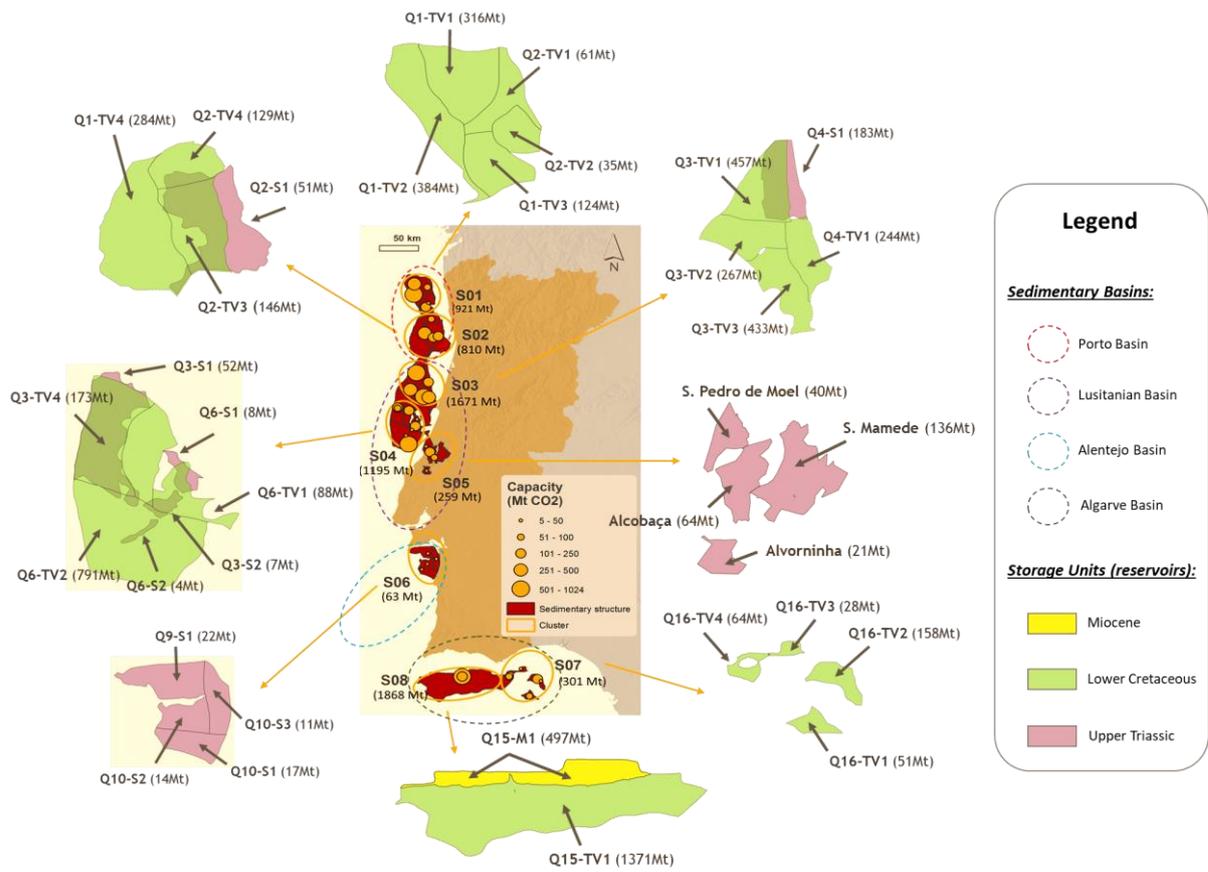


Figure 14: Localization of six storage points in Portugal [62]

The most promising region in continental Portugal is being investigated in an ongoing European project, supported by hydrocarbon exploration activities. The total storage capacity offshore is approximately 2.9 Gt of CO₂ (central P50), with an uncertainty interval, with onshore units being less capable. [62]

Despite higher costs offshore, better social acceptance for CCUS implementation is expected. Projects such as PilotSTRATEGY, funded by the EU, focus on characterizing locations for injection onshore or offshore in the Lusitanian Basin. Although there is no specific CO₂ storage Atlas currently available, there is a CCS Roadmap for Portugal with potential areas based on previous studies. [62]

2.7.3 Summary

Portugal aligns with the European Green Deal, aiming for carbon neutrality by 2050. Currently, there are no past or ongoing large-scale projects for CO₂ capture, transport, or storage. The PilotSTRATEGY project focuses on characterizing areas for storage, involving stakeholders and the public.

There are no full-chain projects, and planning for a CCUS cluster is underway. National legislation outlines requirements for activities, including environmental impact assessments and financial guarantees.

Research is funded by the Foundation for Science and Technology and the National Innovation Agency, covering topics like storage capacity, land planning, well technologies, and social acceptance. Institutions such as universities and national labs are involved in research. Additionally, Portugal has participated in European research projects like FP7 COMET and STRATEGY CCUS.

Public awareness of CCS is growing, with workshops and seminars conducted in recent years. While there are no specific national advocates for CCS, the country is committed to the European Green Deal and carbon neutrality.

According to the study "A Qualification study and assessment of the CO₂ storage capacity, siting and costs in Portugal," the optimal areas for storage align with the major industrial zones emitting the highest concentrations of CO₂, as depicted in images 15 and 16 compared to image 14. This alignment is advantageous, streamlining the transportation phase, cutting costs, and facilitating CO₂ storage.

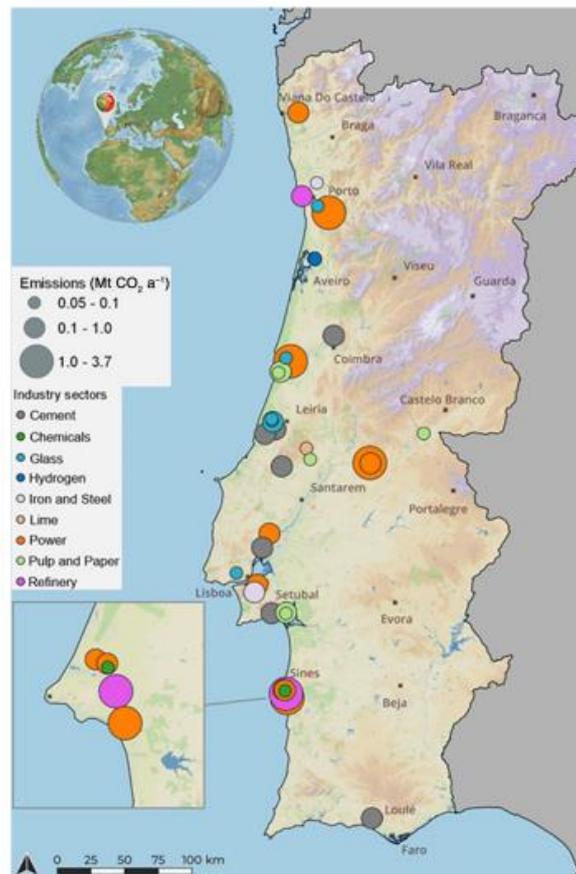


Figure 15: Geological distribution of main CO₂ emission in Portugal [63]

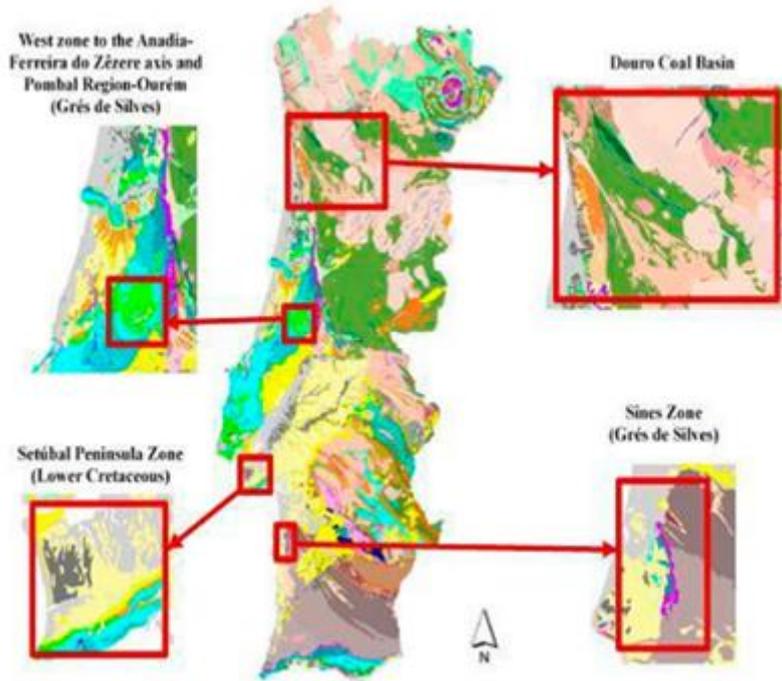


Figure 16: Optimal zones for Portugal CO2 Storage

3. Material And Methods

Simulating complex processes, such as CO₂ injection into porous materials, necessitates the use of advanced mathematical methods and specialized simulation tools. In this context, mathematical models are employed to describe the behaviour of CO₂ flow and its interaction with a porous medium. These models are crucial for understanding intricate phenomena and predicting outcomes in physical environments that are challenging to analyse directly.

In this study, several key mathematical methods are implemented. The mass transport equation describes the evolution of CO₂ concentration over time and space, considering transport flows, diffusion, and sources or sinks. The diffusion equation focuses on CO₂ diffusion through porous material due to concentration gradients. Additionally, the mass conservation equation ensures that mass is neither created nor destroyed in the closed system, providing a solid foundation for fluid and porous material analysis.

The Peng-Robinson equation is used to model the behaviour of CO₂ in its supercritical state, offering crucial information about pressure, temperature, and molar volume. This thermodynamic approach allows for an accurate representation of fluid properties under specific conditions.

To conduct these complex simulations, ANSYS Fluent is employed—a leading computational fluid dynamics (CFD) software. ANSYS Fluent enables the application of advanced numerical methods, such as the finite element method, to solve the differential equations governing CO₂ flow and its interaction with porous material.

This software not only provides a robust platform for modelling complex physical phenomena but also integrates specific tools for simulating thermo-fluid-dynamic processes. Its capability to handle intricate geometries, consider initial and boundary conditions, and analyse detailed results makes ANSYS Fluent the ideal choice for simulating CO₂ injection in porous materials.

Utilizing ANSYS Fluent for simulation purposes is motivated by several key factors. Firstly, ANSYS Fluent has established itself as a tool of high precision and reliability, consistently delivering accurate simulations of complex fluid flows that closely mirror physical reality. Its proven track record instils confidence in the accuracy of results.

Secondly, the software's versatility is a standout feature. ANSYS Fluent goes beyond merely modelling fluid flow; it excels in capturing thermal and chemical interactions. This capability allows for a comprehensive representation of the intricate CO₂ injection process into porous materials, where multiple phenomena are at play.

The user-friendly interface of ANSYS Fluent is another significant advantage. Its intuitive graphical interface simplifies the task of defining geometries, specifying conditions, and conducting result analyses. This ease of use streamlines the entire simulation process, making it accessible to a broad spectrum of users, from engineers to researchers.

Lastly, ANSYS's commitment to continuous development adds to the software's appeal. Users benefit from access to the latest tools and technological enhancements in numerical simulation. This commitment ensures that ANSYS Fluent remains at the forefront of simulation software, incorporating innovations that continually enhance its capabilities.

In summary, ANSYS Fluent stands out as a preferred choice for simulation endeavours due to its proven accuracy, versatile modelling capabilities, user-friendly interface, and the ongoing commitment of ANSYS to advancing the field of numerical simulation. This combination makes it a powerful tool for informed decision-making and advancements across various industries. [64]

3.1. Description of the Mathematical Model

In this section, a detailed description of the mathematical model to be employed for simulating CO₂ injection into the porous material will be presented. The model is based on a set of fundamental equations governing the behaviour of CO₂ flow and its interaction with the porous medium. The following provides an overview of the key equations and mathematical concepts involved:

3.1.1 Mass Transport Equation:

The mass transport equation is pivotal in describing how CO₂ moves through the porous material during injection. It is expressed as follows [65] :

$$\frac{\partial C}{\partial t} = -\frac{\partial(J)}{\partial x} + R \text{ Equation 5: mass transport [66]}$$

Where:

- $\partial C/\partial t$ is the rate of change of concentration with respect to time (partial derivative of C with respect to t).
- $\partial(J)/\partial x$ is the spatial gradient of mass flux (partial derivative of J with respect to x).
- R represents sources or sinks of mass within the system

This equation describes how the concentration of the substance C changes with time t and position in space due to transport flows, diffusion, and sources or sinks of the substance. [66]

Diffusion Equation:

The diffusion equation elucidates how CO₂ diffuses through the porous material due to concentration gradients. Its general form is [67,68]:

$$\frac{\partial C}{\partial t} = D\nabla^2 C \text{ Equation 6: Diffusion [67,68]}$$

Where:

- C is the concentration of the substance (CO_2) as a function of time and position.
- t is time.
- D is the diffusion coefficient of the substance in the medium.
- ∇ is the nabla operator, denoting spatial gradient.

This equation describes how the concentration of the substance C changes with time t and position in space due to the diffusion process, where the substance moves from areas of higher concentration to areas of lower concentration. [67,68]

3.1.2 Mass Conservation Equation:

The mass conservation equation, also known as the continuity equation, is a fundamental principle in fluid dynamics that expresses the conservation of mass within a fluid flow. In its general form, the mass conservation equation can be stated as [66]:

Where:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0 \quad \text{Equation 7: Mass Conservation Equation [66]}$$

In a differential form (for a three-dimensional system):

Where:

- $\partial \rho / \partial t$ represents the rate of change of mass density (ρ) with respect to time (t).
- $\nabla \cdot (\rho \mathbf{v})$ is the divergence of the mass flow rate ($\rho \mathbf{v}$), which is the product of mass density and velocity vector (\mathbf{v}).
- The equation states that the change in mass density over time in a given region is equal to the net mass flow rate into or out of that region.

In an integral form [66]:

$$\oint \rho \mathbf{v} \cdot d\mathbf{A} = -d/dt \iiint \rho \, dV$$

Where:

- \oint represents the closed surface integral, which accounts for the mass flow rate across the closed surface.
- The right-hand side of the equation represents the rate of change of total mass within a volume ($\iiint \rho \, dV$) over time (t).

In simpler terms, the conservation of mass equation asserts that mass cannot be created or destroyed within a closed system. It is commonly used in fluid dynamics, thermodynamics, and other branches of physics and engineering to analyse and predict the behaviour of fluids and substances in various processes, including fluid flow, chemical reactions, and transport phenomena. [65]

Peng-Robinson Equation

The Peng-Robinson equation is a state equation used to describe the behaviour of fluids, including CO₂ in its supercritical state. This equation is employed to calculate the relationship between pressure (P), molar volume (v), temperature (T), and other thermodynamic properties under supercritical conditions. [69,70]

The general form of the Peng-Robinson equation is as follows:

$$P = \frac{RT}{v-b} - \frac{a(T)}{v(v+b)+b(v-b)} \quad \text{Equation 8: State for Supercritical CO}_2 \text{ [70]}$$

Where:

- P is the pressure of the supercritical CO₂.
- R is the gas constant.
- T is the temperature.
- v is the molar volume (volume per mole) of CO₂.
- $a(T)$ and b are temperature-dependent parameters specific to the Peng-Robinson equation.

In this equation, the term $a(T)$ represents the attractive forces between CO₂ molecules, and b accounts for the excluded volume of the molecules. The Peng-Robinson equation is widely used for modelling the behaviour of supercritical CO₂ and other fluids in various engineering and scientific applications, including carbon capture and storage, enhanced oil recovery, and supercritical fluid extraction.

In the case of supercritical CO₂, the values of (T) and b would be determined specifically for carbon dioxide based on its thermodynamic behaviour in the supercritical state and the specific temperature and pressure conditions of the system.

This equation of state is used in modelling and calculating thermodynamic properties of supercritical CO₂ in various applications, such as carbon capture and storage, chemical engineering, and scientific research. Specific values of the parameters (T) and b for CO₂ can be found in technical literature and thermodynamic databases [69,70,71]

Boundary Conditions and Initial Conditions

To solve the model, boundary conditions must be established to describe how CO₂ is introduced into the system and how it interacts with the porous material. Additionally, initial conditions will define the concentration of CO₂ within the material at the outset of the simulation.

This mathematical model will be implemented using numerical methods, such as the finite element method, to calculate how CO₂ flows and distributes within the porous material during the injection process.

3.2.2 Numerical Methods

In the simulation of supercritical CO₂ injection into a porous material using ANSYS, key mathematical and physical concepts are applied, including Darcy's Laws, to model the process:

Darcy's Laws: These laws describe fluid flow through porous media and are crucial in the simulation. The first law of Darcy relates the flow rate to the pressure gradient and the permeability of the porous medium:

$$Q = -kA \frac{dP}{xd} \text{ Equation 9: Darcy's Law 1}$$

The second law of Darcy relates the flow velocity to the fluid viscosity and the pressure difference:

$$v = -\frac{\mu}{k} \frac{dP}{dx} \text{ Equation 10: Darcy equation fluid viscosity}$$

Transport and Diffusion Equations: These are used to describe the movement and diffusion of supercritical CO₂ within the porous material. These equations consider concentration, CO₂ properties, as well as initial and boundary conditions. [72,73]

Supercritical CO₂ State Equations: These equations model how properties of CO₂, such as density and viscosity, change with pressure and temperature in the supercritical state.

Permeability and Porosity: These parameters characterize the porous material's ability to allow CO₂ flow. Permeability describes CO₂'s ease of movement, while porosity represents the volume of void spaces within the material.

Numerical Methods: ANSYS employs numerical simulation methods, such as finite elements or finite volumes, to solve the equations and model the flow and diffusion of CO₂ in the porous material.

Results Analysis: After simulation, results are analysed to understand how CO₂ moves within the material, how concentrations change, and how it's distributed throughout the system.

In summary, ANSYS utilizes Darcy's Laws and other fundamental equations to simulate supercritical CO₂ injection into a porous material. This involves modelling flow, diffusion, and physical interactions in the system, providing valuable insights into the injection process and its effects on the porous material.

4. Simulation

In this section, we will delve into the aspects of the simulation process to investigate the injection of supercritical CO₂ into a porous material, specifically sandstone, which we will saturate with brine using ANSYS. Simulations serve as a tool to explore complex phenomena and gather information about intricate processes that occur in real-world scenarios. In this context, the focus is on understanding the behaviour of supercritical CO₂ within a porous medium and its implications.

1. Importance of Simulation

Simulation offers a controlled virtual environment where various parameters, conditions, and interactions can be manipulated and observed. By replicating real-world conditions, simulations enable us to explore different scenarios, optimize strategies, and predict outcomes. In the case of supercritical CO₂ injection, understanding how the CO₂ interacts with the porous material, its movement, and the resulting changes is crucial for informed decision-making and sustainable practices.

2. Objectives of the Simulation

The main objective of this simulation is to understand the intricate dynamics involved in the process of injecting supercritical CO₂ into a porous material. By using ANSYS, our goal is to examine the general behaviour of CO₂ how it flows, diffuses, and interacts within the material, and understand how these interactions impact the overall system. This simulation provides, in a very general sense, fundamental aspects of CO₂ injection, allowing us to gain a slightly better understanding of its behaviour in the initial stages of the injection process.

3. Key Components of the Simulation

The simulation process involves several key components:

- **Mathematical Models:** Fundamental mathematical equations, such as Darcy's Laws, transport equations, and equations of state for supercritical CO₂, form the basis for describing the physical behaviour of the system.
- **Numerical Methods:** ANSYS employs numerical techniques, like finite element or finite volume methods, to discretize and solve these equations within the digital environment.
- **Material Properties:** Accurate material properties, such as porosity, permeability, and density, are essential for creating a faithful representation of the porous material and its interactions with CO₂.
- **Boundary and Initial Conditions:** Defining appropriate boundary and initial conditions ensures that the simulation starts from a realistic state and accurately simulates the injection process.

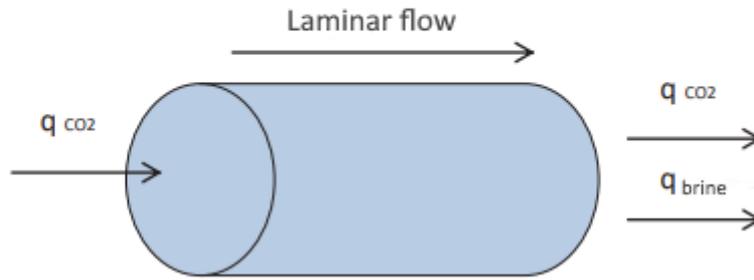


Figure 17: Model simulation

- Result Analysis: Post-simulation analysis allows us to interpret the behaviour of supercritical CO₂ within the porous material, observe concentration changes, and understand the distribution patterns.

4.1.1. Geometry Design

For the creation of our simulation model, we will apply a feature provided by ANSYS known as Design Modeler. This tool allows us to design our model effectively, catering to the specific needs of our study.

In this study, the design of a test specimen has been chosen based on reviewing various projects where CO₂ permeability tests in a porous medium are conducted using specimens of this type. We have choose to have three test specimens with the same diameter and size [74,75,76,77,78].

The chosen diameter for the simulation is 3,8 cm, while the corresponding length are 7,7 cm.

The process of creating this test specimen within ANSYS is straightforward. By selecting the XY plane as our starting point, we proceed to craft a circle using the design tools at our disposal. Once the circular shape is established, we proceed to give it volume, thus forming the basis of our test specimen. The process ensures that our models accurately represent the real-world conditions we aim to simulate.

Below, we've provided visual representations of the initial steps involved in the ANSYS environment for the creation of our model.

Through the utilization of Design Modeler, we are empowered to construct these test specimens in a meticulous manner, setting the stage for the subsequent simulation stages. This systematic approach allows us to ensure accuracy and reliability in our simulation outcomes, enabling a comprehensive exploration of the behaviours and interactions we intend to study.

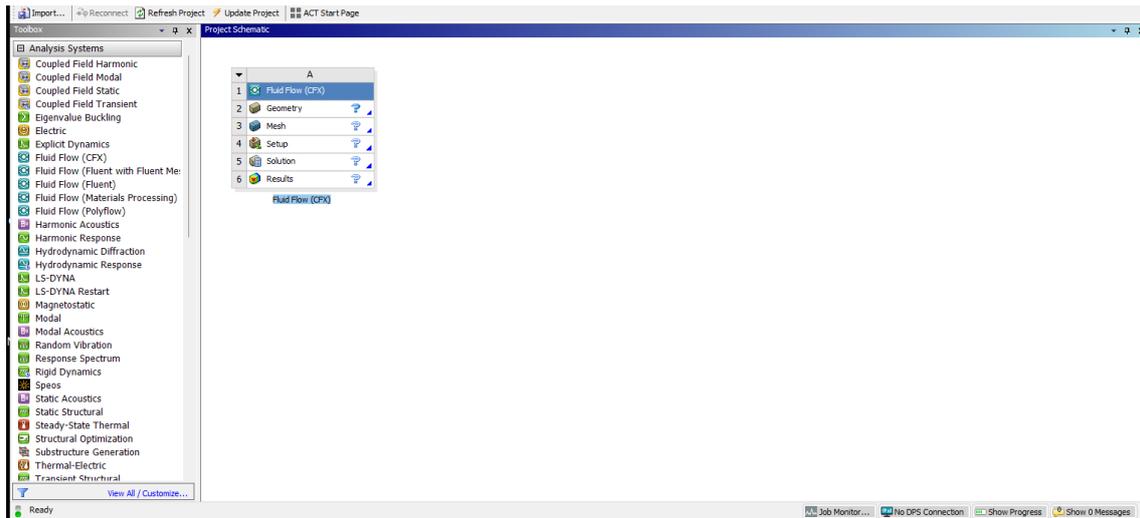


Figure 18: main menu, where you can select which modelling process the project will follow, in this case CFX.

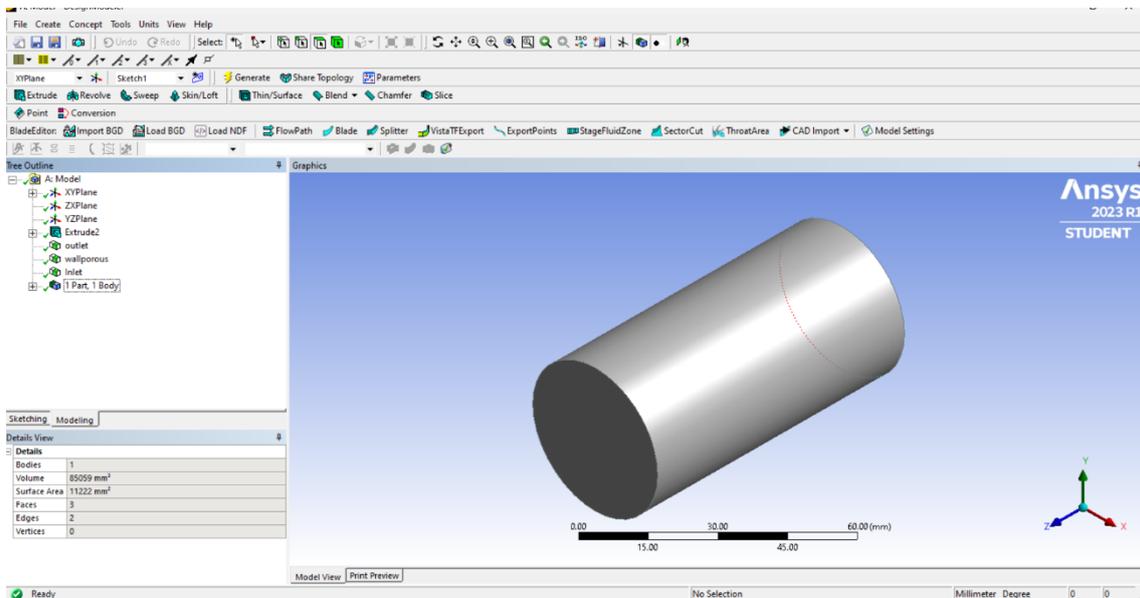


Figure 19: Cylinder Model experiments

In the early stages of our project, we conducted practical tests ,for both CFD (Computational Fluid Dynamics and CFX, two simulation modules within ANSYS. These tests served as a starting point to familiarize ourselves with the capabilities of these simulation tools. However, as we progressed in our project, we needed to make a critical decision regarding which simulation platform to use for our specific study on the permeability of supercritical CO₂ in a saturated sandstone test specimen.

The differences between ANSYS CFD and CFX and why we ultimately chose CFX for our project are as follows:

General vs. Specialized Focus: ANSYS CFD is a more general simulation module used for a wide range of fluid dynamics applications. On the other hand, CFX is more specialized in simulating complex flows and is particularly well-suited for problems involving multiphase and turbulent flows.

Mass and Heat Transfer: Both modules can handle mass and heat transfer, but CFX excels in modelling multiphase flows and turbulent flows, which are crucial in our study of CO₂ permeability in a porous medium.

Porosity Compatibility: CFX can effectively handle geometries representing porous media with porosity, which is essential for simulating a saturated sandstone test specimen.

Flexibility in Problem Formulation: Both modules offer flexibility in problem formulation, but CFX can be especially adaptable for specific problems involving complex and multiphase flows.

Industry Experience: CFX is used in industry to solve computational fluid dynamics problems in complex applications, providing confidence in its ability to address real-world problems.

In summary, while we explored both ANSYS CFD and CFX through practical tests, we chose ANSYS CFX for our project due to its specialization in complex flows, multiphase flows, and its capacity to handle specific problems involving permeability in porous media. This ensures that we have the necessary tools and expertise to effectively address the complex aspects of our research on the permeability of supercritical CO₂ in a saturated sandstone test specimen.

Breaking down our test piece into distinct sections, we identify three key zones: the entrance, the exit, and the wall. This division allows us to meticulously define and delineate the unique characteristics of each zone, enhancing the precision of our simulation process.

The "inlet" zone marks the point of entry for the fluid into our system. It is here that the CO₂ is introduced, initiating the intricate interaction with the porous medium within the wall zone.

Conversely, the "outlet" zone represents the location where the outcome of the CO₂ and porous medium interaction within the wall zone culminates. This section captures the result of the CO₂'s journey through the porous material, showcasing how it has been altered and influenced by the porous medium's properties.

Through this strategic breakdown of our test specimen and the careful establishment of distinct zones, we pave the way for a more targeted and insightful simulation process. Such meticulous structuring empowers us to unravel the intricate dynamics of CO₂ injection into porous materials with heightened accuracy and a comprehensive understanding of the phenomena involved.

4.2. Creation Of Meshing

Following the meticulous creation of our design using ANSYS Design Modeler, the next crucial step in our simulation journey is the generation of a mesh. Meshing, a fundamental aspect,

involves dividing our geometry into smaller, interconnected elements to facilitate precise numerical analysis.

By selecting the body of our geometry within the CFX software, the program generates a mesh that aligns with the complexities of our model. In our specific case, we've made strategic choices during the meshing process. Opting for a medium smoothing approach in the mesh size, we prioritize accuracy and reliability of the simulation results. This choice enhances our ability to capture intricate details and gradients within the system, particularly crucial in studying CO₂ injection into porous materials.

The mesh we've employed consists of 4535 cells and 348754 nodes, reflecting the fine level of detail we've incorporated to ensure comprehensive analysis. This mesh serves as the underlying foundation for our simulation, capturing the intricate nuances of the fluid's behaviour within the porous medium.

In essence, meshing is a pivotal bridge between our initial geometry and the simulation outcomes. It transforms our intricate design into a network of interconnected elements, laying the groundwork for detailed numerical analysis. The careful selection of mesh parameters and settings is essential, as it directly influences the precision and reliability of our simulation results.

Through the amalgamation of geometry design and meshing, we create a systematic approach that ensures our simulation process is both accurate and insightful. This synergy allows us to delve into the intricacies of CO₂ injection into porous materials, unravelling its behaviour and effects with a comprehensive understanding.

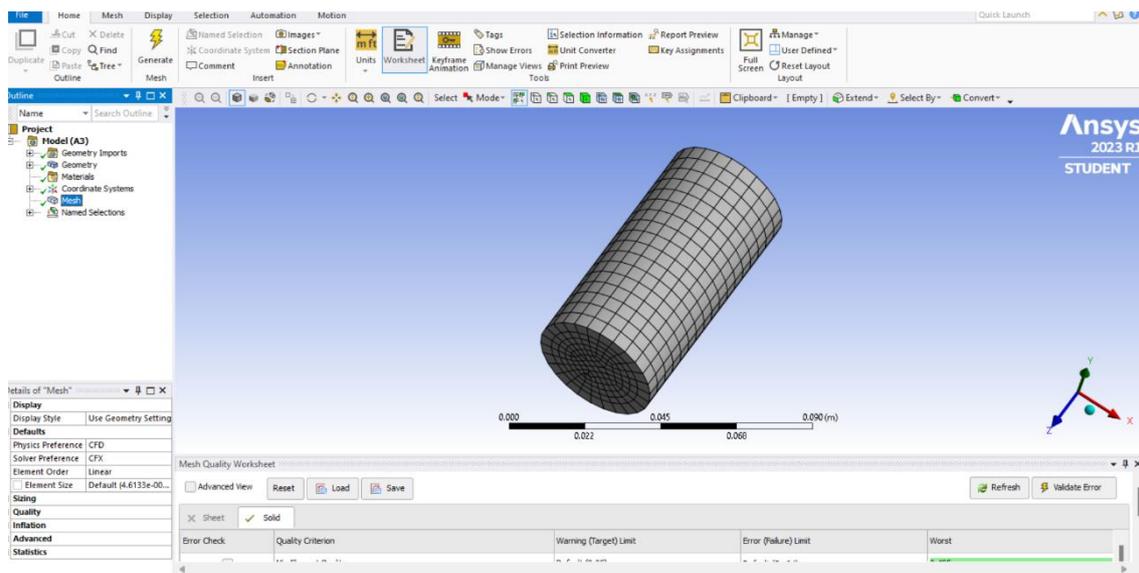


Figure 20: Mesh

4.3. Data Simulation

After defining our model and meticulously meshing it, we went on to set the parameters of our project and describe the characteristics of our simulation. The choice of data from different projects is made to leverage the availability and relevance of existing information.

The study used specific permeability and resistance loss coefficient values, set at 1×10^{-12} (m²) and 1×10^{12} (m⁻¹), respectively [73].

The input pressure was defined as 1MPa and the output pressure as atmospheric pressure. [73].

The test sample "Sample 1B" has a porosity of 0.211(21.1%) and a Klinkenberg permeability of 1.789×10^{-10} m², the test sample "Sample 1B" has an approximate pore volume of about $2,3 \times 10^{-5}$ m³. [74,75,76,77,78].

In summary, in this experiment we are evaluating the behaviour of CO₂ injection in brine-saturated sandstone.

5. Result Analysis

5.1. Results

Now, let's delve into the results obtained from the simulation. To start, we will examine Figure 26, which illustrates how the pressure is distributed during the injection of CO₂ into the sample.

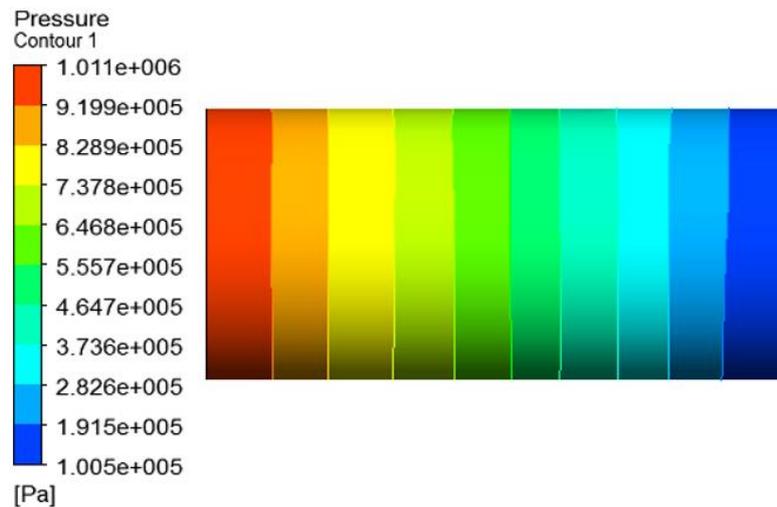


Figure 21 : Distribution of Pressure During CO₂ Injection in the Sample

Figure 21 illustrates how the pressure changes along the axial length of the central sample, from the entry point (on the left side) to the exit point (on the right side). As expected, this pressure gradually decreases as we move towards the outlet. What this means is that as the fluid, in this case carbon dioxide, flows through the sample, it experiences a steady reduction in pressure. This decrease in pressure is a consequence of the resistance the fluid encounters as it moves through the porous medium of the test tube. As more time elapses during the experiment, this pressure decrease begins to slow in its rate of change, indicating that the sample is moving from being initially saturated with brine to being saturated primarily with carbon dioxide, which alters the flow properties in the test tube and affects the observed pressure drop.

Transitioning from the pressure analysis, we now delve into the velocity of CO₂, which can be observed in Figure 22.

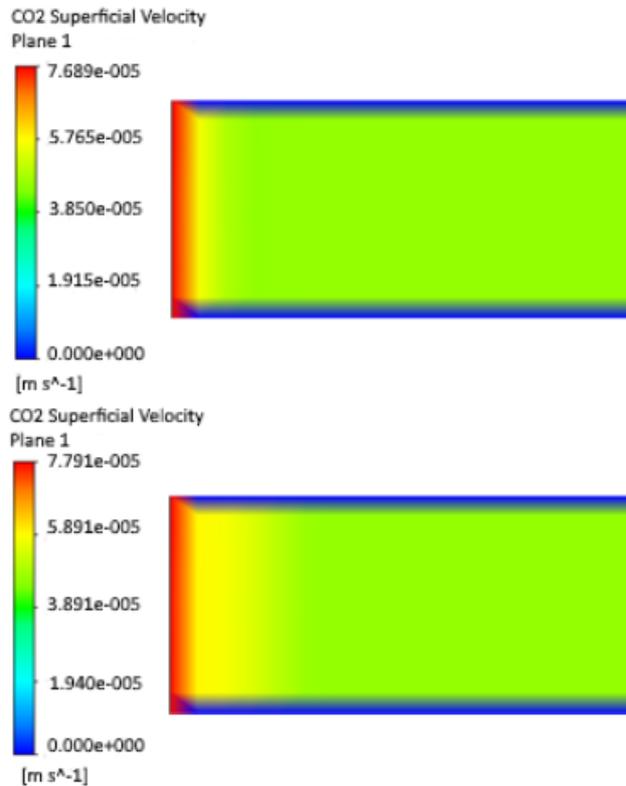


Figure 22 The evolution of CO₂ velocity over time, specifically at 50 seconds of injection (above) and 150 seconds of injection (below), is depicted in the following figures.

The velocity of carbon dioxide (CO₂) within the core sample changes as the injection progresses. In Figure 22, we can observe that the gas velocity gradually decreases from the centre of the sample towards the outer walls. This decrease is attributed to a "non-slip wall condition," signifying that the velocity of CO₂ in contact with the sample's walls is equal to zero due to the interaction between the fluid and the surface of the sample.

As time progresses, it becomes evident that the velocity of CO₂ increases as it invades a larger portion of the core sample, as depicted in the figure from 50 seconds to 150 seconds. This increase in velocity is a result of how the relative permeability properties of the two fluids interact during the process. In summary, as CO₂ advances and displaces brine within the sample, its velocity increases due to these fluid interactions and sample properties.

It's important to note that this representation is a simplification and may not fully reflect real-life conditions, as in actual situations, there may be some slippage at the sample's surface, which would affect the velocity of CO₂ at the boundaries.

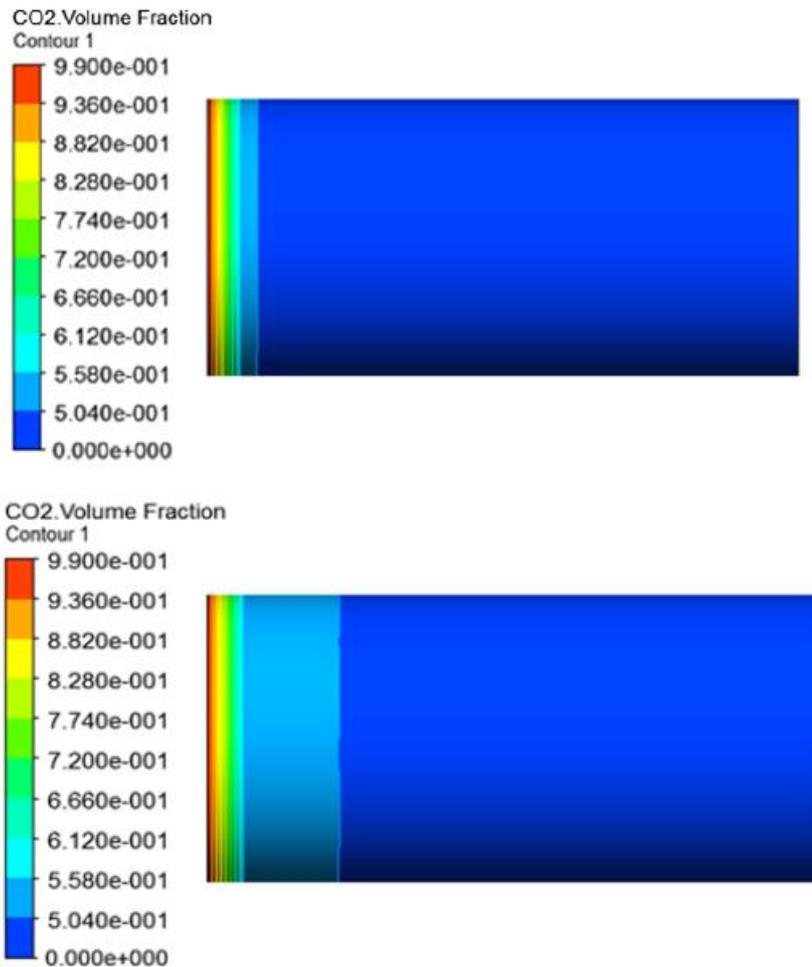


Figure 23 Distribution of Injected CO₂ Fractional Volume Along the Core Sample, Initiated Fifty Seconds After Injection and One Hundred Fifty Seconds Later.

In Figure 23, two separate images depict the volume fraction of carbon dioxide (CO₂) within the sample at different time intervals during the injection process. The top image represents the CO₂ volume fraction at 50 seconds after the start of injection, while the bottom image shows the same parameter at 150 seconds.

These images provide a visual representation of how the distribution of CO₂ within the sample changes over time. Initially, at 50 seconds, it can be observed that CO₂ has begun to penetrate the formation, but a significant presence of water still exists within the sample. This suggests that the displacement of water by CO₂ is underway but has not reached its maximum extent.

Moving to the bottom image, corresponding to 150 seconds of injection, it is evident that CO₂ has penetrated deeper into the formation, and the water phase has been displaced to a greater extent. This indicates that over time, CO₂ continues to enter the sample and progressively displaces the water phase, gradually occupying a larger portion of the total sample volume.

In summary, these images illustrate the gradual process of water displacement by CO₂ within the sample, showing how the volume fraction of CO₂ increases as the injection progresses and the aqueous phase is displaced.

6. CCS Projects

Lastly, I would like to share the projects that exist around the world for CO₂ storage. There are several ongoing CO₂ storage projects around the world. These projects aim to capture and store CO₂ emissions to mitigate climate change and reduce greenhouse gas emissions:

1. Sleipner Project (Norway): Operated by Equinor, the Sleipner project is one of the world's first and largest offshore CO₂ storage projects. It involves the capture and injection of CO₂ from the Sleipner natural gas field into a deep saline aquifer beneath the North Sea. [79]

2. Gorgon Project (Australia): The Gorgon project, operated by Chevron, is a large-scale CO₂ storage initiative that injects CO₂ from a natural gas facility on Barrow Island into a deep reservoir beneath the island. [80]

3. Quest Project (Canada): Operated by Shell, the Quest project in Alberta, Canada, is a carbon capture and storage (CCS) facility that captures CO₂ emissions from a bitumen upgrading plant and stores it in deep geological formations. [81]

4. Petra Nova Project (USA): Located in Texas, USA, the Petra Nova project is a joint venture between NRG Energy and JX Nippon Oil & Gas Exploration. It captures CO₂ emissions from a coal-fired power plant and uses enhanced oil recovery (EOR) to inject the CO₂ into oil reservoirs for storage. [82]

5. Boundary Dam CCS Project (Canada): Operated by SaskPower, the Boundary Dam project in Saskatchewan, Canada, is the world's first commercial-scale CCS facility at a coal-fired power plant. It captures CO₂ emissions and stores them in a deep saline aquifer. [83]

6. Gassnova Project (Norway): The Norwegian government's Gassnova agency is funding several CCS projects, including the Northern Lights project, which aims to develop a full-scale CO₂ transport and storage infrastructure in the North Sea. [84]

7. Decatur Project (USA): The Decatur project, located in Illinois, USA, is a CCS facility operated by ADM, which captures CO₂ emissions from an ethanol production plant and stores them in a saline reservoir. [85]

These are just a few examples of the many CO₂ storage projects currently underway globally. The development of these projects reflects the growing recognition of the importance of carbon capture and storage technologies in addressing climate change and transitioning to a low-carbon future.

7. Conclusions

This project has addressed several interconnected and fundamental objectives that have contributed to a deeper understanding of carbon dioxide (CO₂) mitigation and environmental preservation on a global scale. Initially, a comprehensive analysis of the global environmental situation was conducted, identifying current challenges related to climate change and environmental degradation. Additionally, technologies for Carbon Capture and Storage (CCS) and associated projects worldwide were explored.

Throughout this project, the significance of CO₂ as a crucial technique for mitigating climate change has been emphasized. Global goals have been established to reduce emissions and move towards emissions neutrality by 2050. Despite inherent challenges, significant efforts are underway in this direction.

In the realm of CO₂ storage, various approaches have been examined, including storage in depleted reservoirs or in oil and gas fields. Given that these currently constitute the primary sources of energy globally and are also the most polluting sectors, oil companies show notable interest in CO₂ storage projects to reduce their emissions. However, it has been demonstrated that storage in saline aquifers has significant potential and is considered an optimal form of storage.

Concerning Portugal, diverse studies indicate that its coastal area has high potential for storing CO₂ in these saline aquifers, with several projects currently underway to explore this possibility.

Regarding simulations, it is crucial to highlight that for a comprehensive understanding of the results, a detailed study of parameters such as permeability, relative porosity, and the states of CO₂ (behaviour based on pressure and temperature) is essential. These factors play a critical role in interpreting the results and assessing the feasibility of CO₂ injection into the porous medium. Additionally, the importance of conducting laboratory tests to validate the results obtained through simulations is emphasized. Unfortunately, in this project, a laboratory test could not be conducted due to material and time constraints.

In conclusion, CO₂ storage techniques present a promising option in the fight against climate change. Simulation tools like ANSYS Fluent facilitate modelling situations close to reality, resulting in significant cost savings, a crucial factor in any project.

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9. Annex

