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Comprehensive analysis of an ongoing CO2 storage project

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COMPREHENSIVE ANALYSIS OF AN ONGOING CO₂ STORAGE PROJECT
By

Daniel Moreno

Thesis submitted to the
Benjamin M. Statler College of Engineering and Mineral Resources
At West Virginia University
In partial fulfillment of the requirements
for the degree of

Master of Science
in
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Approved by

Shahab D. Mohaghegh, PhD., Chair

Samuel Ameri, M.S.

Brian Anderson, PhD.

Grant Bromhal, PhD.

Department of Petroleum and Natural Gas Engineering

Morgantown, West Virginia

2013

Keywords: CO₂ sequestration, CCS, Trapping Mechanisms.

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Abstract

Comprehensive Analysis of an Ongoing CO₂ Storage Project;

Impact of Boundary Condition, Cap Rock Characteristic & Trapping Mechanisms as well as Post-Injection Site Care

Daniel Moreno, West Virginia University

Increase in CO₂ emission has become an important issue over the years due to its environmental impacts as a greenhouse gas. The fact that these emissions are primarily derived from energy consumption and that 85% of the primary power is supplied by fossil fuels (Orr, 2004), makes the reduction of CO₂ emissions a major challenge. CO₂ sequestration in the geological formations has been identified as an alternative to counter the impact of the emissions. CO₂ sequestration refers to the capture and long term storage of CO₂.

In order to properly assess the viability of CO₂ sequestration in a geological formation as a “safe” and long term solution, several questions have to be answered: Is this formation capable of trapping the amount of CO₂ to be injected? Does the seal of this formation (the cap rock) have the proper characteristics to ensure a low risk structural trapping? Which trapping mechanisms are present and what kind of interactions (geochemical, geomechanical, etc.) are we to expect as we inject the CO₂? These questions are addressed and evaluated in this research.

The proposed research addresses these questions in the context of an ongoing CO₂ storage project in a deep saline aquifer located in the Citronelle field in Mobile, Alabama. A full field reservoir model was built using information from the actual field site and reservoir scale simulations are performed. Initially we evaluated different trapping mechanisms (residual or capillary trapping, solubility, mineral and structural trapping) and their contribution to the storage process. Quality and integrity of the cap rock, representing the ability to trap “mobile” CO₂ structurally, is studied to assess the potential risk of leakage. Additionally, impact of the nature of the edge boundary conditions on the pressure and saturation distribution throughout the reservoir is studied.

Finally, in order to ensure the long term storage of the CO₂, a Post-Injection Site Care (PISC) study is performed. Pressure stabilization time is assessed within acceptable thresholds, allowing for possible post-stabilization leakage of brine or CO₂ detection.

Dedication

This thesis is dedicated to my family, who has supported me being near and far in every step of the way that I have chosen. To my parents Diego Moreno and Valentina de Moreno for your guidance, trust and wholehearted help, I cannot find words to express my gratitude. Furthermore, to my siblings Diego, David, Neida and Gustavo for always being my pillars and source of inspiration.

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Chapter 1– Introduction

Balancing the global energy demand with a decrease in anthropogenic CO₂ emissions to mitigate climate change has emerged as one of the most pressing challenges of this century. Carbon capture and storage (CCS) is currently the most attractive option to reduce billions of tons of CO₂. Thus far, the deployment of CCS has been delayed by uncertainty about geologic storage capacities, sustainable injection rates and the time span over which storage could be extended.

Different domains that represent viable candidates for large-scale CO₂ storage have been identified over the past decades, such as depleted oil and gas reservoirs, unmineable coal seams, ocean storage and deep saline formations (Figure 1).

Figure 1 Possible domains for CO₂ storage

Within the different domain options, deep saline aquifers offer the largest storage potential and are widely distributed throughout the globe in all sedimentary basins. Deep saline aquifers are sedimentary rocks saturated with formation brines containing high concentrations of dissolved salts, which are unsuitable for human consumption. To ensure that particular deep saline

aquifer is a viable option for large-scale CO₂ storage, it has to be properly studied and characterized, as well as satisfying conditions such as proper sealing capabilities and storage capacities.

In order to properly assess the viability of CO₂ sequestration in a geological formation as a “safe” and long term solution, several questions have to be answered: Is this formation capable of trapping the amount of CO₂ to be injected? Does the seal of this formation (the cap rock) have the proper characteristics to ensure a low risk structural trapping? Which trapping mechanisms are present and what kind of interactions (geochemical, geomechanical, etc.) are we to expect as we inject the CO₂? These questions are addressed and evaluated in this research.

The objective of this research is to perform an integral comprehensive analysis that encloses the aforementioned interrogatives by studying the Impact of the nature of the Boundary Condition, Cap Rock Characteristics & Trapping Mechanisms as well as Post-Injection Site Care on an ongoing CO₂ storage project in a deep saline aquifer located in the Citronelle field in Mobile, Alabama.

The comprehensive analysis was performed on an ongoing CO₂ storage project conducted by the U.S. Department of Energy (DOE) Southeast Regional Carbon Sequestration Partnership (SECARB), the Electric Power Research Institute (EPRI) and the Southern Company to demonstrate commercial-scale storage of CO₂ captured from an existing coal-fired power plant. Injection is taking place in a deep saline aquifer formation (Paluxy formation) in the Citronelle field in Mobile, Alabama at depths between 9,400 ft and 10,500 ft. Injection of CO₂ started in August, 2012 with a target of 182,500 tons of CO₂ per year for the duration of 3 years.

Chapter 2– Literature Review

2. Literature Review

2.1 History CO₂ Storage

While CO₂ has been widely used for enhanced oil recovery (EOR) for decades, industry scale CO₂ capture and storage (CCS) was first achieved in 1996 by Statoil and its partners in the North Sea, Sleipner gas field, 150 miles west of Stavanger, Norway. The produced natural gas in the Sleipner field contains approximately 9% of CO₂ and market specifications demanded that this concentration was to be reduced to 2.5%. Additionally, the Carbon Tax that Statoil is required to pay per metric ton of CO₂ released to the atmosphere is approximately US \$50. Consequently, since Statoil was required to separate CO₂ and incurred in large expenses when CO₂ was released to the atmosphere, carbon capture and storage (CCS) became economically viable. Statoil separates the CO₂ from gas produced from the Heimdal formation using and Mono-ethanol amine (MEA) solvent and injection occurs in the Utsira formation at a depth of approximately 3300 ft using a single highly deviated injection well as it can be observed in Figure 2. Since 1996, the Sleipner CCS project has injected over 10 million metric tons of CO₂¹ and they plan to continue until 2020, representing the first industry-scale CCS and the footing for future successful CCS projects.

¹ Statoil Annual Report 2008 – Sleipner CCS –
http://www.statoil.com/AnnualReport2008/en/Sustainability/Climate/Pages/5-3-2-3_SleipnerCCS.aspx

Figure 2 Diagram of operations in the Sleipner field, North Sea, Norway

Source: Schlumberger – CO₂ Capture and Storage –A Solution Within

Later in 1999, the first transnational EOR project that involved CO₂ capture, transport and storage was started by a partnership of the PanCanadian Resources, now EnCana Corporation, Saskatchewan Industry and Resources, the Petroleum Technology Research Center (PTRC) and the International Energy Agency (IEA). This project involves the transport of CO₂ through a pipeline of more of 200 miles from a coal gasification facility located northwest of Beulah, North Dakota, USA to the Weyburn oilfield near Regina, Saskatchewan, Canada as shown in Figure 3.

Figure 3 Pipeline diagram that transports CO₂ from the Great Plains Synfuels Plant in Beulah, ND to the Weyburn Oilfield in Regina, Saskatchewan, Canada

Before the pipeline was built, the Great Plains Synfuels Plant released most of the CO₂ that it produced to the atmosphere. Presently, the produced CO₂ is compressed at the plant to a pressure of approximately 2200 psi and delivered to the Weyburn field through the pipeline under supercritical conditions. After the CO₂ reaches the Weyburn field it is injected to the subsurface into the Mississippian Midale Beds at an average depth of 4655 ft. Prior to the start of CO₂ injection, the International Energy Agency (IEA) performed a comprehensive geological study of the Weyburn CO₂ in storage site, concluding that the geology of the Weyburn field was suitable for long term CCS. The primary reservoir seals were determined to have the proper characteristics to form extensive and thick barriers to upwards buoyancy driven fluid migration and faults and fractures present did not show any fluid conductance.

Approximately 5,000 metric tons of CO₂ are transported and injected daily into the Weyburn oil field to supply the CO₂ storage and EOR operations. During the project's lifetime it is estimated that over 22 million metric tons of anthropogenic CO₂ will be securely stored in the Weyburn Field. Furthermore, from the oil production point of view the daily production was estimated to be 30,000 barrels per day as of 10,000 barrels per day that would be producing if CO₂ injection had not occurred.

Plenty of Industrial scale projects are underway or in planning stage in this past decade, as stated by the Global CCS Institute² (The Global Status of CCS, 2012), who has identified at 75 large scale integrated CCS projects that are either currently operating or in construction as of September 2012 (Figure 4 and Figure 5). The combined capture capacity of these projects represent approximately 36 million metric tons per year (Mtpa) of CO₂. Additionally, 59 large scale integrated CCS projects have been identified to be in planning stages of development, with an additional capture capacity of more than 110 Mtpa. The Global CCS institute defines Large scale integrated CCS projects as those that involve capture, transport and CO₂ storage at a scale of at least 800,000 tonnes of CO₂ annually for coal-based power plants or at least 400,000 tonnes of CO₂ annually for other industrial based operations which emissions are considerable including natural gas based power generation.

² Global CCS Institute – The Global Status of CCS – 2012
<http://cdn.globalccsinstitute.com/sites/default/files/publications/47936/global-status-ccs-2012.pdf>

Figure 4 Large Scale Integrated CCS projects in their different stages per country - September 2012

Figure 5 Identified Large Scale Integrated CCS projects location.

2.2 Possible domains for CO₂ storage

2.2.1 Depleted Oil and Gas Reservoirs

The integrity and safety demonstrated by the fact that oil and gas has been trapped for millions of years in these formations, by either structural or stratigraphic traps, makes depleted oil and gas reservoirs optimum candidates for CO₂ storage. Usually, these formations extensively studied and characterized, and in most of the cases, fluid models have been developed to forecast fluid displacement behavior. Probably, one of the most appealing aspects when considering depleted oil and gas reservoirs as domains for CO₂ storage is that the underground and surface infrastructure (wells, equipment and pipelines) is already available and could be used for CO₂ storage injection, with minor or even without modifications. Additionally, the injection of different gases, including CO₂, into oil and gas reservoirs as a technique to enhance oil or gas recovery has been widely practiced in the oil and gas industry. The experience gained can be adapted to guide the CO₂ sequestration injection. The sequestration of CO₂ in nearly depleted or even developing oil and gas reservoirs can simultaneously reduce greenhouse gas emissions and increase oil recovery.

Although depleted oil and gas reservoirs represent an attractive candidate for CO₂ storage it still has limitations, being the most important, restricted storage capacity not only because of geological characteristics of any particular formation but also due to changes in the system such as interfacial tension difference oil-brine systems and CO₂ brine systems. Li, Z. et al. (2006) determined that the sealing pressure of caprocks for CO₂ is significantly reduced compared with that for the original hydrocarbons due to the much lower interfacial tension (IFT) of the CO₂ /water system. As a result, the sealing capacity of caprocks that retained the oil and gas in the first place may not be sufficient to prevent the injected CO₂ from migrating through the caprocks by volume flow at the same range of pressures than when hydrocarbons were present. Therefore, it is crucial to re-evaluate the sealing capacity of the caprock once an oil or gas reservoir is selected as a CO₂ storage site. Furthermore, the calculation of the storage capacity for a given reservoir shows that once the reservoir pressure reaches a certain high level, a continuous increase in pressure alone is not effective in enhancing the storage capacity. However, much more capacity can be achieved by removing a portion of the remaining water in the reservoir.

2.2.2 Ocean Storage

There has been limited experience with handling CO₂ in the deep sea that could form a basis for the development of ocean CO₂ storage technologies. Before they could be deployed, such technologies would require further development and field testing. Associated with the limited level of development, estimates of the costs of ocean CO₂ storage technologies are at a primitive state, however, the costs of the actual dispersal technologies are expected to be low in comparison to the costs of CO₂ capture and transport to the deep sea. Proximity to the deep sea is a factor, as the deep oceans are remote to many sources of CO₂. Ocean storage would require CO₂ transport by ship or deep-sea pipelines. Pipelines and drilling platforms, especially in oil and gas applications, are reaching ever-greater depths, yet not on the scale or to the depth relevant for ocean CO₂ storage. No insurmountable technical barrier to storage of CO₂ in the oceans is apparent. Putting CO₂ directly into the deep ocean means that the chemical environment of the deep ocean would be altered immediately and given that only rudimentary understanding of deep-sea ecosystems exists, only a limited and preliminary assessment of potential ecosystem effects can be given. Nonetheless, the potential of the ocean as a possible domain for CO₂ storage cannot be ignored due to fact that it would represent the largest storage capacity up to 1,000 Gt-Carbon (Gt-carbon = 1 billion tons of carbon) (Rhudy et al. 2003)³.

Still, the major concern regarding oceans as possible CO₂ storage candidate relies on the retention time after CO₂ is released; the retention time for CO₂ released in the oceans is generally expected to be on the order of hundreds of years, being less than that represented by other options such as storage in geological formations. Additionally, Brewer et al. (2001)⁴ determined that the released liquid CO₂ at depths deeper than approximately 9000 ft is denser than sea water, and with the use of video imaging systems they observed that when CO₂ is released below this depth it descends, as opposed when CO₂ is released at shallower depths it

³ Rhudy, R. G., Bock, B. R. "CO₂ Storage and sink Enhancements: Developing Comparable Economics" DOE technical paper, February 2003.

⁴ Brewer, P. G., Peltzer, E. T., "Direct Experiments on the Ocean Disposal of Fossil Fuel CO₂" SPE 71454. October, 2001

would rise back up to the water surface in form of liquid CO₂ bubbles. However, they were not able to determine the retention time for the released CO₂ below 9000 ft in their experiments.

2.2.3 Unmineable Coal beds

Usually, these kinds of formations are located either at extremely deep locations or in a form of a very thin layer, making their recovery not economically feasible. However, these formations have large internal surface areas and typically contain considerable amounts of adsorbed methane gas. An enhanced coal bed methane recovery method that has been widely study is by injection of CO₂ into the coal seam, taking advantage over the fact that coal has a higher affinity to adsorb gaseous CO₂ than methane (Orr et al. 2004)⁵(Figure 6), as CO₂ is injected into the formation, it flows through the fracture networks in the coal matrix and displace the adsorbed methane as it adsorbs the CO₂ into the coals pore surface, remaining sequestered in the coal seam (Odusote et al 2004)⁶, ultimately providing a storage sink for the injected CO₂.

Figure 6 Relative adsorption of CO₂, CH₄ and N₂ of a coal sample.

⁵ Orr Jr, F.M. "Storage of Carbon dioxide in Geological Formation." Distinguished Author Series. SPE 88842. September 2004.

⁶ Odusote, O., Ertekin, T. Smith, D., Bromhal G., Sams, N.W., Jikich, S., "Carbon Dioxide Sequestration in Coal Seams: A parametric Study and Development of a Practical Prediction/Screening Tool Using Neuro-Simulation" SPE 90055, September 2004.

2.2.4 Deep Saline Formations

Deep saline aquifers offer the largest storage potential of all the geological CO₂ storage options and are widely distributed throughout the globe in all sedimentary basins. Deep saline aquifers are sedimentary rocks saturated with formation brines containing high concentrations of dissolved salts, which are unsuitable for human consumption.

Even though storage of CO₂ in deep saline formations does not produce value-added by-products, such as additional production from CO₂ EOR (Enhanced Oil Recovery), it has other advantages. Most existing large CO₂ point sources are within easy access to a saline formation injection point, and therefore storage in saline formations is compatible with a strategy of transforming large portions of energy and industrial assets to near-zero carbon emissions via low-cost carbon storage retrofits. In the other hand, it is likely that available information regarding the characterization of these aquifers, is less or even non-existing compared to that available in oil and gas reservoirs (Orr et al., 2004)⁷. This is true for existing infrastructure that could be used for CO₂ injection as well.

2.3 Trapping Mechanisms CO₂ storage

CO₂ trapping mechanisms in geologic storage are the specific processes that hold CO₂ underground in porous formations after it is injected. There are four main trapping mechanisms that are widely recognized: the fundamental confinement of mobile CO₂ phase under low-permeability caprocks, or structural trapping, the dissolution of CO₂ in in situ fluid, or solubility trapping, conversion of CO₂ to mineral precipitates, or mineral trapping, and trapping by surface tension (capillary force) and, correspondingly, remaining in porous media as an immobile CO₂ phase, or residual CO₂ trapping. These trapping mechanisms are described in detail in the following sub-sections.

⁷ Orr Jr, F.M. "Storage of Carbon dioxide in Geological Formation." Distinguished Author Series. SPE 88842. September 2004.

2.3.1 Structural Trapping

This is the most dominant of the trapping mechanisms. Once injected, the supercritical CO₂ can be more buoyant than other liquids that might be present in the pore space. The CO₂ will therefore migrate upwards through the porous medium until it reaches the top of the formation where it meets (and is trapped by) an impermeable layer of cap-rock (confining unit). Once the injected CO₂ reaches this barrier, it will stay sequestered in a “mobile” phase, that in case of failure of the confining unit to contain it, the CO₂ could migrate to other formations and eventually the atmosphere. Even though, when selecting a site as a candidate for CO₂ storage one of the factors thoroughly studied is the characteristics of the confining unit, to ensure that it will act as a proper seal or barrier for CO₂ migration, this trapping mechanism still represents a higher risk scenario in terms of leakage when compared to others.

2.3.2 Residual Trapping

This phase of trapping happens very quickly as the porous rock acts like a tight, rigid sponge. As the supercritical CO₂ is injected into the formation it displaces the present fluids as it moves through the porous rock. As the CO₂ continues to move, formation fluid again replaces it, but some of the CO₂ will be left behind as disconnected droplets in the pore spaces which are immobile (Figure 7). Often, this is how the oil was held for millions of years.

Figure 7 Residually trapped CO₂ illustration - Source: The Cooperative Research Centre for Greenhouse Gas Technologies (CO2CRC) - http://www.co2crc.com.au/publications/all_factsheets

The relative permeability hysteresis plays a very important role when determining the contribution that this trapping mechanism could have within the CO₂ storage process, where

accounting for this irreversibility phenomena leads to a spread out distribution of trapped and immobile CO_2 , as opposed to a concentrated distribution of mobile CO_2 (Juanes et al. 2005)⁸.

2.3.3 Solubility Trapping

This trapping mechanism refers to amount of CO_2 that dissolves within the formation fluid. The solubility of CO_2 in water increases with increasing pressure and decreases with increasing temperature and increasing water salinity as observed by Bennion et al. (2006)⁹. As some CO_2 dissolves in water, the water becomes denser, and begins to sink downwards (Figure 8). This allows the CO_2 to become more dispersed in the water, and over time, the amount of CO_2 dissolved in the water can increase. If the reservoir formation is thin, the extent to which mixing occurs through a convective flow is limited.

Figure 8 Illustration of CO_2 dissolution in brine.

⁸ Juanes, R., E.J. Spiteri, F.M. Orr and M.J. Blunt, "Impact of relative permeability hysteresis on geological CO_2 storage, Water resources: W12418 Res 42 doi: 10.1029/2005WR004806

⁹ Bennion B., Bachu S., "Dependence on Temperature, Pressure and Salinity of the IFT and Relative Permeability displacement Characteristics of CO_2 Injected in Deep Saline Aquifers" SPE 102138. September 2006

2.3.4 Mineral Trapping

Mineral trapping is the permanent sequestration of CO₂ through chemical reactions with dissolved minerals in the reservoir brine and with the minerals in the reservoir rock itself. However, the mineral trapping mechanism is slow and is expected to occur over very long time periods. Through field studies and numerical modeling, it has been determined that CO₂ is primarily trapped through precipitation of calcite (CaCO₃), siderite (FeCO₃), dolomite (CaMg(CO₃)) and dawsonite (NaAlCO₃(OH)₂). In order for mineral trapping through carbonate precipitation to occur, primary minerals rich in Mg, Fe, Na and Ca, such as feldspars and clays, must be present. Therefore, immature sandstones having an abundance of fresh rock fragments (unweathered igneous and metamorphic minerals and clays rich in Mg, Fe and Ca) are most effective (Bachu et al., 1994; Pruess et al., 2001; Xu et al., 2002). The abundance and ratios of these primary minerals can have a tremendous effect on the type of secondary minerals that are precipitated as well as on the overall total amount of CO₂ sequestered through mineral trapping.

This trapping processes take place over many years at different rates from days to years to thousands of years, but in general, geologically stored CO₂ becomes more securely trapped with time (Figure 9). Demonstrations of various geological storage of CO₂ are already being carried out in a range of projects of varying scale.

Figure 9 Increasing security vs. time and contribution degree of different trapping mechanisms

Source: <http://www.co2crc.com.au/aboutccs/safety.html>

2.4 Previous Analysis on CO₂ Storage in Deep Saline Aquifers

Saline aquifers are considered to be one of the most viable candidates for CO₂ storage due to their large storage capacity, considerable amount of studies have been performed describing CO₂-Brine systems and the trapping mechanisms present during the CO₂ storage process. Bennion (et al. 2006) studied the dependence on temperature, pressure and salinity of the interfacial tension between CO₂ and brine saline aquifers observing that Interfacial tension is found to have a strong dependency on pressure, being significantly reduced by increases in the pressure. However increasing temperature or brine salinity has an opposite effect. Additionally he found that the variation of interfacial tension with pressure is roughly proportional to the variation of the viscosity ratio of the brine/CO₂ displacement over the same pressure range. Ide (et al. 2006) studied the effects of gravitational forces on CO₂ storage in saline aquifers analyzing his findings by the relative importance of viscous and gravity forces with a term he defined as gravity to viscous ratio (N_{gv}). This ratio is defined as :

$$N_{gv} = \frac{k_v L \Delta \rho g}{H u \mu}$$

Where:

k_v : vertical permeability.

L : Aquifer length.

$\Delta \rho$: density difference between phases.

H : Aquifer height

u : average flow velocity

μ : viscosity of the bryne

In this study it was determined that as N_{gv} increased, the fluid displacement was dominated by gravity forces. Nevertheless, as this ratio decreases viscous forces become more important and the fluid displacement is sensitively affected by the permeability distribution. Finally, it was observed that when gravitational force is weaker than viscous force for displacement, significantly more CO₂ is trapped residually (by capillary pressure) than when the gravitational force is dominant.

Kumar (et al. 2004) studied the effects of capillary trapping on CO₂ storage finding that as the mean permeability increases so will the migration and injectivity of CO₂, as well that as salinity of the aquifer increases the dissolution of CO₂ into brine will decrease. Additional findings suggest that low residual gas saturation values lead to increased gas migration and dissolution into brine, on the other hand high values of residual saturations lead to increased amount of CO₂ residually trapped. Later in 2005 R. Juanes (et al. 2005) studied the impacts of relative permeability hysteresis on geological CO₂ storage finding that accounting for hysteresis effects leads to a spread out distribution of trapped CO₂, as opposed to a concentrated distribution of mobile CO₂.

Chapter 3 – Methodology

3. Citronelle Field Modeling

3.1 Field Background

The unitized portion of the Citronelle oilfield occupies approximately 16,380 acres of surface area, and is located in Mobile County approximately 30 miles north of the city of Mobile. The oilfield surrounds the city of Citronelle and covers portions of Township 2 North, Ranges 2 West and 3 West; and Township 1 North, Ranges 2 West and 3 West (Figure 10). The proposed CO₂ injection site is located in the Southeast Unit (Figure 11). The Southeast Unit extends for 1,520 acres in portions of Sections 4, 5, 8, 9 and 10 in Township 1 North, Range 2 West and portions of Sections 32 and 33 in Township 2 North, Range 2 West.

Figure 10 Location of the Citronelle Field

Figure 11 Southeast Unit, Citronelle field. (Injection Site)

This project is a part of a CO₂ storage research project conducted by the U.S. Department of Energy (DOE) Southeast Regional Carbon Sequestration Partnership (SECARB), the Electric Power Research Institute (EPRI) and the Southern Company to demonstrate commercial-scale storage of CO₂ captured from an existing coal-fired power plant.

The injection target zone is the Paluxy formation. This formation is deep saline aquifer reservoir with numerous reservoir seals and confining units, making it a perfect candidate to storage CO₂ for a long-term, located at the depth of about 9,400 to 10,500ft (Figure 12). The Paluxy formation represents a coarsening-upward succession of variegated shale and sandstone. Little is known about the depositional environment of the Paluxy Formation of southwestern Alabama because few cores have been taken or preserved. The occurrence of redbeds in this interval appears indicative of periodic oxidation and exposure. The coarsening-upward nature of the

formation has been interpreted as the product of progradational infilling of the sedimentary basin (Mancini and Puckett, 2002).

Based on the logs from the injection well, twenty seven individual sandstones in the Paluxy formation were identified as potential storage reservoirs for CO₂. Seventeen sand layers which are the thickest and most extensive ones were selected for the injection. The Citronelle Dome, a broad, gently dipping anticline, provides the Citronelle Field with structural closure at all stratigraphic horizons of Jurassic through Tertiary age including the Paluxy formation. Moreover, there is an apparent lack of faulting at the Citronelle dome structure.

Formation Tops	Depth (ft bgs)	Interval Thickness (ft)
Bottom of Fresh Water (<1,000 mg/l)	~1,000	
Base of USDW (<10,000 mg/l)	~1,200	
Selma Chalk Group (seal)	4,560	1,310
Eutaw	5,870	150
Tuscaloosa Group		
Upper Tuscaloosa	6,020	720
Middle Tuscaloosa (seal)	6,740	210
Lower Tuscaloosa	6,950	410
Washita-Fredericksburg (seal)	7,360	2,040
Paluxy Formation (target)	9,400	1,110
Mooringsport Formation	10,510	240
Ferry Lake Anhydrite	10,750	190
Rodessa Formation (oil reservoir)	10,940	-

Cretaceous	Upper	Selma Group		Confining Unit
		Eutaw Formation		Minor Saline Reservoir
		Tuscaloosa Group	Upper	Minor Saline Reservoir
			Middle	Confining Unit
			Lower	Saline Reservoir
	Lower	Washita-Fredericksburg Interval	Dantzler sand	Saline Reservoir
			Basal Shale	Primary Confining Unit
		Paluxy Formation	'Upper' 'Middle' 'Lower'	Proposed Injection Zone
		Mooringsport Formation		Confining Unit
		Ferry Lake Anhydrite		Confining Unit

Figure 12 Stratigraphic Column of the Citronelle field

The main confining unit is the basal shale of the Washita-Fredericksburg interval and has an average thickness of 180 ft in the vicinity of the injection site. The aquifers on top and bottom of this confining unit (including Paluxy) represent exhibit extremely low groundwater velocities, which is favorable in terms on long term CO₂ sequestration.

3.2 Geological Model

The main structure of the Paluxy formation is based the interpretation of 16 well logs in three cross sections. From the well logs of the injection well (D-9-7), 27 sand layers were identified as potential storage candidates for CO₂ storage. The prospective sandstones where injection of CO₂

would take place were selected based on Spontaneous Potential response allowing us to identify the sand and shale layers, low resistivity readings that indicate saline formation fluids and significant separation between deep and shallow induction that would indicate permeability.

The injection well (D-9-7) was considered as a reference well in three cross sections (Figure 13), used to construct stratigraphic cross-sections and correlate the prospective sandstones in neighboring wells using available Spontaneous Potential and resistivity logs. At least two distinctive sedimentary environments are suggested by the depositional patterns in the Paluxy, an early fluvial-deltaic to marginal marine shoreline deposit followed by later fluvial-continental incised valley fills. These led to the accumulation of thicker, multi-story aggradational channel fill sandstone units in the upper Paluxy Formation¹⁰.

Figure 13 Location of cross sections (left) and sand layers in well D-9-7(right)

In the upper Paluxy, the ‘fining-upward’ character of individual sandstones coupled with ‘blocky’, irregular bottom sand surfaces is characteristic of fluvial sand deposits that result from infilling of erosional topography by aggradation (Pashin et al., 2008). Therefore, the top of the individual sand bodies should be relatively flat and correlate between wells assuming a flat stratigraphic horizon. This approach was used in all the stratigraphic cross-sections to correlate the individual sandstones identified in the D-9-7 well to their full extent in neighboring wells

¹⁰ SECARB Phase III Anthropogenic Test, Volume 1 of 2 – Class V Experimental Injection Well Permit Application for Proposed Injection Well No. 1 and Observation Well No. 1 – Prepared for: Alabama Department of Environmental Management, Prepared by: Denbury Resources, Incorporated Plano, Texas

(Figure 14). The sand correlations identified in these cross-sections were then mapped aerially to evaluate the lateral continuity of individual sandstones.

Areal dimensions of some of the thicker sandstones are on the order of 6 square miles or 3,840 acres. The total thickness of sand layers is approximately 470 ft ranging from 10 to 80 ft. Structural and Iso-pach maps of the sand layers would be used to make reservoir simulation model. Finally, 17 of the layers were selected for injection based on their thickness and extension. These layers represent approximately 82% of the net sand thickness (385 ft) (Figure 15).

Figure 14 Correlated sand layers of cross section B-B'

Figure 15 Paluxy formation Individual sandstone layers

A Cartesian Grid system was created to discretize the structure of the Paluxy formation. A base case model was created with 125 gridblocks in “i” direction and 125 gridblocks in “j” with dimensions of 133.33 ft in both directions. Vertically, each one of the 17 geological layers was divided equally into 3 simulation layers, with a total number of 51 simulation layers as it can be observed in Figure 16.

Figure 16 Structure of the Paluxy formation - Grid system

Well logs from 40 offset wells that are within the area of study has been acquired and interpreted. Porosity values at these offset wells will be used as control points in the static model.

To have a more reliable model to simulate the actual injection dynamics, we needed to build a heterogeneous model, which would capture, as much as possible, the complexities of the actual reservoir's geology. To develop the heterogeneity in the lateral direction, more well logs from the Citronelle field were acquired. Some well logs in the immediate vicinity of the injection well D-9-7 within the 1-mile from the injection well, were already available. This allows the full representation of the actual injection area.

The resistivity logs are used in the injection depth which is from about 9400ft to about 10500ft. The logs were digitized utilizing the NEURALOG viewer. The Archie equation used by Advanced Resources International, Inc. (ARI) has been used to calculate the porosity values using the resistivity logs.

$$\phi = \left(\frac{a}{\left(\frac{R_t}{R_w} \right) * S_w^n} \right)^{1/m} \quad 11$$

Where

a = tortuosity factor = 1; default value

m = cementation factor = 2.25; best match to Citronelle oilfield porosity logs

n = saturation exponent = 2; common default value

R_w = resistivity of the formation water = 0.045; best match to Citronelle oilfield porosity logs

S_w = Water saturation = 0.95; assuming only residual gas saturation

φ = porosity

R_t = True formation resistivity = obtained from logs.

The weighted average for porosity values were calculated by taking the thickness of each layer into account.

¹¹ SECARB Phase III Anthropogenic Test, Volume 1 of 2 – Class V Experimental Injection Well Permit Application for Proposed Injection Well No. 1 and Observation Well No. 1 – Prepared for: Alabama Department of Environmental Management, Prepared by: Denbury Resources, Incorporated Plano, Texas

The static model was populated with geo-statistical methods using these new 40 control points.
17 porosity maps were generated (one per geological layer) .

Figure 17 Porosity distribution

An example of calculated porosity from one of the well logs can be observed in Figure 18.

D-9-8			
top	bottom	$\phi(\text{resistivity})$	$\phi(\text{Induction})$
9648.2	9658.1	0.1160	0.1596
9658.1	9667.9	0.1769	0.2139
9752.7	9759.1	0.0892	0.1711
9759.1	9765.6	0.0809	0.1774
9765.6	9772.0	0.0755	0.1669
9822.8	9829.9	0.1214	0.1313
9829.9	9836.9	0.1280	0.1272
9836.9	9844.0	0.1263	0.1237
9925.8	9929.3	0.1300	0.1259
9929.3	9932.9	0.1282	0.1313
9932.9	9936.4	0.1332	0.1578
9967.7	9969.7	0.1136	0.1745
9969.7	9971.6	0.1015	0.1785
9971.6	9973.6	0.0982	0.1765
9971.4	9972.9	0.0977	0.1781
9972.9	9974.4	0.0987	0.1746
9974.4	9975.9	0.0985	0.1734
10159.2	10162.3	0.0966	0.1464
10162.3	10165.3	0.0869	0.1242
10165.3	10168.4	0.0805	0.1178
10231.6	10241.3	0.1319	0.1425
10241.3	10251.1	0.1057	0.1590
10251.1	10260.8	0.1177	0.1291
10324.3	10341.2	0.1279	0.1374
10341.2	10358.2	0.1153	0.1755
10358.2	10375.1	0.1044	0.1438

Figure 18 Porosity Calculation from Induction logs and Resistivity logs wel D-9-8

Regarding the permeability of the formation, an initial interpretation was reported by ARI with the use of available core data from neighboring wells. Figure 19, shows the proposed porosity-permeability correlation provided in the ARI report¹². Based on the shown plot, a large amount of outliers can be seen; moreover many of the data points are not following the same trend. In order to rectify this, four different clusters were determined and ranked as the best to the worst rock types. The new correlations between the porosity and permeability for the four different rock types were defined. (Figure 19)

Figure 19 The porosity-permeability correlation proposed by ARI and the four initial clusters.

Additional information was provided to enhance this interpretation, represented by core data coming from the proposed observation well (D-9-8) located east of the injection well. This information was included in the initial interpretation and a new permeability – porosity cross plot was generated (Figure 20); from where 5 distinctive realizations can in terms of permeability can be inferred.

¹² SECARB Phase III Anthropogenic Test, Volume 1 of 2 – Class V Experimental Injection Well Permit Application for Proposed Injection Well No. 1 and Observation Well No. 1 – Prepared for: Alabama Department of Environmental Management, Prepared by: Denbury Resources, Incorporated Plano, Texas

Figure 20 Cross plot of Permeability-Porosity including core data form well D-9-8

These different realizations could determine how “tight” or “conductive” the reservoir would be. They were defined based on their trend and permeability range as very conductive, conductive, average, tight and very tight (Figure 21). For the purpose of this study the conductive realization was used in the model.

Figure 21 Permeability Realizations based on Permeability vs Porosity cross plot

Other parameters such as reservoir temperature were employed in the model. The reservoir temperature of the Paluxy Formation is estimated to be 230° Fahrenheit based on the regional thermal gradient as determined from bottom-hole temperature measurements.

Few data regarding the geochemical composition of the Paluxy Formation and other deep saline reservoirs in southwestern Alabama are available. The average value of approximately 180,000 mg/l was used in the model (based on a water sample taken during the Mississippi Test Site CO₂ injection test at Plant Daniel, Escatawpa, Jackson County, Mississippi, in 2008).

Regarding rock fluid description, no relative permeability data was available for the creation of the model. The relative permeability profile used in the base case model (Figure 22) corresponds to the history math of the injection pilot test at the test site in Escatawpa, Jackson County, Mississippi.

Figure 22 Base Case Relative Permeability profile

3.3 Simulation Model

The simulation of CO₂ injection and storage was performed using a commercial numerical simulator; the compositional simulator GEM (Generalized Equation of State Model) developed

by CMG (Computer Modeling Group). GEM is capable of simulating multiphase flow, multi-component fluids and modeling reservoir management processes such as CO₂ injection.

The composition of the injected fluid will be primarily CO₂, having a nominal concentration greater than 99 percent and an oxygen concentration of approximately 110 parts per million. While trace amounts of water, nitrogen, and oxygen are expected to make up a small portion of the injection stream, they are not expected to affect the behavior of the CO₂ injected into the subsurface. As such, the model assumes a 100 percent pure CO₂ stream.

The main operational constraint to the model is rate of CO₂ injected; an injection profile was designed to reach the target of 547,500 tons of CO₂ in a period of 3 years. Additionally a maximum bottomhole pressure was established as a secondary operational constraint to ensure that the fracture pressure is not surpassed during the injection of CO₂. A conservative upper bottomhole pressure limit of 6,300 psia (0.6 psi/ft at approximately 10,500 ft) was imposed. An example of the injection profile and bottomhole pressure behavior can be observed form Figure 23.

Figure 23 Rate and Bottomhole pressure constraints.

3.3.1 Trapping Mechanism Modeling

The simulation and modeling techniques used describe the behavior of the four main trapping mechanisms (structural, residual, solubility and mineral trapping) are the ones described by L. Nghiem (et. al 2010)¹³ when studying the simulation and optimization of trapping processes for CO₂ storage in saline aquifers. Four scenarios based on different relative permeability profiles were defined in order to study its effects on the contribution that each one of the four main trapping mechanisms provides during the CO₂ sequestration process. This will finally allow determining the “safest” and “riskiest” scenario in terms of CO₂ mobility.

The relative permeability profiles chosen for this study correspond to experimental data for supercritical CO₂ / Brine systems from the West Canadian Sedimentary Basin describing both drainage and imbibition processes (Bennion & Bachu et al., 2006)¹⁴. These parameters are the values that the GEM simulator will use for its rock-fluid data interpretation and can be observed in Figure 24.

Figure 24 Drainage and Imbibition Relative Permeability profiles experimental data for supercritical CO₂ / Brine systems from the West Canadian Sedimentary Basin

¹³ Long Nghiem, Vijay Shrivastava, Bruce Kohse, Mohamed Hassam, and Chaodong Yang, Computer Modelling Group Ltd. "Simulation and Optimization of Trapping Processes for CO₂ Storage in Saline Aquifers" SPE 139429

¹⁴ D. Bennion, S. Bachu, "Drainage and Imbibition Relative Permeability relationships for supercritical CO₂ / Brine Systems in Intergranular Sandstones, Carbonate, Shale and Anhydrite Rocks" SPE Europec 2006, Vienna, Austria. SPE 99326

3.3.1.1 Structural Trapping

The single most important factor for securing CO₂ is the presence of a thick and fine-textured rock that serves as a seal above the sequestration reservoir. The seal should provide an effective permeability and capillary barrier to upward migration; the effects of the properties of this seal or confining unit are studied thoroughly in section 3.4 (Seal quality analysis).

Once injected, the supercritical CO₂ can be more buoyant than other liquids that might be present in the pore space. The CO₂ will therefore percolate up through the porous rocks until it reaches the top of the formation where it meets (and is trapped by) an impermeable layer (confining unit). Furthermore, once the injected CO₂ reaches this impermeable layer

3.3.1.2 Residual or Capillary Trapping Modeling

Simulating and Modeling of residual trapping was performed with the use of the Land's model described by Land C.S (et al. 1968)¹⁵. Figure 25 describes the Land's residual gas trapping model. When the CO₂ saturation increases, the gas relative permeability follows the drainage curve (Black). If at any given saturation (S_{gi}*) on the drainage curve, the gas saturation reverses its course and decreases, the gas follows the imbibition curve (Red) which refers to the irreversibility of the process (Hysteresis).

¹⁵ Land, C.S. 1968. Calculation of Imbibition Relative Permeability for Two and Three Phase flow from rock Properties. SPE J.8(2): 149-156. SPE-1942-PA. doi: 10.2118/1942-PA

Figure 25 Land's residual gas trapping model.

The Land's coefficient "C" is defined as:

$$C = \frac{1}{S_{gt,max}} - \frac{1}{S_{g,max}}$$

Where $S_{g,max}$ refers to the maximum gas saturation that could be attained and $S_{gt,max}$ is the maximum trapped gas saturation. The residual gas saturation for any given gas saturation (S_{gi}^*) is defined as:

$$S_{gt}^*(S_{gi}^*) = \frac{S_{gi}^*}{1 + C * S_{gi}^*}$$

3.3.1.3 Solubility Trapping Modeling

The second CO₂ storage mechanism is CO₂ dissolution in reservoir water. CO₂ is soluble in water, and when injected into a pressurized saline reservoir some of the CO₂ will dissolve in the formation water. The amount of CO₂ ultimately dissolved in water is affected by several factors including temperature and pressure within the reservoir, salinity of the reservoir water and reservoir heterogeneity and geometry.

The CO₂ solubility in brine is modeled as a phase-equilibrium process, which is governed by the equality of fugacities in the gas and aqueous phase :

$$f_{ig} = f_{ia}, \quad i = 1, \dots, n_c$$

The fugacity of the component “i” in the gas phase (f_{ig}) is calculated with the equation of state (Peng-Robinson). In this model the fugacity of the component “i” in the aqueous phase (f_{ia}) is modeled with Henry’s laws:

$$f_{ia} = H_i * y_{ia}$$

Henry’s constant (H_i) is a function of pressure, temperature and water salinity, which has to be input in addition to basic water properties (density, compressibility and viscosity). A survey of Henry’s constant correlations for important gases associated with greenhouse gas (GHG) sequestration in saline reservoirs was conducted. Harvey (1996)¹⁶ published correlations to determine Henry’s constants for many gaseous components including CO₂, N₂, H₂S and CH₄. These correlations have been implemented in GEM-GHG and the default values were used in the simulation.

3.3.1.4 Mineral Trapping Modeling.

The CMG-GEM simulator, with the use of the greenhouse gas module (GHG), can evaluate the chemical reactions among chemical species in the aqueous phase and the

¹⁶ Harvey, A. (1996), “Semiempirical Correlation for Henry’s Constants over Large Temperature Ranges,” American Institute of Chemical Engineers Journal, 42(5), 1491–1494.

dissolution/precipitation of minerals. To describe the chemical reactions, it is useful to define the number of chemical reactions and to define the number of components in gas, aqueous, and mineral phases. This process is thoroughly described by L. Nghiem (et. al 2010)¹⁷.

Despite the fact that when creating this model no mineralogy data was available, the following (most common) reactions expected in sandstone were modeled and they are summarized as follows:

3.4 Seal Quality Analysis

The main confining unit of the Paluxy formation is within the Washita-Fredericksburg interval as mentioned in section 3.1, where it is thoroughly described. The Washita-Fredericksburg interval is formed by the Danztler Sand, which is an aquifer with similar characteristics as those of the Paluxy formation, and the Basal Shale, being this last one the main confining unit.

Quality and integrity of the cap rock, representing the ability to trap “mobile” CO₂ structurally, is studied to assess the potential risk of leakage, as well as the impact that the properties of this confining unit may have on pressure and saturation distributions within the Paluxy formation.

In order to perform this analysis, a new cross-section was generated including wells near the area of interest (D-9-3, D-9-7, D-9-9) as shown in Figure 26 to assess properties of this seal. The Washita-Fredericksburg interval is located at depths between 7360 ft and 9400 ft. By using the

¹⁷ Long Nghiem, Vijay Shrivastava, Bruce Kohse, Mohamed Hassam, and Chaodong Yang , Computer Modelling Group Ltd.” Simulation and Optimization of Trapping Processes for CO₂ Storage in Saline Aquifers” SPE 139429

Spontaneous Potential (SP) log it was possible to identify the top and bottom of the Basal shale, finding that throughout the area of interest the thickness of this shale ranges within 170 ft and 240 ft (Figure 27) .

Figure 26 Cross-section A-A'

Figure 27 Well log interpretation of Cross-section A-A'

Finally, these two additional geological layers (Basal Shale and Danztler Sand) were included in the base model corresponding to the formations within the Washita-Fredericksburg interval (Figure 28). Each geological layer was initially divided in three simulation layers.

Figure 28 Inclusion of the Washita-Fredericksburg geological layers

Figure 29 Simulation layers corresponding to the Basal Shale (confining unit)

A sensitivity analysis was performed in terms of thickness and permeability of the Basal Shale; nine (9) different scenarios were designed, with a range of thickness between 150 ft and 250 ft and permeability within 10^{-3} darcy and 10^{-7} darcy for a period of 500 years. These scenarios are summarized in Table 1.

Table 1 Scenarios for sensitivity analysis on the effects of the Basal Shale permeability and thickness

<i>Scenarios</i>	<i>Thickness (ft)</i>	<i>Permeability (Darcy)</i>
1	150	10^{-3}
2	150	10^{-5}
3	150	10^{-7}
4	200	10^{-3}
5	200	10^{-5}
6	200	10^{-7}
7	250	10^{-3}
8	250	10^{-5}
9	250	10^{-7}

Based on the initial results of this simulations, it was determined that the vertical resolution when modeling the confining unit needed to be increased. Two particular factors made this necessity quite evident; the first one corresponded to the maximum amount of CO₂ present within the seal layers. Since this geological layer was divided in three simulation layers, the dimension of the gridblocks in the vertical direction is between 50 ft and 83 ft depending on the scenario. This did not allowed to perceive the vertical gradual changes of CO₂ mole fraction within the confining unit; hence, a proper assessment of depth of invasion of CO₂ within this confining unit could not be preformed. The second factor corresponds to the migration behavior of the CO₂ within the confining unit, implying that this migration would occur initially vertically only from the well gridblock and then move horizontally within the shale. After thorough analysis, it was decided to locally refine the gridblocks that corresponded to the confining unit in order to better grasp the complexity of the process taking place. This refinement was made such that the vertical dimensions of the gridblocks would not exceed 2 ft and the simulation of the nine previously defined scenarios was performed (Figure 30).

Figure 30 Grid refinement of the simulation layers of the confining unit

3.5 Boundary Conditions Effect Study

In this section an assessment is made to determine the effects that different boundary conditions may have on pressure distribution throughout the Plauxy formation. Two different boundary conditions were applied to the model; No-flow boundary and a Constant pressure boundary. In order to achieve this, different methods were tried when modifying the base case model. Finally, it was decided to connect an aquifer to the north, south, east and west boundaries of the model to maintain a constant initial pressure condition (Figure 31). A Fetckovich aquifer was included in the model with an R-ratio of 100. The default values in the CMG-builder were used since the main purpose of this aquifer is limited to pressure preservation.

Figure 31 Boundary conditions: No-Flow boundary (left) and Constant Pressure Boundary (right)

This effect was studied using three different scenarios in terms of permeability of the confining unit, since it was demonstrated in section 3.3.2 that this parameter will have the larger effect in pressure build up within the Plauxy formation, particularly in the top layer which is in permanent contact with the seal. These simulations were performed for a period of 500 years with both boundary conditions and the scenarios are summarized in Table 2.

Table 2 Scenarios for Boundary condition effect study.

Scenarios	Thickness (ft)	Permeability (Darcy)	Boundary Condition
1	150	10^{-3}	No- flow
2	150	10^{-5}	No- flow
3	150	10^{-7}	No- flow
4	150	10^{-3}	Aquifer
5	150	10^{-5}	Aquifer
6	150	10^{-7}	Aquifer

3.6 Post Injection Site Care Study (PISC)

In November 2010, the Administrator of the Environmental Protection Agency (EPA) signed the Federal Requirements under the Underground Injection Control (UIC) for CO₂ sequestration wells, Final Rule, as authorized by the Safe Drinking Water Act (SDWA). The final rule establishes new federal requirements for the underground injection of carbon dioxide for the purpose of long term underground storage, or geologic sequestration, and a new well class –Class VI– to ensure the protection of underground sources of drinking water (USDWs) from injection related activities.

EPA’s proposed rulemaking, describes the technical criteria for the geologic site characterization, fluid movement, area of review (AoR) and corrective action, well construction, operation, mechanical integrity testing, monitoring, well plugging as well as post-injection site care and site closure to protect underground sources of drinking water (USDWs).

Post Injection Site Care regarding the Citronelle field CO₂ sequestration project is bounded within the legal framework established by the following regulations:

- Code of Federal Regulations – Title 40 – Protection of Environment.- Chapter I, Subchapter D- part 146, section 146.93 “Post-injection site care and closure”.
- Alabama Department Of Environmental Management Water Division -Water Quality Control Administrative Code 335-6-8-.25 Class VI Well Post-Injection Site Care and Site Closure Requirements.

Regarding post injection site care and closure, these regulations establish the following:

Post-injection site care and site closure.

- a. The owner or operator of a Class VI well must prepare, maintain, and comply with a plan for post-injection site care and site closure that meets the requirements of paragraph (a)(2) of this section and is acceptable to the Director. The requirement to maintain and implement an approved plan is directly enforceable regardless of whether the requirement is a condition of the permit.
 1. The owner or operator must submit the post-injection site care and site closure plan as a part of the permit application to be approved by the Director.
 2. The post-injection site care and site closure plan must include the following information:
 - i. The pressure differential between pre-injection and predicted post-injection pressures in the injection zone(s);
 - ii. The predicted position of the carbon dioxide plume and associated pressure front at site closure as demonstrated in the area of review evaluation required under § 146.84(c)(1) ;
 - iii. A description of post-injection monitoring location, methods, and proposed frequency;
 - iv. A proposed schedule for submitting post-injection site care monitoring results to the Director pursuant to § 146.91(e); and,
 - v. The duration of the post-injection site care timeframe and, if approved by the Director, the demonstration of the alternative post-injection site care timeframe that ensures non-endangerment of USDWs.

3. Upon cessation of injection, owners or operators of Class VI wells must either submit an amended post-injection site care and site closure plan or demonstrate to the Director through monitoring data and modeling results that no amendment to the plan is needed. Any amendments to the post-injection site care and site closure plan must be approved by the Director, be incorporated into the permit, and are subject to the permit modification requirements at § 144.39 or § 144.41 of this chapter, as appropriate.
 4. At any time during the life of the geologic sequestration project, the owner or operator may modify and resubmit the post-injection site care and site closure plan for the Director's approval within 30 days of such change.
- b. The owner or operator shall monitor the site following the cessation of injection to show the position of the carbon dioxide plume and pressure front and demonstrate that USDWs are not being endangered.
1. Following the cessation of injection, the owner or operator shall continue to conduct monitoring as specified in the Director-approved post-injection site care and site closure plan for at least 50 years or for the duration of the alternative timeframe approved by the Director pursuant to requirements in paragraph (c) of this section, unless he/she makes a demonstration under (b)(2) of this section. The monitoring must continue until the geologic sequestration project no longer poses an endangerment to USDWs and the demonstration under (b)(2) of this section is submitted and approved by the Director.
 2. If the owner or operator can demonstrate to the satisfaction of the Director before 50 years or prior to the end of the approved alternative timeframe based on monitoring and other site-specific data, that the geologic sequestration project no longer poses an endangerment to USDWs, the Director may approve an amendment to the post-injection site care and site closure plan to reduce the frequency of monitoring or

may authorize site closure before the end of the 50-year period or prior to the end of the approved alternative timeframe, where he or she has substantial evidence that the geologic sequestration project no longer poses a risk of endangerment to USDWs.

3. Prior to authorization for site closure, the owner or operator must submit to the Director for review and approval a demonstration, based on monitoring and other site-specific data, that no additional monitoring is needed to ensure that the geologic sequestration project does not pose an endangerment to USDWs.

4. If the demonstration in paragraph (b)(3) of this section cannot be made (i.e., additional monitoring is needed to ensure that the geologic sequestration project does not pose an endangerment to USDWs) at the end of the 50-year period or at the end of the approved alternative timeframe, or if the Director does not approve the demonstration, the owner or operator must submit to the Director a plan to continue post-injection site care until a demonstration can be made and approved by the Director.

The main focus of the post injection site care study being performed within this thesis is to determine the time when a maximum yearly pressure differential has been achieved (stabilization time) based on thresholds of 10 psi, 5 psi and 2 psi per year. For this purpose, a code was generated using Microsoft's Visual Basic for Applications to manage the yearly pressure data generated in all the simulation runs, for each one of the 15,625 gridblocks located in the Paluxy formation top layer. Additionally, the technical requirements established in section a – 2 of these regulations to generate a proper post injection site care study are included in Appendix "B" for right after injection has stopped, as well as monitoring periods of 50 years and 500 years.

Chapter 4 –Results and Discussion

4. Results and discussion

In this section the results of the different studies performed in this comprehensive analysis are portrayed. Initially, the results regarding the trapping mechanisms will be shown and analyzed comparing the contribution of the main trapping mechanisms that play a role in the CO₂ sequestration process, when in presence of different relative permeability profiles. Subsequently, the results regarding the seal quality study will be presented, where the confining unit properties (thickness and permeability) impacts on invasion depth (within the seal), saturation and pressure distribution (last layer of the paluxy formation) are assessed.

Afterwards, the findings corresponding to the nature of the Boundary Condition and Post Injection Site Care study will be presented. Finally, an integration of all the different aspects that comprise this comprehensive study is performed, in order to determine the most favorable scenario in terms of risk.

4.1 Trapping Mechanisms

After performing the simulations for a period of 500 years, as described in section 3.3.1, the sensitivity analysis was performed on the effects of different relative permeability profiles on the contribution and behavior of each one of the four main trapping mechanisms (residual, structural, solubility and mineral trapping). The four different scenarios are summarized in Table 3 and Figure 32.

Table 3 Relative permeability profiles summary

Scenario	Relative Permeability profile	Residual Gas Saturation (%)	Critical Gas Saturation (%)	Maximum Krg
1	Cardium #1	30.09	20.37	0.1166
2	Cardium #2	28.98	1.08	0.1219
3	Viking Sandstone	25.81	11.10	0.2583
4	Nisku #2	10.66	2.93	0.53291

Figure 32 Drainage and Imbibition Relative Permeability profiles experimental data for supercritical CO₂ / Brine systems from the West Canadian Sedimentary Basin

The individual results of each one of these scenarios are listed as follows in sections 4.1.1 through 4.1.4.

4.1.1 Scenario 1 – Cardium #1

Figure 33 Scenario 1 - Gas Saturation, 500 years - vertical cross-section of the well site

Figure 34 Scenario 1 - Dynamic trapped gas, 500 years - vertical cross-section of the well site

Gas Saturation 2512-01-01 J layer: 83

File: citronelle - ci
 User: Dan
 Date: 8/13/2012
 Scale: 1:21001
 Z/X: 7.00:1
 Axis Units: ft

0.59
 0.53
 0.47
 0.41
 0.36
 0.30
 0.24
 0.18
 0.12
 0.07
 0.01

0.00 0.25 0.50 0.75

Figure 36 Scenario 2 - Gas Saturation, 500 years - vertical cross-section of the well site

Figure 37 Scenario 2 - Dynamic trapped gas, 500 years - vertical cross-section of the well site

Figure 38 Scenario 2 - 500 years - Trapping mechanisms contribution

4.1.3 Scenario 3 – Viking Sandstone

Figure 39 Scenario 3 - Gas Saturation, 500 years - vertical cross-section of the well site

Figure 40 Scenario 3 - Dynamic trapped gas, 500 years - vertical cross-section of the well site

Figure 41 Scenario 3 - 500 years - Trapping mechanisms contribution

4.1.4 Scenario 4 – Nisku #2

Figure 42 Scenario 4 - Gas Saturation, 500 years - vertical cross-section of the well site

Figure 43 Scenario 3 - Dynamic trapped gas, 500 years - vertical cross-section of the well site

Figure 44 Scenario 3 - 500 years - Trapping mechanisms contribution

After thorough analysis of these presented results we can observe that, even do the profiles differ in range on relative permeability to CO_2 , CO_2 critical saturations as well as in the range of CO_2 saturation, the main parameter that can be distinguished driving this behavior is the residual saturations corresponding to each one of the profiles. As the residual saturations are higher, it will represent higher amounts of residually or capillary trapped CO_2 as it can be observed in the comparison in Figure 45.

Figure 45 Comparison of amount of capillary trapped CO_2 for the different relative permeability profiles - 500 years

This behavior can also be observed in terms of dissolved CO₂ as shown in Figure 46.

Figure 46 Comparison of amount of dissolved CO₂ for the different relative permeability profiles - 500 years

The contribution that each one of the trapping mechanisms provides to the CO₂ storage process was quantified. This is possible by knowing the total amount of CO₂ injected into the formation (15,045.36 MMCF or 550,596.35 tons of CO₂) and comparing it to the amounts of CO₂ trapped by the different mechanisms (Figure 47). Mineral trapping is also included not showing a significant contribution to this process in the first 500 years, detailed knowledge of the mineralogy of the formation is necessary to make a proper assessment of the contribution of this mechanism.

Additionally we can observe which relative permeability profile will represent a “safer” scenario in terms of CO₂ mobility in case of that a leakage would occur. The relative permeability profile corresponding to Scenario 1 (Cardium #1) results in a 54.7% of the CO₂ residually or capillary trapped, 28.25% dissolved into the brine and 17% structurally trapped, implying that more than 80% of the CO₂ will remain immobile in the formation in the event of failure of the confining unit or any other mean of leakage. As opposed from the relative permeability profile corresponding to Scenario 4 (Nisku #2), in which more than 80% of the CO₂ is structurally trapped and only 20%

of the injected amount is trapped by different mechanisms, representing an scenario where 80% of the injected CO₂ will be still mobile and able to migrate in event of a leakage.

Figure 47 Trapping Mechanisms Contribution - 500 years

4.2. Seal Quality study

When performing the sensitivity analysis based on the properties of the confining unit (thickness and permeability) two different aspects were studied. The first aspect corresponds to what was defined as depth of invasion; the depth of invasion represents the maximum depth (within the seal) where there is presence of CO₂, acting as an indicator of how the confining unit has been compromised by “allowing” the migration of the injected CO₂ within itself. As described in section 3.4, nine different scenarios were defined in order to perform this analysis, and the CO₂ mole fraction was used to observe the CO₂ invasion within the confining unit. Figure 48, Figure 49 and Figure 50 correspond to three different scenarios where the thickness of the confining

unit is 200 ft and the permeability is varies within 10^{-3} darcy and 10^{-7} (scenarios 4,5,6). In these figures we can observe that as permeability decrease, so will the invasion of CO_2 within the confining unit. It is proper to mention that the high permeability scenario (1 md), is not characteristic of shale formations, particularly a formation that would be selected as a proper confining unit when selecting CO_2 storage formation targets.

Figure 48 Scenario 4 ($h=200\text{ft}$ and $k=10^{-3}$ md)- Global mole fraction after 500 years

Global Mole Fraction(CO2) 2502-01-01 J layer: 56

Figure 49 Scenario 5 ($h=200\text{ft}$ and $k=10^{-5}\text{md}$)- Global mole fraction after 500 years

Gas Mole Fraction(CO2) 2512-01-01 J layer: 56

Figure 50 Scenario 6 ($h=200\text{ft}$ and $k=10^{-7}\text{md}$)- Global mole fraction after 500 years

This same analysis was performed to all the scenarios and they are included in Appendix “A”. After analyzing the results for all the scenarios available, it was observed that permeability is the main factor that determines the depth of invasion of the within the confining unit, with the exception of those scenarios considered to have high permeability (10^{-3} darcy or 1 md). In these scenarios, the confining unit is fully breached by the injected CO₂ and the depth of invasion will then be the same as the thickness of the seal in those particular scenarios. These results are summarized in figure, where as mentioned earlier the high permeability scenarios the depth of invasion ranges within 150 ft and 250 ft (full seal breach), contrasting from the scenarios where permeability is 10^{-5} and 10^{-7} darcy that the maximum depth of invasion is 22 ft and 8 ft respectively.

Figure 51 CO₂ Depth of invasion within the confining unit - all scenarios comparison

The second aspect analyzed in the context of this study, was the impact that the variations of the properties of the confining unit have on saturation and pressure distribution within the first layer of the Paluxy formation. This layer is the most extensive and conductive layer in the Paluxy formation, also is the layer that is in permanent contact with the confining unit.

Regarding the saturation distribution in the first layer of the Paluxy formation, it was observed that a change in the permeability of the confining unit has the most significant impact, as

opposed to variations in thickness. This is due to the fact that, when in presence of a quite conductive confining unit, the changes in the saturation profiles are mainly driven by “fluid loss” represented by the ability of the CO₂ to migrate within this confining unit and as the permeability of the confining unit is decreased, less CO₂ will be able to migrate upwards within the seal; hence higher concentrations of CO₂ will remain in the Paluxy formation migrating mainly horizontally once they reach this “impermeable” layer. This behavior was observed in the nine scenarios that were defined for this study as shown in Figure 52.

Figure 52 Saturation distribution – Paluxy formation top layer- after 500 years - all scenarios

As expected, the same behavior was observed in the pressure distribution profiles. This behavior can be attributed to the fact that, as permeability in the confining unit is decreased, less pressure dissipation will occur as a consequence of CO₂ migration upwards and out of the

Paluxy formation, therefore the post injection pressure distribution will no longer be govern as much by “fluid loss” as by CO₂ plume migration itself. Figure 53 summarizes the results of the simulations for a period of 500 years for all the defined scenarios.

Figure 53 Pressure distribution – Paluxy formation top layer- after 500 years - all scenarios

4.3. Boundary Condition study

As described in section 3.5, a sensitivity analysis was performed, in order to determine the effects that the nature of the boundary condition would have on the pressure distribution throughout the reservoir. The layer of interest, once again is the top layer of the Paluxy

formation as well as two particular locations: location of the injection well and monitoring well. Additionally, based on the findings in the Seal Quality study 6 different scenarios were determined in order to perform this analysis and they are summarized in Table 4.

Table 4 Scenarios defined for the boundary condition study

Scenarios	Thickness (ft)	Permeability of the confining unit (Darcy)	Boundary Condition
1	150	10^{-3}	No- flow
2	150	10^{-5}	No- flow
3	150	10^{-7}	No- flow
4	150	10^{-3}	Aquifer
5	150	10^{-5}	Aquifer
6	150	10^{-7}	Aquifer

The difference between the pressure distributions after 500 years and initial reservoir pressure is been used as indicator of the effects of the nature of the boundary condition. For comparison purposes these scenarios have been divided into three categories in terms of the permeability of the confining unit: High permeability, Medium Permeability and Low permeability that correspond to the values of permeability of 10^{-3} , 10^{-5} and 10^{-7} darcy respectively. These results are summarized the following sections.

4.3.1 High permeability scenarios (10-3darcy)

Figure 55 Pressure difference with initial reservoir pressure after 500 years - high permeability scenario

Figure 54 Pressure profile comparison @Injection well - 500 years

Figure 56 Pressure profile comparison @Observation well - 500 years

4.3.2 Medium permeability scenarios (10-5darcy)

Figure 57 Pressure difference with initial reservoir pressure after 500 years - Medium permeability scenario

Figure 58 Pressure profile comparison @Injection well - 500 years

Figure 59 Pressure profile comparison @ Observation well - 500 years

4.3.3 Low permeability scenarios (10⁻⁷darcy)

Figure 60 Pressure difference with initial reservoir pressure after 500 years - Low permeability scenario

Figure 61 Pressure profile comparison @Injection well - 500 years

Figure 62 Pressure profile comparison @Observation well - 500 years

From these results important observations can be made. In the scenarios where the imposed boundary condition consist of a constant pressure boundary the average reservoir pressure, after 500 years of monitoring, stabilizes to the initial reservoir pressure, opposed to when the boundary condition consist of a no-flow condition. When a no-flow boundary is imposed to the system, a pressure gain (difference between initial average reservoir pressure and average reservoir pressure after 500 years) is observed and varies with the properties of the confining unit, which represents the “upper” boundary of the top layer of the Paluxy formation. Depending on how permeable this confining unit might be and in order to be consistent with the pre-defined scenarios, as observed in the Seal quality study in section 3.4, the pressure dissipation will be either “fluid loss” driven or it will depend mainly on the CO₂ plume migration and system response to it. Figure illustrates the pressure gain in the system as the permeability of the confining unit varies.

Figure 63 Pressure gain in the reservoir after 500 years

It is proper to mention that even do a higher average reservoir pressure is observed after 500 years of monitoring, these changes only represent an increase in a range of 0.43 % and 3.18% of the initial average reservoir pressure within an area of 6,373.71 acres or 9.95 square miles, after injecting 550,596.35 tons of CO₂.

4.4. Post Injection Site Care study

As stated in section 3.6 ,the main focus of the post injection site care study being performed within this thesis is to determine the time when a maximum yearly pressure differential has been achieved (stabilization time) based on thresholds of 10 psi, 5 psi and 2 psi per year. For this purpose, a code was generated using Microsoft’s Visual Basic for Applications (VBA) to manage the yearly pressure data generated in all the simulation runs, for each one of the 15,625 gridblocks located in the Paluxy formation top layer. In order to perform this analysis, the VBA code extracts pressure data from the CMG-GEM simulation results yearly and determines the pressure difference distribution per year, as well as the time when the maximum pressure difference threshold has been found. Based on the findings from the Seal Quality study, and knowing the greater impact will be caused by changes in the permeability of the confining unit, opposed by the effects the thickness of this seal, a range of “seal conductivity” was defined (permeability*thickness of the confining unit measured in 150). The scenarios used for this study are summarized in Table 5. The results shown in the following sections will correspond to the pressure difference distribution per time step until the corresponding threshold condition has been satisfied and distribution profiles of where in the top layer of the Paluxy formation this condition has been met.

Table 5 Scenarios used in PISC

Scenario	Permeability of the Confining Unit (md)	K*h range of the confining unit (md-ft)	
High Permeability	1	150	250
Medium Permeability	0.01	1.5	2.5
Low Permeability	0.0001	0.015	0.025

In this section the results for one of the scenarios will be analyzed and discussed as an example case, the result for the rest of the cases are included in Appendix “B”.

After calculating and plotting the yearly pressure differentials we could determine that the all the thresholds are met the second year after injection (post-injection monitoring) has stopped. The following figures represent the spatial distribution of this pressure differences for 1 year post injection and 2 years post injection for verification purposes:

Figure 64 Yearly Pressure Difference distribution - 1 year Post-injection

Figure 65 Yearly Pressure Difference distribution - 2 year Post-injection

As observed in Figure 64 and Figure 65, after the first year of post-injection has past, we can still observe large pressure differences particularly in the surroundings of the injection well. This pressure is dissipated after the second year post-injection has elapsed. Comparing them with the 3 predefined thresholds for pressure variation in yearly bases (10 psi, 5 psi and 2 psi), it was possible to determine when and where in the reservoir this conditions were not being satisfied. Figure 66 and Figure 67 represent the pressure difference distribution as before, but this time the formatting was set to determine which parts of the top layer are over or under the pressure

thresholds in order to verify the stabilization times after 1 and 2 years of post-injection monitoring.

Figure 66 Threshold Verification - 1 year post injection

Figure 67 Threshold Verification - 2 year post injection

As observed in Figure 67 the condition for the 3 pre-defined thresholds has been fully satisfied after the second year of post-injection monitoring, hence the pressure is consider to be stabilized under this criteria by the end of the second year after injection has stopped.

4.5. Lessons Learned

After performing the studies considered in this comprehensive analysis, it was possible to grasp the complexity of the processes that takes place in a CO₂ storage project of this magnitude and how it can be affected by different factors, where the degree of uncertainty of the reservoir characteristics, such as relative permeability, nature of the boundary conditions and confining units properties (seal quality), plays a very important role. It has been possible to determine risk scenarios combining these different studies, and how they are impacted by the degree of mobility and long-term fate of the injected CO₂ as well as pressure and saturation alterations within the system.

In terms of rock-fluid interactions, we learned that it is possible to determine the level of risk in terms of CO₂ “mobility” in deep saline formations by proper assessment of relative permeability profiles and its hysteresis, which would trigger and influence the trapping mechanisms that contribute to the CO₂ storage process. Additionally, we observed the benefits of taking advantage of the wettability and capillary effects (residual or capillary trapping) as well as dissolution of CO₂ into brine, representing “safer” scenarios in the event that a leakage would happen, leading to a considerable amount of immobile of CO₂ that would not migrate in case of deterioration or fracture of the confining unit or any other means of leakage. Furthermore, within the scenarios used for this study, it was possible to observe the importance of relative permeability hysteresis, particularly the residual gas saturations and its proportional relation to the amount of CO₂ that could be residually trapped. After quantifying the contribution of the trapping mechanisms, it was observed that the relative permeability profile corresponding to “safer” scenario resulted in a 54.7% of the CO₂ residually or capillary trapped, 28.25% dissolved into the brine and 17% structurally trapped, implying that more than 80% of the CO₂ will remain immobile in the formation in the event of failure of the confining unit or any other mean of leakage. As opposed from the relative permeability profile corresponding to scenario that represented a higher risk, in which more than 80% of the CO₂ is structurally trapped and only 20% of the injected amount is trapped by different mechanisms, representing an scenario where 80% of the injected CO₂ will be still mobile and able to migrate in event of a leakage. Additionally, as residual trapping and CO₂ dissolution would increase, less amount of CO₂ will actually be able to migrate due to bouyance to the first layer of the paluxy formation decreasing its concentration in this area of the reservoir.

Regarding the seal quality study, it was possible to observe the effects that the properties such as permeability and thickness of the confining unit had, not only on its capability to seal and prevent flow to migrate out of the saline formation, but on the Paluxy formation itself. It was observed that changes in the permeability of the confining unit have the most significant impact, as opposed to variations in thickness. This is due to the fact that the changes in the pressure and saturation profiles when in presence of a quite conductive confining unit are mainly driven by “fluid loss” represented by the ability of the CO₂ to migrate from the Paluxy formation to the this confining unit. As the permeability of the confining unit is decreased, less CO₂ will be able to migrate upwards within the seal; hence, higher concentrations of CO₂ will remain in the Paluxy formation migrating mainly horizontally once they reach this “impermeable” layer.

From the boundary condition study we learned that when the imposed boundary condition consists of a constant pressure boundary, the average reservoir pressure eventually stabilizes back to the initial reservoir pressure, opposed by when in presence of a boundary condition that will not allow the pressure to stabilize back to the initial reservoir pressure (no-flow boundary), after 500 years of monitoring, the change in average reservoir pressure will only represent an increase in a range of 0.43 % and 3.18% of the initial average reservoir pressure within an area of 6,373.71 acres or 9.95 square miles, after injecting 550,596.35 tons of CO₂. Furthermore, combined with the seal quality study, this increase in pressure will not represent a major risk in terms of leakage by compromising the integrity of the confining unit.

Finally, it was demonstrated that pressure stabilization times can be determined within acceptable thresholds, representing a powerful tool when applying post-injection monitoring techniques that rely on long term pressure behavior. This is particularly true for technologies such as the ones being developed by the Petroleum Engineering and Analytics lab, in West Virginia University, for leakage detection systems at the reservoir level with the use of smart fields.

Chapter 5

Concluding Remarks

CO₂ storage in deep saline formations is a complex process, sensitive to many different factors that can determine the ability of such formations to sequester CO₂ for very long periods of time. In order to fully grasp the complexity of this process, a comprehensive analysis on an ongoing CO₂ storage project in the Citronelle field located in Mobile, Alabama was performed. This consisted of performing different studies related to the impact of the nature of the boundary condition, trapping mechanisms, confining unit characteristics as well as post-injection site care on the aforementioned CO₂ storage project.

The key findings and conclusions from this comprehensive analysis can be summarized as follows:

- A full field reservoir model was generated with actual field data in order to properly simulate the complexity and heterogeneity of the actual formation in terms of structure and geological properties.
- The CO₂ storage process is significantly controlled and impacted by the formation's relative permeability profile as well as the contribution of the different trapping mechanisms involved.
- A proportional relationship exists between the residual gas saturation of the relative permeability profiles and the amount of CO₂ that will be either residually trapped or dissolved in the formation brine.
- In event that a leakage would occur due to any deterioration or fracture that would compromise the integrity of the confining unit, safer scenarios will be those that have a relative permeability profile which allows to achieve higher amounts of immobile spread out trapped gas (e.g. residually trapped and dissolved CO₂ in formation brine), rather than those where most of the CO₂ would be trapped structurally in a continuous mobile phase. After quantifying the contribution of the trapping mechanisms, it was observed that the relative permeability profile corresponding to "safer" scenario resulted in a 54.7% of the CO₂ residually or capillary trapped, 28.25% dissolved into the brine and 17% structurally trapped, implying that more than 80% of the CO₂ will remain immobile in the formation in the event of failure of the confining unit or any other mean of

leakage, as opposed to the relative permeability profile corresponding to scenario that represented a higher risk, in which more than 80% of the CO₂ is structurally trapped and only 20% of the injected amount is trapped by different mechanisms, representing an scenario where 80% of the injected CO₂ will be still mobile and able to migrate in event of a leakage.

- The properties of the confining unit affect the pressure and saturation distributions of the target storage formation, finding that permeability and thickness of the seal have a significant impact on them. These characteristics can determine if the pressure and saturation behaviors during the CO₂ storage process either will be governed to a certain degree by “fluid loss”, represented by the amount of CO₂ that can migrate to the confining unit (conductive seal), or CO₂ plume migration (tight seal).
- Regarding the impact that the nature of the boundary condition has on the CO₂ storage process, when the imposed boundary condition consists of a constant pressure boundary, the average reservoir pressure eventually stabilizes back to the initial reservoir pressure, opposed to when the boundary condition consists of a no-flow condition. When a no-flow boundary is imposed to the system, a pressure gain (difference between initial average reservoir pressure and average reservoir pressure after 500 years of monitoring) is observed and varies with the properties of the confining unit, which represents the “upper” boundary of the top layer of the Paluxy formation. In the scenarios presented for this study these changes represent an increase of average reservoir pressure in a range of 0.43 % and 3.18% of the initial average reservoir pressure within an area of 6,373.71 acres or 9.95 square miles, after injecting 550,596.35 tons of CO₂.
- It is possible to determine the pressure stabilization time within acceptable yearly pressure difference thresholds (10 psi, 5 psi, 2 psi). Additionally, the time it will take for the pressure to stabilize is deeply impacted by the properties of the confining unit as well as the complexity and heterogeneity of the reservoir.

Recommendations

The comprehensive analysis performed in this research revealed how sensitive the CO₂ storage process is to variations of parameters such as relative permeability profiles, nature of the boundary condition and confining unit characteristics. However, further detailed investigation of several aspects will enhance our understanding of the processes that take place during the injection of CO₂ into deep saline aquifers. The recommended future tasks can be summarized as follows:

- In order to reduce the degree of uncertainty of the petrophysical properties of the reservoir, actual experimental data regarding relative permeability measurement and detailed mineralogy of the Paluxy formation would be a great addition, which will enhance the reservoir model generated to perform this comprehensive study.
- Include the capillary pressure into the reservoir model, based on experimental data, and investigate its impact on the CO₂ storage process, comparing it with the cases where it is not imposed.
- Further characterization of the confining unit is recommended, in order to grasp its heterogeneity, study the effects this will have on its sealing capabilities as well as the effect it will have on pressure and saturation distribution behaviors within the Paluxy formation.

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Appendix “A”

Seal Quality Results invasion determination (before vertical grid refinement)

Realization	Thickness (ft)	Permeability (Darcy)
1	150	10^{-3}

Figure 68 Scenario 1 - CO₂ mole fraction after 500 years (pre- grid refinement)

Realization	Thickness (ft)	Permeability (Darcy)
2	150	10^{-5}

Figure 69 Scenario 2 - CO2 mole fraction after 500 years (pre- grid refinement)

Realization	Thickness (ft)	Permeability (Darcy)
3	150	10^{-7}

Figure 70 Scenario 3 - CO2 mole fraction after 500 years (pre- grid refinement)

Realization	Thickness (ft)	Permeability (Darcy)
4	200	10^{-3}

Figure 71 Scenario 4 - CO₂ mole fraction after 500 years (pre- grid refinement)

Realization	Thickness (ft)	Permeability (Darcy)
5	200	10^{-5}

Figure 72 Scenario 5 - CO₂ mole fraction after 500 years (pre- grid refinement)

Realization	Thickness (ft)	Permeability (Darcy)
6	200	10^{-7}

Figure 73 Scenario 6 - CO2 mole fraction after 500 years (pre- grid refinement)

Realization	Thickness (ft)	Permeability (Darcy)
7	250	10^{-3}

Figure 74 Scenario 7 - CO2 mole fraction after 500 years (pre- grid refinement)

Realization	Thickness (ft)	Permeability (Darcy)
8	250	10^{-5}

Figure 75 Scenario 8 - CO₂ mole fraction after 500 years (pre- grid refinement)

Realization	Thickness (ft)	Permeability (Darcy)
9	250	10^{-7}

Figure 76 Scenario 9 - CO₂ mole fraction after 500 years (pre- grid refinement)

Seal Quality Results invasion determination (post- vertical grid refinement)

<i>Realization</i>	<i>Thickness (ft)</i>	<i>Permeability (Darcy)</i>
1	150	10^{-3}

Figure 77 Scenario 1 - CO₂ mole fraction after 500 years (post- grid refinement)

Realization	Thickness (ft)	Permeability (Darcy)
2	150	10 ⁻⁵

Global Mole Fraction(CO2) 2512-01-01 J layer: 56

Figure 78 Scenario 2 - CO2 mole fraction after 500 years (post- grid refinement)

<i>Realization</i>	<i>Thickness (ft)</i>	<i>Permeability (Darcy)</i>
3	150	10^{-7}

Global Mole Fraction(CO2) 2512-01-01 J layer: 56

Figure 79 Scenario 3 - CO2 mole fraction after 500 years (post- grid refinement)

Realization	Thickness (ft)	Permeability (Darcy)
4	200	10^{-3}

Global Mole Fraction(CO₂) 2512-01-01 J layer: 56

Figure 80 Scenario 4 - CO₂ mole fraction after 500 years (post- grid refinement)

Realization	Thickness (ft)	Permeability (Darcy)
5	200	10^{-5}

Global Mole Fraction(CO2) 2512-01-01 J layer: 56

Figure 81 Scenario 5 - CO2 mole fraction after 500 years (post- grid refinement)

Realization	Thickness (ft)	Permeability (Darcy)
6	200	10^{-7}

Global Mole Fraction(CO₂) 2512-01-01 J layer: 56

Figure 82 Scenario 6 - CO₂ mole fraction after 500 years (post- grid refinement)

Realization	Thickness (ft)	Permeability (Darcy)
7	250	10 ⁻³

Global Mole Fraction(CO2) 2512-01-01 J layer: 56

Figure 83 Scenario 7- CO2 mole fraction after 500 years (post- grid refinement)

Realization	Thickness (ft)	Permeability (Darcy)
8	250	10^{-5}

Global Mole Fraction(CO2) 2512-01-01 J layer: 56

Figure 84 Scenario 8 - CO2 mole fraction after 500 years (post- grid refinement)

Realization	Thickness (ft)	Permeability (Darcy)
9	250	10 ⁻⁷

Global Mole Fraction(CO2) 2512-01-01 J layer: 56

Figure 85 Scenario 9 - CO2 mole fraction after 500 years (post- grid refinement)

Appendix “B”

Technical requirements for Post-injection Site Care

Delta P 2512-01-01 K layer: 7

Figure 86 Scenario 1 -Pressure front (differential with initial pressure) - After 50 years

Delta P - 500 years 2012-01-01 K layer: 7

Figure 87 Scenario 1 -Pressure front (differential with initial pressure) - After 500 years

Global Mole Fraction(CO₂) 2075-01-01 K layer: 7

Figure 88 Scenario 1 -CO₂ plume front- After 50 years

Global Mole Fraction(CO2) 2512-01-01 K layer: 7

Figure 89 Scenario 1 -CO2 plume front- After 500 years

Delta P - 50 years 2512-01-01 K layer: 7

Figure 90 Scenario 2 -Pressure front (differential with initial pressure) - After 50 years

Delta P - 500 years 2012-01-01 K layer: 7

Figure 91 Scenario 2 -Pressure front (differential with initial pressure) - After 500 years

Global Mole Fraction(CO2) 2075-01-01 K layer: 7

Figure 92 Scenario 2 -CO2 plume front- After 50 years

Global Mole Fraction(CO2) 2512-01-01 K layer: 7

Figure 93 Scenario 2 -CO2 plume front- After 500 years

Delta P - 50 years 2512-01-01 K layer: 7

Figure 94 Scenario 3 -Pressure front (differential with initial pressure) - After 50 years

Delta P - 500 years 2012-01-01 K layer: 7

Figure 95 Scenario 3 -Pressure front (differential with initial pressure) - After 500 years

Global Mole Fraction(CO2) 2075-01-01 K layer: 7

Figure 96 Scenario 3 -CO2 plume front- After 50 years

Global Mole Fraction(CO2) 2512-01-01 K layer: 7

Figure 97 Scenario 3 -CO2 plume front- After 500 years

VBA source code for pressure stabilization time determination

```
Option Explicit
'variable declaration
Dim Layer As String
Dim fname As Variant
Dim j As Double
Dim LineofText As String
Dim p As Variant
Dim pos As Long
Dim i As Double
Dim k As Integer

Dim diffpress As Double
Dim AFTER As String
Dim BEFORE As String
Dim D As Integer
Dim C As Integer
Dim Di As Integer
Dim F As Integer

Sub ini2() ' initialization routine
Call read_txtFile
If MsgBox("do you want to generate differential pressure table?", vbYesNo, "Proceed??") = vbYes
Then Call DeltaP_generate
If MsgBox("Proceed to plot and identify regions_>for trshholds defined->for all times
available", "Proceed?") = vbYes Then Call PLOT_X3
End Sub

Sub read_txtFile()

' ///////////////////////////////////////////////////
' Disable excel application permits - free memory
Application.ScreenUpdating = False
Application.DisplayStatusBar = False
Application.Calculation = xlCalculationManual
Application.EnableEvents = False
' ///////////////////////////////////////////////////

'read file
fname = Application.GetOpenFilename("Text Files (*.txt),*.txt", , "Select Text Data File")
If fname = False Then Exit Sub
Open fname For Input As #1

'initialize read variables
j = 1
pos = 1
i = 1
k = 1

'reading blocks loop
```

```

Do Until pos = (125 * 125 + 5)
    Line Input #1, LineofText
    p = Split(LineofText, " ")

    For i = 1 To UBound(p)
        ActiveSheet.Cells(j, i) = p(i)
    Next
    j = j + 1
    pos = pos + 1
    On Error Resume Next
Loop

'Reading pressure loop

i = 3
pos = 1
Do Until EOF(1) 'loop until end of file

    Line Input #1, LineofText
    p = Split(LineofText, " ")
    k = UBound(p)
    ActiveSheet.Cells(j, i) = p(k)
    j = j + 1
    k = 0
    If p(k) = 1274547.59 Then
        i = i + 1
        j = 1
    End If
    k = i
    On Error Resume Next
Loop

'Close the file.
Close #1

'Arrange titles
Layer = ActiveSheet.Cells(4, 4)
Rows("2:3").Select
Selection.ClearContents
Rows("1:1").Select
Selection.Cut
Rows("4:4").Select
ActiveSheet.Paste
Range("A4").Select
ActiveCell.FormulaR1C1 = "x"
Range("B4").Select
ActiveCell.FormulaR1C1 = "y"
Range("C4").Select
ActiveCell.FormulaR1C1 = "0"
Rows("1:2").Select
Selection.Delete Shift:=xlUp
Columns("A:A").EntireColumn.AutoFit
Columns("B:B").EntireColumn.AutoFit

```

```

ActiveSheet.Cells(1, 1) = Layer
ActiveSheet.Name = InputBox("Realizacion#", "introducir numerod e realizacion")

'/////////////////////////////////////////
'Enable excel application permits
    Application.ScreenUpdating = True
    Application.DisplayStatusBar = True
    Application.Calculation = xlCalculationAutomatic
    Application.EnableEvents = True
'/////////////////////////////////////////

End Sub

Sub DeltaP_generate()

'Read columns
F = 1

Do While ActiveSheet.Cells(2, F) <> ""
    F = F + 1
Loop

'Initialization
i = 1
j = 2
Application.ScreenUpdating = True

'Look up target
With ActiveSheet
    .Cells(15639, 1).Select

'Print Titles for every column (Time steps)
For i = 3 To F - 2
    AFTER = .Cells(2, i)
    BEFORE = .Cells(2, i + 1)
    .Cells(15639, i) = "Time" & AFTER & " - " & BEFORE
Next i

'Print Blocks (X,Y) designation
For j = 2 To 15627 ' rows
    .Cells(j + 15637, 1) = .Cells(j, 1)
    .Cells(j + 15637, 2) = .Cells(j, 2)
Next j

'Print table difference of pressure ->abs(pressure time step+1 - pressure time step)
For i = 3 To F - 2 ' columns
    For j = 3 To 15627 ' rows
        diffpress = Abs(.Cells(j, i + 1) - .Cells(j, i))
        .Cells(j + 15637, i) = diffpress
    
```

```

        Next j
    Next i

'Loop-> locate difference of pressures over 2 psi - determine stabilization time
For i = 3 To F - 2 ' columns
    For j = 15640 To 31277 ' rows
        diffpress = .Cells(j, i)
        If diffpress > 2 Then
            .Cells(j, i).Select
            Selection.Interior.Color = 65535
            D = i
        End If
    Next j
Next i

'Loop-> locate difference of pressures over 5 psi - determine stabilization time
For i = 3 To F - 2 ' columns
    For j = 15640 To 31277 ' rows
        diffpress = .Cells(j, i)
        If diffpress > 5 Then
            .Cells(j, i).Select
            Selection.Interior.Color = 49407
            C = i
        End If
    Next j
Next i

'Loop-> locate difference of pressures over 10 psi - determine stabilization time
For i = 3 To F - 2 ' columns
    For j = 15640 To 31277 ' rows
        diffpress = .Cells(j, i)
        If diffpress > 10 Then
            .Cells(j, i).Select
            Selection.Interior.Color = 255
            Di = i
        End If
    Next j
Next i

'Print stabilization times
.Cells(15639, D).Select
Selection.Interior.Color = 65535
.Cells(15639, C).Select
Selection.Interior.Color = 49407
.Cells(15639, Di).Select
Selection.Interior.Color = 255

'report via Message box stabilization times
MsgBox ("Stabilization time for 2 psi threshold: " & .Cells(15639, D))
MsgBox ("Stabilization time for 5 psi threshold: " & .Cells(15639, C))

```

```

MsgBox ("Stabilization time for 10 psi treshold: " & .Cells(15639, Di))

End With

Application.SendKeys ("^s")

End Sub

Sub PLOT_X3()
Dim NomPlot As String
Dim RealZ As String
Dim tiempo As String

Dim i, j, k, L, C, F As Integer

'Preparation to plot + add new sheet

RealZ = ActiveSheet.Name
MsgBox ("program is going to perfome plot for each timestep on Activesheet")

NomPlot = RealZ & InputBox("name of plot?", "Plotting")
Sheets.Add AFTER:=Sheets(Sheets.Count)
ActiveSheet.Name = NomPlot

Application.ScreenUpdating = False
For C = 0 To 2

    L = 135 * C

    F = 1

    For i = 3 To 37 'columns

        tiempo = Sheets(RealZ).Cells(15639, i)
        Sheets(NomPlot).Cells(1 + L, F) = tiempo

        For j = 1 To 125 'X axis
            Sheets(NomPlot).Cells(1 + L, j + F) = Sheets(RealZ).Cells(15639 + j, 1)
        Next j

        For j = 1 To 125 'y Axis
            Sheets(NomPlot).Cells(j + 1 + L, F) = Sheets(RealZ).Cells(15640 + j * 125, 2)
        Next j

        For j = 1 To 125 'Block pressure data

```

```

        For k = 1 To 125
            Sheets(NomPlot).Cells(j + 1 + L, k + F) = Sheets(RealZ).Cells(15639 + j * 125
                + k, i)
        Next k
    Next j

    ActiveWindow.Zoom = 10

    Sheets(NomPlot).Cells(2 + L, F + 1).Select
    Range(Selection, Selection.End(xlToRight)).Select
    Range(Selection, Selection.End(xlDown)).Select

    'conditional formating

    If C = 0 Then

        Selection.FormatConditions.Add Type:=xlCellValue, Operator:=xlGreater, _
            Formula1:="=10"
        Selection.FormatConditions(Selection.FormatConditions.Count).SetFirstPriority
        With Selection.FormatConditions(1).Interior
            .PatternColorIndex = xlAutomatic
            .Color = 192
            .TintAndShade = 0
        End With
        Selection.FormatConditions(1).StopIfTrue = False
        Selection.FormatConditions.Add Type:=xlCellValue, Operator:=xlBetween, _
            Formula1:="=0", Formula2:="=10"
        Selection.FormatConditions(Selection.FormatConditions.Count).SetFirstPriority
        With Selection.FormatConditions(1).Interior
            .PatternColorIndex = xlAutomatic
            .Color = 15773696
            .TintAndShade = 0
        End With
        Selection.FormatConditions(1).StopIfTrue = False

    ElseIf C = 1 Then

        Selection.FormatConditions.Add Type:=xlCellValue, Operator:=xlGreater, _
            Formula1:="=5"
        Selection.FormatConditions(Selection.FormatConditions.Count).SetFirstPriority
        With Selection.FormatConditions(1).Interior
            .PatternColorIndex = xlAutomatic
            .Color = 180
            .TintAndShade = 0
        End With
        Selection.FormatConditions(1).StopIfTrue = False
        Selection.FormatConditions.Add Type:=xlCellValue, Operator:=xlBetween, _
            Formula1:="=0", Formula2:="=5"
        Selection.FormatConditions(Selection.FormatConditions.Count).SetFirstPriority
        With Selection.FormatConditions(1).Interior
            .PatternColorIndex = xlAutomatic
            .Color = 15773696

```



```

        .TintAndShade = 0
    End With
    Selection.FormatConditions(1).StopIfTrue = False

    ElseIf C = 2 Then

        Selection.FormatConditions.Add Type:=xlCellValue, Operator:=xlGreater, _
            Formula1:="=2"
        Selection.FormatConditions(Selection.FormatConditions.Count).SetFirstPriority
    With Selection.FormatConditions(1).Interior
        .PatternColorIndex = xlAutomatic
        .Color = 170
        .TintAndShade = 0
    End With
    Selection.FormatConditions(1).StopIfTrue = False
    Selection.FormatConditions.Add Type:=xlCellValue, Operator:=xlBetween, _
        Formula1:="=0", Formula2:="=2"
    Selection.FormatConditions(Selection.FormatConditions.Count).SetFirstPriority
    With Selection.FormatConditions(1).Interior
        .PatternColorIndex = xlAutomatic
        .Color = 15773696
        .TintAndShade = 0
    End With
    Selection.FormatConditions(1).StopIfTrue = False

    End If

    F = F + 130

    Next i
Next C

Application.ScreenUpdating = True

End Sub

```

Post Injection Site Care Stabilization Time determination

Scenario 2 (Medium Permeability)

Figure 98 Yearly Pressure Difference distribution - 1 year Post-injection

Figure 99 Yearly Pressure Difference distribution - 9 year Post-injection

Figure 100 Threshold Verification - 1 year post injection

Figure 101 Threshold Verification - 9 year post injection

Scenario 3 (Low Permeability)

Figure 102 Yearly Pressure Difference distribution - 1 year Post-injection

Figure 103 Yearly Pressure Difference distribution - 3 year Post-injection

Figure 104 Threshold Verification - 1 year post injection

Figure 105 Threshold Verification - 3 years post injection