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Systematical Analysis of the Impacts of different operations conditions and geological formation characteristics on Area of Review (AOR), Post Injection Site Care (PISC) and Risk associated with anthropogenic CO₂ Sequestration in Citronelle Dome, Alabama

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*Systematical Analysis of the Impacts of different
operations conditions and geological formation
characteristics on Area of Review (AOR), Post Injection
Site Care (PISC) and Risk associated with anthropogenic
CO₂ Sequestration in Citronelle Dome, Alabama*

By

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Benjamin M. Statler College of Engineering and Mineral Resources

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Injection Site Care

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Abstract

Systematical Analysis of the Impacts of different operations conditions and geological formation characteristics on Area of Review (AoR), Post Injection Site Care (PISC) and Risk associated with anthropogenic CO₂ Sequestration in Citronelle Dome, Alabama

Danilo Arcentales Bastidas

The emission of greenhouse gases (GHG) has been one of the biggest problem concerning the climate change during these years. The concentration of these gases has increased by a disproportionate amount over the last decade due to human activities such as, deforestation, agricultural practices and burning fuel, oil and coal while natural sources are extracted and processed. Being the main cause of global warming, a variety of technology is being applied in order to diminish GHG emissions. There are two ways to achieve this goal: burning less carbon-containing fuel or by storing CO₂ resulting from burning carbon-rich fuels. Potential storage methods include injection into underground geological formations, into deep oceans, or industrial fixation in organic carbonates.

Primary considerations in subsurface sequestration of anthropogenic carbon dioxide (CO₂) are the knowledge on gas storability of geological formation, Saturation and Pressure plume size and Post Injection Site Care (PISC) embracing risks associated with CO₂ leakage and fault reactivation. At a glance, a formation with a reasonable pore volume would appear to be a good candidate for the purpose. However, careful considerations should be taken, since not all high-porosity formations have the capability to store a huge amount of gas for a long period of time. That is the biggest concern when discussing geological CO₂ sequestration, if underground storage is suitable for permanent storage of CO₂. Based on results obtained from CO₂ saturation and pressure, the Plume Size and the Post-Injection Site Care are going to be simulated using reservoir models from Citronelle dome in Alabama. A detailed scenario analysis will be performed to generally quantify the relationships between pressure buildup and injection volume, injection rate and reservoir characteristics. A range of geologic conditions such as thickness of storage, seal thickness, geologic closure, homogeneous vs heterogeneous (permeability, porosity, compressibility variations), salinity levels and fluid-rock interactions are going to be varied in this study to appraise the storage site and quantify the parameters on a scale of importance according to their impact on the response.

Finally, to assess the uncertainty associated with our studies Latin Hypercube Sampling together with experimental design technique, i.e., Plackett-Burman design, is used. Application of Pareto charts and respond surfaces enabled us to determine the most important parameters impacting saturation and pressure plume sizes and quantifying the auto and cross correlation between different parameters impacting saturation and pressure plume size in history matched and upscaled models.

Objective

The objective of this research is to develop a systematical reservoir modeling study of CO₂ sequestration in Citronelle dome, Alabama, taking into account all possible scenarios and conditions to betake the questions of Plume Size and Post Injection Site Care. For addressing questions of how operational conditions and geologic environment impact the overall risk during and after the injection, the purpose is to use simulation capabilities to simulate the Saturation and pressure plume size and the post-injection behavior of the reservoir.

Dedication

This thesis is dedicated to all my family who have made everything in life so that I could achieve all my goals, for all the motivation, guidance and trust that I received from them at any time. A special dedication to my grandfather who passed away during this time.

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List of Abbreviations

Term	Description
AoR	Area of review
CO ₂	Carbon dioxide
CMG	Computer Modeling Group (commercial reservoir simulator)
ΔP	Difference in pressure (relative to pre-injection pressure)
$\Delta P_{\max}$	Maximum difference in pressure (relative to pre-injection pressure)
ΔP_{thr}	Threshold value used to define pressure plume
ft	Feet
kt	Thousand metric tons (i.e., 10 ⁶ kg)
m ₁	Growth rate of CO ₂ plume during early phase of injection
m ₂	Long term growth rate of CO ₂ plume
Mt	Million metric tons (i.e., 10 ⁹ kg)
NETL	National Energy Technology Laboratory
NRAP	National Risk Assessment Partnership
PISC	Post-injection site care
psi	Pounds per square inch
R _i	Effective radius of plume at the end of injection (assumes a circular plume)
R _{max}	Maximum effective radius of pressure plume (assumes a circular plume)
S _{thr}	Threshold value used to define saturation plume
yr	Year
PB	Plackett-Burman
GHG	Greenhouse Gases
LHS	Latin Hypercube Sampling

Chapter 1 – Introduction

Problem Statement

Nowadays, geological capture and storage of carbon dioxide is a technology which is in an advanced development attempting to diminish the emission of CO₂ and tame greenhouse effects. Many studies are being realized due to vague conclusions regarding the geological storage site and its capability to confine and maintain the injected CO₂ for a very long period of time. Since not all high-porosity formations have a suitable storage environment that may boost physical mechanism of gas trapping, careful considerations in operational and geological conditions should be taken.

During the past years, some suitable and appropriate candidates have been found for long-lasting storage of CO₂ such as depleted oil and gas fields, deep saline formations and ocean storage (Figure 1).

Figure 1 Suitable candidates for CO₂ storage.

Source: IEA GHG R&D Programme

Despite having these possible viable candidates for large-scale CO₂ storage, deep saline formations is the most promising storage process with a view to the future. However, it is a recently emerging field.

This involves injecting greenhouse gas emissions in supercritical phase in geological formations thoroughly studied. The deep saline aquifer will be delimited in this study by a cap rock in order to prevent flow emissions toward the surface.

Recently some studies regarding gas storage have been conducted in Citronelle dome, Alabama, where there is an imminent need to develop a model that describes how risk-related performance metrics vary as a function of the size of injection, time of injection and geologic environment. For this purpose Latin Hypercube Sampling (LHS) method is used to have a wide range of different conditions to generate a simulation matrix varying as a function of multiple parameters.

The objective of this research is to perform a systematically reservoir exemplifying studies of CO₂ sequestration in a real project such as Citronelle dome, Alabama, where all relevant scenarios and conditions to address the questions of Saturation and Pressure plume size and Post Injection Site Care (PISC) are considered. Two different cases are going to be evaluated in this analysis, one considering a History Matched Citronelle Model (5km x 5km) and one using an Upscaled Citronelle Model (10km x 10km) keeping the same formation structure than the history matched.

This CO₂ storage project is going to be guided by the U.S. Department of Energy (DOE) and conducted with other groups in National Risk Assessment Partnership (NRAP).

Citronelle Field Background

The proposed storage project is taking place into the saline Paluxy formation in the Citronelle Dome geologic structure, north of Mobile, Alabama (Figure 2), which forms an elliptical structural closure containing multiple opportunities for large capacity CO₂ sequestration and is free of faulting zones. The injector-well applied for this investigation is called D-9-7 located in the Southeast Unit (Figure 3), which will capture CO₂ from a coal-fired power generating facility called power plant Barry and it will be transported to the storage site by a twelve-mile pipeline.

Figure 2 Mobile, Alabama.

Figure 3 Location of Citronelle Field.

Source: A GIANT OPPORTUNITY FOR MULTI-ZONE CARBON STORAGE AND EOR IN THE MISSISSIPPI INTERIOR SALT BASIN OF ALABAMA – (NETL-DOE)

Field History

In Morgan and Blount counties, Alabama, in the late 1880s, and by 1902, traces of petroleum in the form of natural gas were discovered. However, Citronelle Oil Field was discovered in 1955. Within the first 10 years of discovery, 434 productive wells were drilled, which 139 were unitized for water-flood. By May 1966 all wells were unitized, and on December 31, 1973, the field had produced around 107 million bbl of oil (Eaves, 1976)⁵. Nowadays, the Citronelle Operator Unit is studying to demonstrate safe, secure CO₂ injection and storage in extensive saline reservoirs.

Geologic Description

The Paluxy formation located at depths of approximately 9,400 to 10,500 ft. (TVD) consists of 1,100 ft. of sandstone inter-bedded with siltstone and shale. This formation is separated by two extensive shale layers from the Washita Fredericksburg sand (saline reservoir) at the top and the Donovan sand (oil reservoir) at the bottom. According to previous studies made in this field, 17 sand layers were detected and correlated using petro-physical logs and core data (Moreno, 2013)¹¹. Besides the Upper Tuscaloosa Formation, this deep saline aquifer contains multiple geologic confining units that serves as a barrier enclosure to prevent leakage of CO₂ to the surface being one of several well-sealed sandstone formations at this location.

Previous studies of this viable storage candidate stand out that saline reservoirs of Upper Cretaceous age may provide almost a century of CO₂ sequestration capacity. The Massive and

Pilot sands of the lower Tuscaloosa Group, as well as several sandstone units in the upper Tuscaloosa Group and Eutaw Formation provides potentials carbon sinks (Figure 4). These sandstone units have the remarkable characteristic of having high porosity and permeability and low heterogeneity (Pashin et al, 2008-NETL)¹⁴.

System	Series	Stratigraphic Unit	Major Sub Units	Potential Reservoirs and Confining Zones
Tertiary	Pliocene		Citronelle Formation	Freshwater Aquifer
	Miocene	Undifferentiated		Freshwater Aquifer
	Oligocene		Chicasawhay Fm. Bucaturra Clay	Base of USDW
		Vicksburg Group		Local Confining Unit
	Eocene	Jackson Group		Minor Saline Reservoir
		Claiborne Group	Talahatta Fm.	Saline Reservoir
		Wilcox Group	Hatchetigbee Sand Bashi Marl Salt Mountain LS	Saline Reservoir
	Pleistocene			
		Midway Group	Porters Creek Clay	Confining Unit
		Selma Group		Confining Unit
Cretaceous	Upper	Eutaw Formation		Minor Saline Reservoir
		Tuscaloosa Group	Upper Tall. Tall.	Minor Saline Reservoir
			Middle Tall. Tall.	Confining Unit
			Lower Tall. Tall.	Saline Reservoir
			Pilot Sand Massive sand	Saline Reservoir
Cretaceous	Lower	Washita-Fredericksburg	Dantzler sand Basal Shale	Saline Reservoir Primary Confining Unit
		Paluxy Formation	'Upper' 'Middle' 'Lower'	Proposed Injection Zone
		Mooringsport Formation		Confining Unit
		Ferry Lake Anhydrite		Confining Unit
		Donovan Sand	Rodessa Fm.	Oil Reservoir
			'Upper'	Oil Reservoir
			'Middle'	Minor Saline Reservoir
			'Lower'	Oil Reservoir

Figure 4 Stratigraphic column for southwest Alabama.

Source: The SECARB Anthropogenic Test: A US Integrated CO₂ Capture, Transportation and Storage Test

In the upper Paluxy, individual sandstones with irregular bottom sand surfaces are characteristic of fluvial sand deposits that result from infilling of erosional topography by aggradation (Pashin et al., 2008)¹⁴.

Sixteen well logs in three cross sections were used to interpret the structure of the Paluxy formation (Figure 5). The sandstones where the CO₂ will be injected were selected based on the study of an SP log (Figure 6), whose response allow us to identify sand and shale layers, and accordingly confirm whether it is a saline formation and if that formation is capable to receive a large amount of gas (Moreno, 2013)¹¹.

Figure 5 Cross sections (left) and sand layers in well D-9-7 (right).

Source: The SECARB Anthropogenic Test: A US Integrated CO₂ Capture, Transportation and Storage Test

Figure 6 SP Log.

Source <http://www.spec2000.net>

After distinguishing the three cross-sections, the sand correlations were mapped aerially in order to assess their individual continuity. Areal measurements of a percentage of the thicker sandstones are approximated around 6 square miles. The thickness of these sand layers is

approximately 470 ft., where 17 sand-layers were selected for injection based on thickness and their extension. Approximately 385 ft. of the thickness are being represented by these selected layers (Figure 7)⁴.

Sand Layer	Sand Layer Top and Bottom (feet below sea-level)	Thickness (feet)
9420	9,414 – 9,421	6
9430	9,427 – 9,438	12
9460	9,444 – 9,476	32
9520	9,513 - 9,528	15
9540	9,534 - 9,549	15
9570	9,562 - 9,584	22
9620	9,596 - 9,638	42
9670	9,660 - 9,679	19
9710	9,695 - 9,717	22
9740	9,730 - 9,748	18
9800	9,775 - 9,806	30
9840	9,833 - 9,843	10
9870	9,868 - 9,874	6
9900	9,886 - 9,903	18
9940	9,929 - 9,939	10
9970	9,954 - 9,977	24
10030	10,016 - 10,025	9
10040	10,037 - 10,049	11
10060	10,055 - 10,069	15
10100	10,099 - 10,113	15
10130	10,121 - 10,134	13
10230	10,223 - 10,231	7
10310	10,302 - 10,318	16
10370	10,362 - 10,381	20
10400	10,396 - 10,412	16
10470	10,454 - 10,484	31
10500	10,491 - 10,508	18

Figure 7 Individual sandstone layers selected.

Source: *Geologic Characterization of the Lower Cretaceous Paluxy Formation for the Southeast Regional Carbon Sequestration (SECARB) Partnership Phase III Anthropogenic Test*

More well logs were provided with the purpose of developing a heterogeneous model resembling the reservoir's geology. For example, porosity maps were generated by interpreting well logs from 40 existing oilfield wells surrounding the area of review. After gathering all this information, these 40 control points were populated with geo-statistical methods by applying Archie equation in order to calculate the porosity values (Eq. 1)⁴

Equation 1 Archie equation used to calculate porosity values.

$$\phi = \left(\frac{a}{\left(\frac{Rt}{Rw} \right) * S_w^n} \right)^{1/m} \quad \text{Eq.1}$$

Where:

a = tortuosity factor, constant often taken to be 1

Rt = observed bulk resistivity

Rw = formation water resistivity = 0.045; obtained from Citronelle porosity logs

Sw = water saturation = 0.95; assuming residual gas saturation

n = saturation exponent, generally around 2

ϕ = porosity

The values for porosity were calculated by using the thickness of each layer considered (Figure 8).

⁴SECARB 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.

D-9-8			
top	bottom	ϕ (resistivity)	ϕ (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 8 Porosity calculation using induction and resistivity logs from well D-9-8.

Based on the thermal gradient of the region, the reservoir temperature of this formation was set to be 230° Fahrenheit.

Due to unavailability of experimental data, relative permeability curves were obtained from history matching of an injection pilot test in Escatawpa, Mississippi (Figure 9).

Figure 9 Relative Permeability Profile used k_r vs S_w (top), k_r vs S_g (bottom).

CO₂ sequestration Project Status

In a world dependent on fossil fuels, CCGS could be the key to controlling emissions of greenhouse effects. However, several obstacles have stalled projects to implement technology that aims to remove carbon dioxide from the air.

Many companies claim that while there is no an existing obligation, the high costs of CCGS operations won't be worth if the carbon price doesn't go over what we now find in the European emissions trading system. According to a recent report from the World Watch Institute there are only few projects operating large-scale CCGS, and this number has not increased during three years. Even many projects in Europe and North America have been discarded. Canadian power company (TransAlta) abandoned plans for a CCGS facility in Alberta plant because few financial incentives didn't justify the investment.

The International Energy Agency (IEA) believes that applying CCGS technology in fossil fuel plants and other industrial facilities could drastically reduce emissions of greenhouse gases. IEA expects to see over 3,000 plants with CCGS facilities operational by mid-century and thus achieve the objective of reducing CO₂ emissions by 20%. However, no large-scale projects now operating in power plants claims that plans to expand the industry are on hold¹⁸.

The United States has failed to pass a climate policy, and other countries have failed to reach international agreements to reduce carbon emissions by not being involved in the negotiation with the biggest country's polluter in the world (Figure 10). As a result, the system by which companies would benefit by trying to reduce emissions has never come to take shape, and it would be essential after knowing the high costs of CCGS projects.

Figure 10 Countries releasing CO₂ to the atmosphere.

Source: Global CCS Institute - The Global Status of CCS - 2014

The story is similar in Europe, which launched its own carbon market in 2005 under the international agreement known as the Kyoto Protocol. However, its first hurdle was United States' refusal to sign it, and nowadays, the largest carbon emitter, China, and other developing countries are not required to reduce their emissions. The European system has failed to stimulate CCGS projects because the permissions are not sufficient to cover the high costs.

The current problems of CCGS projects are linked to the global economic crisis, which hinders investment. Another obstacle is the failure of international governments to reach a climate agreement to replace the Kyoto Protocol. We have seen that international commitment is difficult to achieve and therefore has not signed any agreement that requires the reduction of emissions.

However, this technology is being pursued by many companies around the world hoping of getting CCGS projects more affordable and to reduce energetic penalties.

Citronelle Numerical Model

Compositional reservoir simulator (CMG-GEM) capable of simulating the multiphase, multi-component fluid flow and storage was used to perform the simulation runs. It also helps to quantify the dynamics of fluid property composition and phase behavior. The maximum bottom-hole pressure is the main operational constraint that is fixed as 6,300 psi. This will assure that the formation is not going to be fractured during the injection of CO₂.

Numerical Models

Two models are developed for this study including history matched and upscaled models.

History Matched Model

In order to discretize the structure of the Paluxy formation a Cartesian grid system is used where first - "history matched model" is generated with a total of 796,875 grid blocks, i.e., 125*125*51 grid in i, j and k directions, that covers 25 square kilometers. This model includes laterally discontinuous low-permeability units distributed vertically within the reservoir. For each layer porosity and permeability maps are generated as shown in Figure 11. Porosity and permeability in this reservoir is between 3-33% and 1-2100 mD respectively. This multi-layer sandstone reservoir was modeled using both semi-open and closed boundary conditions. Figure 11 shows porosity and permeability distributions throughout the reservoir.

Figure 11 Porosity (left) and Permeability (right) distribution.

Upscaled Model

Next, an upscaled model of the Citronelle reservoir was built based on Cartesian grids with total of 1,437,500 grid blocks, i.e., 250*250*23 grids in I, j and k directions covering an area of 100 square kilometers. In this enlarged model, the isopach, porosity and permeability maps were upscaled without destroying the structure of the formation (Figure 12). The permeability range varied between 1-1,000 mD, while the porosity kept the same range as the history matched model. Compressibility of the rock varies between 1. 01 e-05 and 1. 06 e-06 1/psi. Injection rate will vary in a range between 10 kt/yr to 5 Mt/yr while injection time will be fixed to 3 and 30 years. Post-injection time will also set to 50 years for 3 years of injection, and 300 years for 30 years of CO₂ injection period.

Figure 12 Grid top map (left) and permeability distribution (right) for Upscaled Model.

In general, a simulation plan was generated for a better understanding of the relationship between geological/operational parameters and risk metrics implied. An overall range of simulation cases is shown as follows:

1. Models used
 - a. History Matched Model
 - b. Upscaled Model
2. Injection rate
 - a. 5 Mt/year
 - b. 1 Mt/year
 - c. 250 kt/year
 - d. 50 kt/year
 - e. 10 kt/year
3. Injection length
 - a. 3 years of injection
 - b. 30 years of injection
4. Horizontal size of model domain
 - a. Large: 10 km x 10 km
 - b. Small: 5 km x 5 km
5. Dipping angle
 - a. Structural map
6. Closed and semi-open
 - a. Closed (no flow BC at all sides)
 - b. Semi-open (open at lateral sides, closed on top and bottom)
7. Porosity: 3 – 33%
8. Compressibility: 1.01×10^{-5} – 1.06×10^{-6} 1/psi
9. Anisotropy ratio (k_v/k_h): 0.01 – 1

10. Salinity: 10 – 230 g/L

The simulation responses of this study is also listed as follows:

1. Area of review
 - a. Maximum CO₂ saturation at any time during injection
 - b. Maximum pressure increase
2. PISC: long term trapping
 - a. For 3 years of injection: 50 years of post-injection
 - b. For 30 years of injection: 300 years of post-injection

In order to properly sample the multi-dimensional model variable space, Latin Hypercube Sampling method (LHS) is used to generate simulation matrix for the history matched and the upscaled model. LHS is performed based on a statistical distribution of the different model variables as follow (Figure 13):

Figure 13 Statistical distribution of the parameters involved.

First, 35 simulations were performed using history matched model with closed and semi-open boundary condition as depicted in Table 1.

Table 1 Performance metrics for H-M model.

#RUNS	Injection length (yr)	Injection rate (kt/yr)	Post injection length (yr)	Model domain size (km x km)	Reservoir thickness (m)	Permeability (mD)	Porosity	Compressibility (1/psi)	Boundary type
1	30	5000	300	5 x 5	maps	maps	maps	3 x 10 ⁻⁶	closed
2	3	250	50	5 x 5	maps	maps	maps	1 x 10 ⁻⁶	closed
3	30	5000	300	5 x 5	maps	maps	maps	9 x 10 ⁻⁶	closed
4	30	1000	50	5 x 5	maps	maps	maps	9 x 10 ⁻⁶	closed
5	3	250	300	5 x 5	maps	maps	maps	3 x 10 ⁻⁶	closed
6	30	5000	300	5 x 5	maps	maps	maps	1 x 10 ⁻⁶	closed
7	30	5000	50	5 x 5	maps	maps	maps	9 x 10 ⁻⁶	closed
8	30	5000	50	5 x 5	maps	maps	maps	3 x 10 ⁻⁶	closed
9	30	10	50	5 x 5	maps	maps	maps	1 x 10 ⁻⁶	closed
10	30	5000	50	5 x 5	maps	maps	maps	1 x 10 ⁻⁶	closed
11	3	1000	50	5 x 5	maps	maps	maps	9 x 10 ⁻⁶	closed
12	3	5000	300	5 x 5	maps	maps	maps	3 x 10 ⁻⁶	closed
13	3	250	50	5 x 5	maps	maps	maps	1 x 10 ⁻⁶	closed
14	3	250	300	5 x 5	maps	maps	maps	1 x 10 ⁻⁶	closed
15	30	5000	300	5 x 5	maps	maps	maps	1 x 10 ⁻⁶	closed
16	3	50	300	5 x 5	maps	maps	maps	9 x 10 ⁻⁶	closed
17	3	250	50	5 x 5	maps	maps	maps	3 x 10 ⁻⁶	closed
18	3	5000	300	5 x 5	maps	maps	maps	3 x 10 ⁻⁶	closed
19	3	250	50	5 x 5	maps	maps	maps	3 x 10 ⁻⁶	closed
20	3	5000	300	5 x 5	maps	maps	maps	1 x 10 ⁻⁶	closed
21	3	1000	50	5 x 5	maps	maps	maps	9 x 10 ⁻⁶	closed
22	30	1000	50	5 x 5	maps	maps	maps	1 x 10 ⁻⁶	closed
23	3	50	50	5 x 5	maps	maps	maps	1 x 10 ⁻⁶	closed
24	3	1000	300	5 x 5	maps	maps	maps	3 x 10 ⁻⁶	closed
25	30	10	50	5 x 5	maps	maps	maps	3 x 10 ⁻⁶	closed
26	30	1000	50	5 x 5	maps	maps	maps	3 x 10 ⁻⁶	closed
27	30	250	300	5 x 5	maps	maps	maps	9 x 10 ⁻⁶	closed
28	3	10	300	5 x 5	maps	maps	maps	3 x 10 ⁻⁶	closed
29	3	10	300	5 x 5	maps	maps	maps	1 x 10 ⁻⁶	closed

Next, for the upscaled more than 200 simulation runs were performed for a closed and semi-open system with 3 and 30 years of CO₂ injection, Table 2 shows sample of simulation runs performed in this study.

Table 2 Performance metrics for 30 years of injection.

#	inj length (yrs)	res_per m	res_anis	por	thick (m)	compr(1/ps i)	salinity (ppm)	cap_per m (md)	subL_per m (md)
1	30	756.72	0.3127	0.1805	50	3.4E-06	110.37	0.0008	0.0007
3	30	171.45	0.4498	0.246	50	2.93E-06	175.22	0.0032	0.0002
4	30	112.65	0.0176	0.1527	100	1.88E-06	45.429	0.0005	0.0001
5	30	235.87	0.0467	0.2739	50	4.79E-06	200.39	0.0001	0.0073
6	30	42.299	0.0653	0.2797	50	7.39E-06	185.86	0.0001	0.0007
7	30	470.57	0.126	0.0502	50	4.07E-06	70.372	0.0006	0.0003
8	30	12.735	0.0201	0.2141	100	3.74E-06	205.2	0.0002	0.0013
9	30	29.473	0.0385	0.3479	200	1.78E-06	98.361	0.0054	0.002
10	30	20.122	0.011	0.3149	100	1.14E-06	60.308	0.0002	0.0007
11	30	857.51	0.3389	0.1014	200	2.9E-06	25.958	0.0023	0.0002
13	30	379.73	0.0136	0.3352	50	2.65E-06	132.23	0.0002	0.0066
15	30	70.206	0.8805	0.2074	50	3.5E-06	210.72	0.0018	0.0009
16	30	11.023	0.0233	0.2346	200	9.67E-06	186.25	0.0001	0.0033
17	30	39.199	0.5168	0.3043	200	6.75E-06	124.1	0.0015	0.0013
18	30	520.24	0.0226	0.1458	50	1.36E-06	128.39	0.0022	0.0006
19	30	317.45	0.1638	0.1556	200	2.55E-06	153.8	0.0001	0.0047
21	30	25.746	0.2433	0.2258	100	1.43E-06	151.73	0.0035	0.0026
22	30	943.04	0.027	0.2009	100	3.35E-06	120.07	0.0002	0.0004
23	30	434.28	0.0152	0.2611	200	6.29E-06	54.065	0.0002	0.0005
24	30	361.79	0.0378	0.2329	100	5.8E-06	37.768	0.0011	0.0033
25	30	14.957	0.0523	0.1419	100	8.84E-06	135.55	0.0004	0.0008
26	30	333.24	0.1046	0.2237	100	4.2E-06	133.93	0.0003	0.0059
27	30	193.36	0.0284	0.3114	50	4.4E-06	196.4	0.0028	0.0007
28	30	15.685	0.8427	0.0546	100	1.08E-06	191.23	0.0003	0.0015
29	30	92.595	0.4662	0.0662	200	6.6E-06	226.6	0.0005	0.001
30	30	569.83	0.1906	0.27	50	2.78E-06	111.91	0.0014	0.0001
31	30	28.431	0.0404	0.3241	50	1.01E-05	22.417	0.0031	0.0035
32	30	411.52	0.0809	0.1195	200	2.01E-06	166.73	0.0003	0.0083
33	30	17.412	0.6868	0.3229	200	1.26E-06	130.96	0.0056	0.0013
35	30	217.98	0.5468	0.163	50	5.05E-06	29.172	0.0001	0.004
36	30	10.19	0.0948	0.1155	200	5.89E-06	64.315	0.0007	0.0019
37	30	15.902	0.2519	0.1183	100	1.61E-06	221.84	0.0081	0.0011
38	30	283.83	0.0107	0.1232	100	3.95E-06	214.05	0.0001	0.0005
39	30	977.22	0.5843	0.241	50	2.13E-06	216.07	0.002	0.0004
40	30	581.16	0.2842	0.0964	200	2.27E-06	183.18	0.0043	0.0036
41	30	161.78	0.0671	0.1304	50	5.63E-06	53.487	0.0014	0.0002
42	30	299.29	0.0593	0.0646	100	2.52E-06	203.15	0.0003	0.0006
43	30	619.92	0.0428	0.211	200	4.43E-06	126.13	0.0063	0.0004
45	30	536.63	0.0149	0.0613	50	3.52E-06	170.88	0.0003	0.0052
47	30	21.396	0.7496	0.3073	200	1.28E-06	208.72	0.0084	0.0001
48	30	95.902	0.1083	0.2843	50	1.19E-06	118.69	0.001	0.0003
51	30	117.28	0.0183	0.0744	100	1.44E-06	217.77	0.0003	0.0002
52	30	68.805	0.1785	0.0728	50	1.31E-06	74.115	0.0006	0.01
56	30	44.661	0.1173	0.2504	200	7.26E-06	41.714	0.0012	0.0003
57	30	89.567	0.0192	0.0812	100	3.28E-06	148.65	0.0062	0.0004
58	30	40.615	0.1479	0.2205	100	8.24E-06	94.914	0.0021	0.0002
61	30	14.216	0.0124	0.2925	100	2.23E-06	142.22	0.005	0.0001
62	30	24.331	0.2306	0.152	200	6.09E-06	145.41	0.0002	0.0021
63	30	58.051	0.7126	0.1489	100	4.87E-06	83.758	0.0008	0.0005
66	30	120.88	0.0138	0.0851	200	5.26E-06	20.494	0.0017	0.001
67	30	75.396	0.026	0.0862	200	5.46E-06	11.371	0.0052	0.0003
70	30	108.92	0.012	0.1836	50	9.15E-06	207.42	0.0005	0.0002
72	30	11.558	0.9947	0.0795	50	4.27E-06	103.12	0.0011	0.0017
74	30	83.25	0.1325	0.1911	100	1.95E-06	49.088	0.0058	0.0014
75	30	274.87	0.6178	0.2289	50	1.68E-06	34.58	0.0027	0.0004
76	30	135.12	0.7618	0.3449	200	3.07E-06	139.81	0.0004	0.0028
83	30	10.614	0.1579	0.2527	100	1.47E-06	138.86	0.0035	0.0029
85	30	55.916	0.0345	0.1071	200	3.27E-06	146.85	0.002	0.002
86	30	245.49	0.0315	0.1699	50	1.75E-06	159.83	0.0012	0.0034
90	30	684.98	0.3954	0.1886	200	1.06E-06	91.143	0.0006	0.0002
91	30	302.36	0.0832	0.266	100	2.05E-06	13.949	0.004	0.0018
93	30	148.21	0.2043	0.1044	200	1.56E-06	101.51	0.0002	0.0031
94	30	204.84	0.0484	0.3276	100	5.34E-06	72.221	0.0026	0.0024
95	30	451.9	0.3481	0.1877	50	3.18E-06	97.236	0.0008	0.0002
96	30	224.13	0.4145	0.3428	200	2.43E-06	177.23	0.0009	0.0001
97	30	641.15	0.9425	0.1746	100	2.66E-06	69.045	0.0003	0.0071
99	30	46.185	0.0322	0.3322	50	7.72E-06	56.307	0.0067	0.0015

Chapter 2 – Literature Review

CO₂ Sequestration History

Through the years the problem of climate change has been a subject of quite importance around the world. The main reason of this problem has been the amount of carbon emissions and one of the solutions that have been found by specialists is storing CO₂ in natural underground storage. Although it is known that CO₂ emissions don't have the same global warming potential as other GHG, it is considered as the main contributor due to the volume emitted to the atmosphere during fuel combustion. In 2002, the atmosphere received around 24,000 million of metrics tons of CO₂ from fuel combustion.

Around 1996, Statoil and its partners meet the goal of achieving Carbon Dioxide Capture and Storage in the Sleipner field, 250 km west of Stavanger, Norway. The natural gas produced at this field contains 9.5% of CO₂, where instead of purging to the atmosphere the separated gas, the company decided to inject it down a 3km-long well and store it in a porous and permeable reservoir rock called the Utsira Sand (Figure 14). The Utsira Sand has an estimated pore-space volume of about $6 \times 10^{11} m^3$, making it capable to store 50 years emissions from around 20 coal-fired if only 1% of this volume were utilized for CO₂ storage. Around 7 metrics tons of CO₂ per year has been stored since 1996 proving that the storage in aquifers can work in practice. Also no leakage has so far been detected in this project and they plan to continue until 2020, representing the footing for future CCGS projects¹⁷.

Figure 14 Diagram of operations in Sleipner field, Stavanger, Norway.

Source: <http://www.bgs.ac.uk/science/CO2/home.html>

Three years after the beginning of Sleipner project, PanCanadian Resources, now called EnCana Corporation, initiated the first transnational EOR project that consisted in capturing and transporting CO₂ through a 200 miles pipeline from a coal gasification facility located northwest of Beulah, North Dakota, USA, and storing the CO₂ in Weyburn field located close to Regina, Saskatchewan, Canada¹⁷ (Figure 15).

Figure 15 Diagram showing CO₂ transportation from coal gasification facility in Beulah to Weyburn field in Regina, Saskatchewan, Canada.

Source <http://www.canadiangeographic.ca/magazine/jf08/indepth/weyburn.asp>

This field contains a CO₂ 96% pure with some traces of sulfide hydrogen, nitrogen and hydrocarbons and produce oil from the carbonate reservoir called Midale, located at an approximately depth of 1,420 m. In 2000, the International Energy Agency (IEA) began a geological study of the site storage at Weyburn field in which it is concluded that the large-scale CCGS is appropriate since it has some seals that form a barrier to the gas injected avoiding this gas to migrate to surface. About 5,000 metrics tons of CO₂ are injected daily into Weyburn field to supply CO₂ storage and EOR operations.

An estimated made by the United Nations Intergovernmental Panel on Climate Changes says that the world's potential capacity of CO₂ storage is around two trillion tones, and it could be a much larger potential due to the significant studies being performed by many regions around the world.

A hundred of ongoing and proposed geologic storage projects have been depicted in the past decade, as stated by the Global CCS Institute¹⁸, and many more of them would be started or planned encouraged by the promising results obtained.

Possible domain for CO₂ Storage

Several concerns about CO₂ concentrations have specialists to investigate the possible sites where these emissions can be stored. The fact is that all this possible options of storage have many advantages and limitations that will be shown as it follows.

Depleted Oil and Gas Reservoirs

Oil reservoirs are considered sites with a significant potential to store because it is characterized by a geological seal that allows trapping hydrocarbons. The CO₂ could remained underground for several years as long as the seal does not have any damage caused by production operations. One of the most important aspects regarding these sites is that the infrastructure required for the storage such as equipment and pipelines is available. However it has a remarkable limitation on its storage capacity due to geological characteristics of any formation.

The storage on depleted gas reservoirs has been proposed but not attempted due to economic issues when considering the cost of purchasing the CO₂. This reservoirs would contain a geologic seal capable of remaining gas for a long-period of time and it would have the advantage of storing all CO₂ in the same reservoir, at the same pressure and temperature¹³ (Orr et al, 2004).

Ocean Storage

This type of storage has not been investigated in deep due to environmental problems involved that haven't been solved yet and the regulations that are handled with respect to this. Further the technology and equipment that has to be implemented may cause an economical adversity because of the distance that imply transporting CO₂ from a source plant to a deep ocean. In the past, it was thought that this would accelerate ocean acidification, however recent studies show that discharging CO₂ directly to the ocean would reduce atmospheric CO₂ concentrations and their rate of increase. Once the gas is injected it would be distributed in the oceans and it will diminish the pH change in the near-surface ocean⁷ (Herzog et al, 2001). The retention time is another limitation due to the short time of retention of CO₂ in comparison with other possible storage sites.

Unmineable Coal bed

Similar to ocean storage sites, there are just few cases applying this technology around the world, thus it is considered as the least well understood storage site. Although having little experience about this site, many tests are being planned in the U.S., Canada and Australia for useful guidance for future. These formations are located at extremely deep locations and contain considerable amounts of adsorbed methane gas. It is known that the CO₂ adsorb on the surface of coal particles at high pressure which can then be recovered as free gas¹³ (Orr et al, 2004). Flow in this site will occur primarily through the cleats, which are fractures in coal beds and it will diffuses into matrix blocks where the adsorbed CH₄ will be replaced by CO₂.

As a limitation, due to the complexity of physical mechanisms and flows, this site gives us challenges to investigate it more in a short future and determine the feasibility of CO₂ sequestration.

Deep Saline aquifers

Deep saline aquifers are considered as the most important site regarding capacity of storage. They are used to be found close to many CO₂ point sources, such as coal-burning power plants. It consists of sedimentary rocks distributed in sedimentary basins and saturated with formation brines that contain high concentrations of dissolved salts. Considering local hydrologic gradients, the time that this gas can remain within this site can be range from hundreds to thousands years.

On the other hand, most of these sites are often poorly characterized as to their structure in comparison to the other possible domains. Delineating the aquifers may be a problem, even more when structural traps may or not may exist. That being said, there should be an imperative need to have a well-understanding of faults and barriers in order to prevent vertical migration.

Trapping mechanisms

There are four main trapping mechanisms that help keeping the gas underground and they are described in detail as follows in the section below.

Structural trapping

It can be called as stratigraphic trapping and is one of the most dominant trapping mechanisms that exist. After the CO₂ is injected, the gas tends to migrate upward to surface direction due to buoyancy, but this mechanism attempts to prevent the migration by barriers created by low permeability formations and geological structures (Figure 16). Even it creates a confining unit that act as a seal for CO₂ migration, in terms of leakage, this trapping mechanism cannot be considered as the best one in comparison to others.

Figure 16 Illustration of structural trapping mechanism.

Source: http://www.CO2captureproject.org/CO2_trapping.html

Residual trapping

This phase of trapping mechanism usually begins when there is no more gas being injected. Once the supercritical CO₂ is injected, it migrates forming a plume, where at the tail of this plume some of the CO₂ will left behind as disconnected droplets in the tiny pores due to surface tension. As this happens, the injected gas becomes trapped and immobilized by the capillary pressure of water (Figure 17). This trapping mechanism can be considered as one of the most important in terms of safety because the immobile gas stays away from the cap rock¹² (Nghiem et al. 2010).

Figure 17 Illustration of CO₂ residual trapping mechanism.

Source: CO₂CRC - <http://www.CO2crc.com.au/imagelibrary3/storage.php>

Solubility trapping

This type of trapping mechanism details that the CO₂ injected dissolves in fluids in its gaseous and supercritical state. When CO₂ dissolves into the salt water or brine it becomes a denser fluid and so will sink to the bottom of the rock formation over time and help trapping the injected gas more safely (Figure 18). Studied and observed by Bennion et al. (2006), it is said that when the pressure increases the solubility of CO₂ in water increases; on the other hand, when the temperature increases, the solubility of CO₂ in water decreases¹.

Figure 18 Illustration of CO₂ dissolution.

Mineral trapping

Mineral trapping mechanism occurs when the dissolved CO₂ reacts chemically with minerals in the reservoir rock and in the reservoir brine. In order for this process to take place, minerals rich in Mg, Fe, Na and Ca, must be present. Through field studies, it has been determined that the chemical reaction depends on the composition of the reservoir rock, the pressure and temperature of the rock, and the rate of fluid flow through the rock.

Although mineral trapping is a slow process due to the thousands of years it takes, is considered as a very safe storage site because of its effectiveness to blind CO₂ to the rock.

Previous Analysis on CO₂ Storage in Deep Saline Aquifers

Because of having an extensive storage capacity and the support of several studies previously conducted, deep saline aquifer is considered as the most promising candidate for this next study. Regarding CO₂-brine systems, Bennion (et al. 2006) studied the dependence on temperature, pressure and water salinity of the interfacial tension between CO₂ fresh water and brine saline aquifers concluding that interfacial tension increases when water salinity or temperature increases, and the CO₂ solubility decreases in brine as salinity increases. When considering the pressure, they found that the interfacial tension reduces by increasing the pressure¹.

Moreno (2013) studied which out of four relative permeability profiles will represent the safest scenario in case of a leakage due to any fracture¹¹. He concluded that the safest scenario will be the one that have a relative permeability profile that can hold a high amount of immobile spread out trapped gas by mostly applying residual or solubility trapping mechanism. Besides this aspect, Moreno (2013) also analyzed the impact on pressure and saturation distribution in the first layer of the formation when the properties of the confining unit are varied.

Haghighat (et al. 2013) developed a tool called Intelligent Leakage System in order to predict the performance of Citronelle reservoir when a leakage occurs, and also to identify the location and amount of the CO₂ leakage before it reaches the surface⁶. Using two Permanent Down-hole Gauges (PDGs) in the observation well, high frequency pressure data was collected, processed

and transformed into an appropriate format by using Descriptive Statistics. This study will give plenty of time to take decisions when a leakage occurs.

Characterization of Reservoir Behavior as a function of operational and geological conditions

One of the main objectives of this project is to have an advance understanding of how pressure and saturation plume size behave in a deep saline aquifer as a function of operational and geological conditions.

Careful considerations need to be taken due to two main risks associated with storing carbon dioxide in deep saline aquifers, i.e., groundwater contamination and seismicity induced by the injection of CO₂. Aiming to characterize the reservoir behavior over time, three main metrics were identified and quantified including pressure differential plume area, CO₂ plume area and pressure differential at a location in the reservoir. These metrics will be discussed in following sections.

As it was remarked previously, a Latin Hypercube Sampling method (LHS) is applied to generate a matrix of a set of variables for reservoir characterization. The geological parameters considered for this objective are: reservoir anisotropy, salinity, porosity, reservoir permeability, thickness, compressibility and the permeability for the layer on top of the formation called as cap rock and the layer at bottom of the formation.

Latin Hypercube Sampling

Latin Hypercube Sampling (LHS) is a statistical method used to generate random and multivariate samples from a probability distribution (Iman, 1984)⁸. The probability distribution can be depicted by using a cumulative curve as it is showed in Figure 19.

Figure 19 Latin Hypercube Sampling Illustration.

<https://mathieu.fenniak.net/latin-hypercube-sampling/>

The vertical axis represents the cumulative probability that the variable may fall at or below the horizontal axis value.

Experimental design

Experimental design or Design of Experiments (DOE) is a systematic and statistical procedure for planning experiments that helps us to determine the relationship between the parameters that are impacting the process and the output of that process. The data that is obtained from this procedure can be evaluated so better conclusions can be drawn. There are several design of experiments that can be applied, however, we will apply Plackett-Burman Design for this study.

Plackett – Burman Design

Plackett-Burman design is a special category of two level fractional factorial designs, where you can gather a wide range of information even from a small amount of data. You can easily evaluate many factors to see which ones are the most important or which ones are the “heavy hitters” taking out of consideration those unimportant ones. That means, that just a few specifically chosen runs are conducted to analyze the main parameters. However, one downside of this design is its efficiency, because it won’t tell you the relationship between two factors.

Pareto charts

Pareto chart is a type of distribution diagram that contain bars and a line graph, where the parameters or variables used for the analysis can be represented on a scale of importance. It classifies the parameters using dimensionless statistics to scale the effects in terms of standard deviations. These are t-value obtained from t-test and p-value using statistical significance.

In simple words, the purpose of a Pareto chart is to highlight the most important among a set of variables (Figure 20).

Figure 20 Schematic of a Pareto chart.

http://file.scirp.org/Html/6-2200435_24928.htm

Normal charts

A Normal plot is a technique that can identify departures from normality and quantify the effect polarity of each parameter on an output. In a normal plot, the data is plotted vs. values selected to make these points look close to a straight line if the data is normally distributed.

Chapter 3 – Methodology

General Methodology

For a better clarification purposes, the methodology of this study is presented in the next figure as follows (Figure21):

Figure 21 Methodology Flowchart.

Site specific application of AoR and PISC tool

As it was mentioned, the pressure expansion and CO₂ plume size during injection and post injection is investigated. For the purpose three metrics were identified to evaluate and analyze the reservoir behavior during injection and post-injection including the CO₂ plume area (saturation plume size), the pressure differential plume area, and the pressure differential at specific locations in the reservoir. Figures 22 and 23 clearly shows the CO₂ saturation and pressure distributions at the end of 3 and 30 years of CO₂ injection in upscaled Citronelle reservoir.

Figure 22 CO₂ Saturation distribution (left) and pressure distribution (right) at the end of 3 years of injection for the history matched model.

Figure 23 CO₂ Saturation distribution (left) and pressure distribution (right) at the end of 30 years of injection for the upscaled matched model.

Different thresholds are assigned to pressure and saturation to study the CO₂ plume size and pressure area, i.e., 1, 5 and 10 bar for pressure and 0.01 and 0.2 for CO₂ saturation. For each pressure and saturation threshold the plume size and pressure area is obtained from simulation results of CMG-GEM using in-house program developed by Seth King at NETL, results are then compared and used toward study of the reservoir fluid dynamics behavior.

Main Metrics

CO₂ Saturation Plume

The current analysis tracked for this first metric is based on the evolution of the saturation plume size over time while injecting and for post-injection, which would help us to determine how site risks behaves over time. Figure 24, shows schematic that describes the behavior of saturation plume size over time. The plume size expanded very fast during the injection period (early phase), and then slows down after injection ends (long-term phase). Despite the fact that plumes didn't always have a roundabout shape, they were assumed as such, aiming to derive the radius of the plume from the calculated plume area. Growth rate of plume size expansion at early and late time can be characterized with slopes of m_1 and m_2 :

Figure 24 Time evolution of CO₂ saturation plume size.

Area of Pressure Plume

Similar to saturation plume size here to study the area of pressure plume, multiple thresholds were selected. As it is detailed in the schematic (Figure 25a), the pressure plume size shows a different profile in comparison with CO₂ saturation plume; the pressure plume size starts increasing at the beginning of the injection until it reaches its highest point usually sometime after injection ends. Then, the plume size starts decreasing with different rate depending on the boundary condition applied (closed or semi-open). Figure 25b shows the behavior of pressure plume in case of closed boundary condition. The effective radius of the pressure plume was obtained by assuming a circular shape of the plume area.

Figure 25 a) Schematic of usual pressure plume behavior b) Time evolution of pressure plume size for a specific threshold for a closed boundary condition.

Pressure at a Specific Location in the Reservoir

Finally, the pressure plume size was analyzed at various distances from the injection point including 1, 2 and 3 km. Figure 26, shows the schematic of pressure dynamics at a specific location away from the injection point. Pressure profile shows rapid increase during injection and reaches its maximum pressure at the end of injection period. After injection stops pressure starts decaying. The rate of pressure decay is directly related to the specific boundary condition applied. The maximum pressure at specific location can be reached at the end of injection or sometime after injection stops depending on the distance from the injection point and also reservoir heterogeneity. It is important to note that the pressure differential was calculated assuming reservoir is in hydrostatic equilibrium before injection starts.

Figure 26 Time evolution of pressure at a particular point in reservoir.

An analysis on how pressure is changing during three years of injection and fifty years of post-injection is performed investigating the dynamics of pressure buildups at 1, 2 and 3 kilometers away from the injection point. Comparing all different cases where the injection rate is close to 50 kt/yr we can clearly see that the pressure increases rapidly at different locations and suddenly declines after shutting in the injector well. However, the pressure stabilization is reached almost 20 years after the injection stops (Figure 27).

Figure 27 Pressure buildup vs time at 1, 2 and 3 km away from injection point for a closed system.

Chapter 4 – Detailed Analysis of Reservoir Behavior

Systematic approach has been implemented to perform the sensitivity analysis for both reservoir models, i.e, history matched and upscaled, to find the most important parameters impacting the saturation and pressure plume size. This includes determining the parameters of interests, performing a screening analysis to find the “heavy hitters” using Plackett-Burman (PB) analysis, performing comprehensive analysis to understand the non-linear behavior of important parameters and finally generating the response surfaces. Here to perform the design of experiments, Minitab software has been used.

Analysis of Results

Conventional approach to analysis the simulation results is to plot the pressure and saturation plume size versus injection rate. Here expectation is to see larger plume size by increasing the injection rate; however, since the problem involves multi-variables with special and temporal auto and cross correlations the simulation response might not be intuitive. Where higher injection rate might lead to smaller plume size simply due to higher thickness and porosity and lower permeability values assigned for that specific realization of simulation runs in compare to the realization of simulation runs where low injection rate is associated with higher permeability, lower porosity and thickness. Therefore, there is critical need to obtain a dimensionless number represents the overall impact of different variables and their correlations to simulation response.

For the purpose a dimensionless number “ Ψ ” is defined including the most important parameters obtained from PB design analysis (will be discussed in next sub-section). Figure 28 shows the simulation response vs dimensionless number for two cases of closed and semi-open boundary conditions. There is a clear linear trend observed when saturation plume size is plotted against the dimensionless number. A similar linear trend between pressure plume size and dimensionless number is also obtained and illustrated in Figure 29. In the case of pressure plume size unlike saturation plume size different critical values obtained for different pressure thresholds above which the pressure plume reaches the boundary of the reservoir.

a)

Figure 28 a) Saturation Plume Size vs Dimensionless number using Upscaled model for closed system; b) Saturation Plume Size vs Dimensionless number using Upscaled model for semi-open system.

b)

Figure 29 Pressure Plume Size vs Dimensionless number using Upscaled model for closed system.

Following is the definition of dimensionless number Ψ :

$$\Psi = \frac{q \times t}{\phi \times h \times \log(k)}$$

Where:

q = injection rate

t = injection length

h = thickness

k = permeability

ϕ = porosity

Sensitivity analysis have been performed to see the impacts of different parameters on dimensionless number Ψ as shown in Figure 30:

Figure 30 Linear relationship between dimensionless number and risk metrics.

Plackett-Burman Design

Systematic approach has been used for both reservoir models to find the most important parameters affecting the dynamics of CO₂ saturation and pressure plume size. This includes determining the parameters of interests, performing a screening analysis to find the “heavy hitters” using Plackett-Burman analysis of history matched model, performing a comprehensive analysis to understand the non-linear behavior of important parameters using both history-matched and upscaled models.

Plackett-Burman (PB) design used here is the most compact two-level design that requires (n+1) runs where n is the number of factors or variables. In PB design all the columns in Table 3 and 4 are orthogonal to each other and can analyze all the main effects. Table 3 shows the 7 parameters selected and their level of variation, however, in order to perform the significance test instead of 8 runs we use a design matrix with 12 runs for both models. Table 3 and 4 show the terminology of two-level design matrix for history matched and upscaled models where the highest value for the factors are represented with (+1), and the low values with (-1). In this study saturation and pressure plume size have been used as simulation response.

Table 3 Parameter setting of PB design.

Parameter	-1	+1	Unit
A: Permeability	10.19	977.224	md
B: <u>kv/kh</u>	0.010654	0.994728	NA
C: Porosity	0.05017	0.34789	%
D: Thickness	50	200	m
E: Compressibility	1.06E-06	1.01E-05	1/psi
F: Salinity	11.37096	228.1210	Ppm
G: <u>Inj rate</u>	20	4274	<u>Kt/yr</u>

Table 4 PB design for 7 variables, -1=low value, +1=high value, 12 realizations.

	Factor 1	Factor 2	Factor 3	Factor 4	Factor 5	Factor 6	Factor 7
RUN	A: Permeability	B: <u>kv/kh</u>	C: Porosity	D: Thickness	E: Compressibility	F: Salinity	G: <u>Inj rate</u>
	md	NA	%	m	1/psi	ppm	<u>Kt/yr</u>
1	-1	1	1	-1	1	-1	-1
2	-1	-1	1	1	1	-1	1
3	-1	1	1	1	-1	1	1
4	1	-1	-1	-1	1	1	1
5	1	1	-1	1	-1	-1	-1
6	-1	-1	-1	-1	-1	-1	-1
7	1	1	1	-1	1	1	-1
8	1	-1	1	-1	-1	-1	1
9	-1	1	-1	-1	-1	1	1
10	1	1	-1	1	1	-1	1
11	1	-1	1	1	-1	1	-1
12	-1	-1	-1	1	1	1	-1

A student version of software called Minitab (version 17) is used to develop this qualitative assessment analysis and to perform the distribution diagrams and plots.

Pareto and Normal Plot charts

In this study, Pareto chart, normal plot of the standardized effects and 3D surface responses are used for the analysis. The Pareto chart displays the relative size of the effects and present the contribution of the simulation response, i.e., pressure and saturation plume size. In this design Pareto chart analyzes the uncertainty into three different classes. The variable has certainly significant impact in simulation response if it falls above a line defined based on confidence intervals and has no significant impact on simulation results if it falls below the line. From the following Pareto charts, figures 31-33, we can tell that reservoir permeability and injection rate have significant influence on the pressure and saturation plume size for all the thresholds and boundary conditions.

Following, we presented more detailed studies on each scenario. Figure 31 shows that the main parameters impacting the size of a CO₂ saturation plume are reservoir permeability, injection

rate, porosity and compressibility; these are showing a higher impact on the simulation response. However, salinity, reservoir anisotropy and thickness show a very low impact.

In the normal probability plot of the effects, points that do not fall near the line usually indicate important effects. Important effects are larger and generally further from the fitted line than unimportant effects. Unimportant effects tend to be smaller and centered on zero. Also, normal plot can tell the effect polarity of each variable. For example in Figure 31, the standard effect of reservoir permeability is positive, that means in higher permeability reservoir, saturation plume expands faster. Normal plots also show that reservoir permeability, injection rate and compressibility have positive correlation with saturation size whereas porosity has negative correlation.

Figure 31 Pareto and Normal plot charts of Upscaled model using saturation plume size for closed system.

Similar analysis was performed using pressure plume size as a simulation response, with 1, 5 and 10 bar pressure thresholds. Figure 32 summarizes the Pareto and normal plot analysis for pressure plume size with different pressure thresholds.

Figure 32 Pareto and Normal plot charts of Upscaled model using pressure plume size for closed system.

As discussed earlier Plackett-Burman design is a two-level design. In order to break down the aliasing in two-level design a standard method is to use fold-over technique. Typically the fold-over is performed by simply changing the signs of all columns in design of experiment table 4. Full fold-over significantly increases the resolution of the results, more discussions can be found in Hunter 2005³. Figure 33 shows the Pareto chart obtained from analysis of fully fold-over PB design that is in agreement with our previous observations and shows robustness of the calculations.

Figure 33 Pareto charts of Upscaled model using pressure plume size for 1 and 5 bar of thresholds.

Boundary condition effect

Different boundary conditions can impact the rate and magnitude of pressure and saturation change in the reservoir. Here, to investigate the impact of using different boundary conditions on simulation response and to study the possibility of having significant impact of boundary condition on uncertainty analysis, we introduced the closed and semi-open boundary condition as new variables in our study for history matched model and compared the simulation responses and uncertainty analysis of these two cases.

A closed system with a no-flow boundary is defined by setting an impermeable barrier as a cap rock at the north boundary and also setting a low-perm layer at the top of the south boundary (Figure 34).

Figure 34 3D view of a closed system.

For the semi-open system, we will perform the same north and south impermeable boundaries, however, a flow boundary condition will be applied by setting an aquifer surrounding the storage site (Figure 35). More detailed information and results will be discussed in the following subsections.

Figure 35 3D view of a semi-open system.

Table 5 shows the Plackett-Burman design used to compare these two cases.

Table 5 Performance metrics using History Matched Model for boundary condition study.

#RUNS	Injection time (yr)	Injection rate (kt/yr)	Post injection length (yr)	Compressibility (1/psi)	Boundary type	salinity	kv/kh
PB-HM RUNS							
1	3	10	30	0.0000101	semiopen	11.37	0.994728
2	3	25	30	0.0000101	semiopen	11.37	0.994728
3	3	10	30	0.0000101	semiopen	228.121	0.010654
4	3	10	30	0.00000106	semiopen	228.121	0.994728
5	3	25	30	0.0000101	closed	228.121	0.010654
6	3	25	30	0.00000106	semiopen	228.121	0.010654
7	3	10	30	0.0000101	closed	11.37	0.010654
8	3	10	30	0.00000106	closed	11.37	0.010654
9	3	10	30	0.00000106	closed	228.121	0.994728
10	3	25	30	0.0000101	closed	228.121	0.994728
11	3	25	30	0.00000106	closed	11.37	0.994728
12	3	25	30	0.00000106	semiopen	11.37	0.010654

Similar to previous cases discussed earlier, saturation and pressure plume sizes were used as simulation response for both semi-open and closed systems (Figure 36-37). Figure 38 shows the Pareto and normal plots describing the importance and correlation of each parameter impacting saturation and pressure plume size. Injection rate and boundary condition show significant impact on plume size, furthermore, injection rate shows positive correlation with plume size and closed boundary shows negative correlation. That implies applying the barrier to plume extension and retardation effect on saturation and pressure dissipation in the reservoir.

Figure 36 Saturation plume size distribution during injection for a semi-open system using History Matched model.

Figure 37 Pressure plume size distribution during injection for a semi-open system using History Matched model.

Figure 38 Pareto and Normal plot charts of History Matched model using pressure plume size for closed system.

Response Surface

Response surfaces are usually used to explore the relationships between significant parameters obtained through application of Pareto charts and simulation response, i.e., saturation and pressure plume size in this study. Surface responses can also be used as a proxy to the system or as an optimization strategy. In reservoir simulation studies, developing a relationship between porosity, permeability and reservoir response usually attracts huge interest. Figure 39 shows the surface responses developed to find the regression between porosity, permeability and pressure plume size with different pressure thresholds using upscaled model with closed boundary condition. For more detailed studies few exploratory runs need to be performed to validate the accuracy of the surface responses and regressions generated between porosity, permeability and pressure plume size.

Figure 39 Surface plots of AOR vs porosity and permeability for different pressure and saturation thresholds for upscaled model.

Commercial and Non Commercial Software employed

The software described as follows were used for different in this study:

- Computer Modeling Group (CMG), General Equation of State Model (GEM), Commercial Numerical Simulator Software.
- Minitab 17, free Statistical Software.
- Microsoft Excel 2013.
- Python ver2.7, Programming language.

Chapter 5 – Conclusions

Concluding Remarks

CO₂ storage in deep saline aquifers requires an advanced understanding of reservoir rock and fluid properties and interactions and also impact of different geological and operational conditions on fluid dynamics during and after injection of anthropogenic carbon dioxide (CO₂) in the reservoir. This can be summarized in two underlying questions:

- How does a reservoir's performance change as a function of injection volumes and rates of CO₂?
- How does a reservoir respond as a function of time when CO₂ injection stops?

To answer these questions series of simulation runs performed on wide range of geological and operational conditions following statistical approach that ensures the correct sampling of multi-dimensional space of model variables. The key finding for this study can be summarized as follows:

- The CO₂ plume profile increases during the injection period and it stabilizes in a slower growth rate after injection. The growth rate after injection stops depends on multiple geological and operational variables and their correlations.
- The pressure plume profile depicts rapid increase during injection until it reaches its maximum value before it begins to decrease after injection stops.
- The pressure plume profile of the specific points near the injection well shows a fast increase during the injection and a rapid decrease after injection stop.
- The plume degradation after injection stops could last few years depending on the amount of CO₂ injected, porosity, permeability and boundary condition of the formation.
- Injection rate, reservoir permeability and boundary condition show higher impact on saturation and pressure plume size.

Qualitative assessment of the geological and operational conditions on CO₂ plume size and pressure presented based on extensive simulations runs and uncertainty analysis. The outcome of this study is also compared and found to be in good agreement with similar studies performed within the National Risk Assessment Partnership (NRAP) project. Table 6 shows details of our qualitative assessment.

Qualitative Assessment

Table 6 Qualitative Assessment for parameters used.

Parameter	Impact on Pressure	Impact on Saturation	Observations
Porosity	Medium	High	For closed systems, the impact of porosity can be higher, depending on pressure threshold and injection rate.
Permeability (k)	High	High	For closed systems, the impact of permeability can be lower, depending on pressure threshold and injection rate.
Compressibility	Low-Medium	Low	Compressibility will have a higher impact on pressure for a closed system where the pore volume is within an order of magnitude of the injected volume.
Thickness	Low-Medium	Low-Medium	There is some variability between reservoirs on whether thickness impacts pressure or saturation plume size more.
$k_h:k_v$	Low	Low-Medium	
Salinity	Low	Low	
Caprock Permeability	Low-Medium	Low	Caprock permeability has more impact when the mass injected is not too high and caprock permeability is low.
Boundary Conditions	Medium-High	Low	Boundary conditions are important for higher injection volumes or smaller reservoirs.

Recommendations and Future Work

After a comprehensive and systematical analysis performed during this project, few recommendations for future studies can be detailed as follows:

- Conduct a detailed study of fault reactivation and induced seismicity associated with CO₂ sequestration due to the contamination and hydrocarbon migration upward to ground water resources.
- A better understanding of in-situ stress changes during CO₂ injection period that will help us to optimize CO₂ sequestration design while assessing the potential seismicity risk associated with these activities.
- Perform a deep analysis of reservoir characterization in deep saline aquifers by doing an exhaustive study with different boundary conditions.
- A more detailed study for post injection behavior.

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Appendix

Appendix A: CMG Inputs: A1: History Matched Model

Grid Top (ft) 2012-01-01

Figure 40 (A1.1) History Matched Citronelle Grid Top map

Grid Thickness (ft) 2012-01-01

Figure 41 (A1. 2) History Matched Citronelle Grid Thickness map.

Porosity 2012-01-01

Figure 42 (A1. 3) History Matched Citronelle Porosity map.

A2: Upscaled Model

Grid Top (ft) 2012-01-01

Figure 43 (A2. 1) Upscaled Citronelle Grid Top map.

Appendix B: CMG Outputs: Pressure and Saturation Plume Sizes

B1. History Matched Model

Figure 44 (B1. 1) Gas Saturation Plume Size History Matched Model

Figure 45 (B1. 2) Pressure Plume Size History Matched Model

Figure 46 (B1. 3) Gas Saturation Plume Size History Matched Model

Figure 47 (B1. 4) Pressure Plume Size History Matched Model

B2. Upscaled Model

Figure 48 (B2. 1) Gas Saturation Plume Size Upscaled Model

Figure 49 (B2. 2) Pressure Plume Size Upscaled Model

Figure 50 (B2. 3) Gas Saturation Plume Size Upscaled Model

Figure 51 (B2. 4) Pressure Plume Size Upscaled Model

Figure 52 (B2. 5) Gas Saturation in 3D view-Upscaled Model