POLITECNICO DI TORINO

Department of Environment, Land and Infrastructure Engineering

Master of Science in Petroleum & Mining Engineering

UNDERGROUND STORAGE OF HYDROGEN AND CARBON DIOXIDE

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Abstract

A huge part of the world economy is associated with petroleum and coal. From decades we are depending on fossil fuels in many ways such as chemical products, pharmaceuticals, fertilizers, solvents and plastics. But the application of organic fuel in fulfilling energy demands leads to global pollution in environment, depletion of ozone layer and increase in carbon dioxide. According to Global CCS Institute, the amount of CO_2 has gone from 280 ppm to over 400 ppm over the past 300 years. So in this aspect there is a need of new energy source which is more sustainable and to reduce global warming CO_2 can be stored underground. Therefore in this project firstly there will be a discussion about hydrogen as an energy carrier and its future in industry. Secondly I will discuss about the carbon storage in aquifers.

Deep saline storage aquifers are the most enchanting and captivating storage sites for research works because of their plentiful occurrence in the regions with high awareness towards sustainable environment such as USA, UK and Europe. Different aspects of CO_2 injection and storage such as geochemical reactions with rock minerals, geo-mechanical effects, hydrodynamic behavior of CO_2-brine system and pre and post injection processes have been discussed in previous literature and experimentation. Yet a substantial amount of work is required to be done on the development of a preliminary process for nominating a suitable aquifer for CCS operation. Site selection and characterization is very essential part of CCS operation so in this project an up to date and extensive screening criterion for CO_2 storage in deep aquifers has been presented on the basis of strong literature review.

A newly developed screening criterion has covered most of the factors which should be considered before selecting a particular aquifer for carbon dioxide storage operation. A lot of work has been done on CO_2 sequestration in aquifers, but most of the previous researchers used homogenous aquifer models to perform experimental and simulation work. So there is a knowledge gap about the impact of the aquifer permeability on the storage capacity. For this purpose Lorenz coefficient was used to express the aquifer heterogeneity degree.

The purpose of this work is to calculate the different degrees of heterogeneity through the Lorenz coefficient and investigate its influence on CO_2 storage capacity and injectivity. To this end permeability heterogeneity is simulated in aquifer models starting from homogenous system to highly heterogeneous system. Lorenz coefficients vary from 0.1 to 0.9 according to the level of heterogeneity present in the aquifer. Three different aquifer models with porosity values of 0.1, 0.2 and 0.3 are used for this study. Modeling of each aquifer model is performed for three different levels of heterogeneities and in this way, simulation of nine cases is carried out for three different aquifer models with different porosity values. CO2STORE module of Eclipse300 Simulator is used for the purpose of this study. Sensitivity analyses are performed to conclude the effect of permeability heterogeneity on CO_2 storage capacity for three different cases of porosities.

DEDICATION

TO ALMIGHTY GOD

TO MY WONDERFUL PARENTS

Zain Rasheed

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I would first like to express my deepest gratitude to God Almighty, without whom none of this would have been possible.

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1 Overview

1.1 Aim of the study

The aim of this research is to enlighten the importance of hydrogen gas as an alternate to fossil fuels and to get the understanding of CO_2 storage in aquifers. This theme would be accomplished by obtaining following objectives:

- To understand the significant aspects of underground storage of carbon dioxide and hydrogen gas.
- To govern critical parameters and update screening criteria for selection of an aquifer for CO_2 storage based on literature survey.
- To simulate proposed parameters in the selection of aquifer for CO_2 storage by using Eclipse to confirm the selection.
- To calculate the different levels of heterogeneity through Lorenz coefficient and investigate the influence of it on CO_2 storage capacity and injectivity.

1.2 Anticipated Outcomes / Results

- State of the art of UHS and CCS operations will provide the significant aspects of these processes and on the basis of literature review evaluate the research gap present.
- A screening criterion would be available in order to choose the best aquifer for safe and large scale storage of CO_2.
- Calculation of heterogeneity was a problem before but the use of Lorenz coefficient in this aspect will provide an innovation to this field.
- Sensitivity Analysis of different heterogeneities revealed the most suitable condition for CO_2 sequestration in deep saline aquifers.
- Dynamic simulation study with Eclipse software has shown the real time variations after the injection of carbon dioxide. It will evaluate the fate of CO_2 plume, its migration and trapping abilities.

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2 Underground Hydrogen Storage (UHS)

2.1 State of art

Petroleum is integral to many industries, and is of vital importance to many nations as the foundation of their industries. The percentage of world energy supply from fossils according to IEA 2011 is petroleum (36.3%), coal (20.2%), and natural gas (24.5%). But the application of organic fuel in fulfilling energy demands leads to global pollution in environment, depletion of ozone layer and oxygen, and increase in greenhouse gases.

According to World Energy Outlook (WEO), without a transition in the global energy system, the Earth will get warm more than 2°C. It also states that, even after the implementations on new carbon-constraining policies announced by governments, CO_2 will rise twenty percent by 2040, which can lead to 3.6°C rise in average temperature of the globe.

IEA Executive Director Maria van der Hoeven and Chief Economist Fatih Birol stated that world must give transparent direction at the Paris climate change negotiations in 2015 in order to spur an increase in low-carbon investment four-times the current level in the report on November 2014. Otherwise, as indicated in the central scenario, the entire global carbon dioxide (CO2) budget for 2100 needed to keep warming under 2°C is used up by 2040.

For this reason, it mandatory to limit the immediate production and consumption of these fuels which leads to social and environmental impacts associated with. Reduction of air pollution, water use and contamination, and local disruption should be done to avoid global warming. In this particular aspect there is a need to find a sustainable energy source that is free of air pollution and which is not known to be toxic to living organisms. Moreover a huge amount of energy is needed to overcome the energy demands that are being compensated by fossil fuels.

Hydrogen is being substantiated as an alternate carbon free energy source and is being tested as a fuel cell for vehicles, as an enabler for carbon capture and sequestration technology for power generation and refineries. The dream of hydrogen being the main industry driving energy source is delayed due to both technical and economic issues such as high cost performance challenges of fuel cells and problems related to storage, production and transportation.

2.2 Hydrogen as Energy

Hydrogen is considered as one of the simplest elements on Earth. It is one of the most plentiful elements present on Earth constituting about three quarters of the universe by mass.

Hydrogen is an inexhaustible emerging energy to very much extent, and will be the foundation of the overall world economy in the recent years of 21st century due to its utilization in various industries, such as electricity, internal combustion engines and turbines. Renewable energy includes many types, e.g., solar energy, wind power, geothermal energy and so on. In case there is such huge amount of energy, it will be a waste if we do not make use of them. For this, people have tried to convert the available free energy into hydrogen and then store it in many ways for a certain period and retrieve it.

There are many types of renewable energy, such as, solar energy, wind power, geothermal energy etc., and these sources have the potential to generate enough amount of energy that can fulfill the ever increasing global energy demand. Therefore a considerable amount of research is being conducted to exploit these sources of energy to its fullest and converting the available free energy to hydrogen and then store it so that it can be retrieved later.

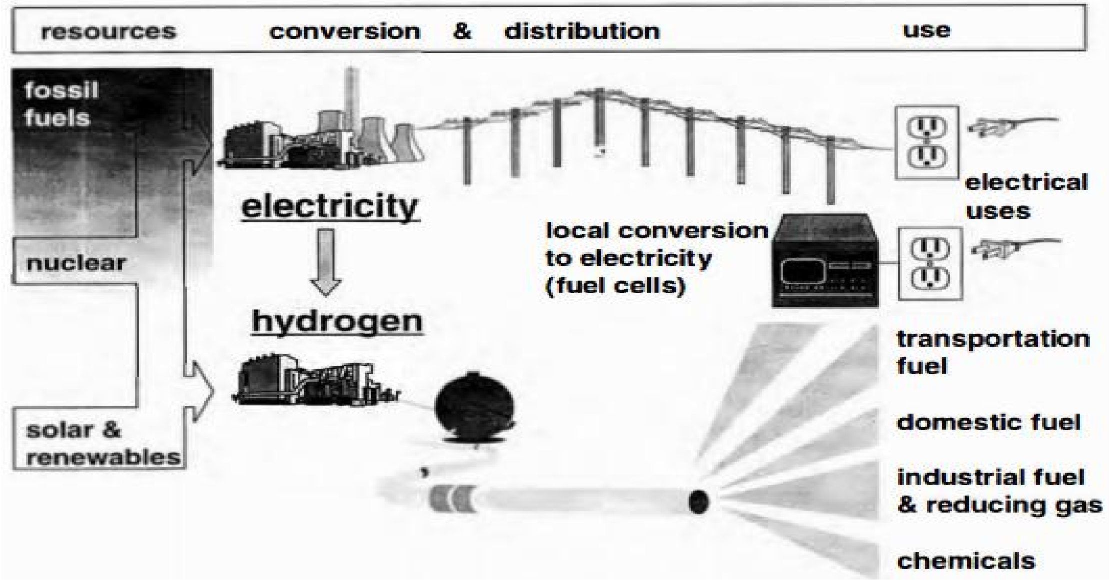

Figure 1 Hydrogen Energy System (Sherif, Barbir et al. 2003)

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2.3 Applications of Hydrogen

2.3.1 Rocket fuel

Main and the primary use of hydrogen are as a rocket fuel. For the very first time in the mid of 20th century The National Aeronautics and Space Administration (NASA) used liquid hydrogen as a rocket fuel. Hydrogen fuel cells to power the electrical systems on spacecraft were also invented by scientists of NASA.

2.3.2 Hydrogen fuel cells

In a fuel cell hydrogen and oxygen react with each other and generate electricity. The byproducts of the reaction are water and heat which can also be brought to use. Fuel cells are alternate to batteries. The output of both fuel and batteries is same but the charge of fuel cells can be never ending if the supply of the hydrogen is continuous. Pure hydrogen is necessary for the more reliable operation of fuel cells. Also fossil fuels like methane, methanol, or even oil can be transformed to generate the hydrogen for fuel cells. Even methanol can be used directly without any reform in special types of fuel cells.

Fuel cells have a good range of application in the powering of portable electronic appliances. Fuel cells can be used to provide electrical power to cell phone, computers and laptops on a small scale. And on a larger scale they also have a capacity to power the buildings and can be very handy in the areas where we don’t have electric grid systems.

2.3.3 Hydrogen as a fuel for Vehicles

Hydrogen is an alternate to conventional fuels because it doesn’t produce any pollution and it is also efficient than batteries due to high capability of fuel cells. Hydrogen fuel cell vehicles have leisure and environmental benefits of driving on electricity as compared to conventional cars which use gasoline and other fossil fuels.

There is a difference between the refueling process of both gasoline and hydrogen. At hydrogen refueling stations there is pressurized hydrogen gas filled in the car. And in less than 10 minutes latest models of electric H_2 cars can be refilled. Some leases may cover the cost of refueling entirely. The range of these cars is almost similar to the conventional ones but is a lot better than vehicles that depend on battery cells.

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Electric vehicles with hydrogen fuel cells are in operation in some countries. In California (USA) there are many hydrogen vehicles and they have almost sixty hydrogen refueling stations. Many companies around the globe played their role and invested a lot of money in shifting world's attention towards the use of hydrogen cars due to its environmental friendly emissions.

2.4 Production of Hydrogen

The major processes specific for the manufacturing of H_2 are partial oxidation, electrolysis of water, steam reforming, and coal gasification (Sherif, Barbir et al. 2003):

Partial oxidation $CH_{1.8} + 0.98\ H_2O + 0.52\ O_2 \rightarrow CO_2 + 1.88\ H_2$

Water electrolysis $2H_2 \rightarrow 2H_2 + O_2$

Steam reforming $CH_4 + 2H_2O \rightarrow CO_2 + 4H_2$

Coal gasification $CH_{0.8} + 0.6\ H_2O + 0.7\ O_2 \rightarrow CO_2 + H_2$

The feasibility of the process for the manufacture of hydrogen can be decided on the basis of number of factors for all these methods and according to availability of resources one can choose the best suitable method.

The main processes of hydrogen production on a larger scale are (Potter 2011)

- Thermal
- Electrochemical
- Biological
- Other

2.4.1 Thermic Hydrogen Production

- Steam Methane Reforming (SMR)
- Coal Gasification
- Partial oxidization of Fossil fuels
- Multistep Thermochemical Water Splitting

2.4.2 Electrochemical Hydrogen Production

- Aqueous Alkaline Electrolysis
- Concentrated Solar Energy

2.4.3 Biological Hydrogen Production

- Biomass Gasification
- Biomass Pyrolysis
- Algae Based Systems

2.4.4 Other Hydrogen Production Systems

- Refinement of the by products

2.5 Storage of Hydrogen:

In accordance with all the benefits and applications of hydrogen mentioned above there is a need to store hydrogen for future.

There are many ways to store hydrogen and the best method depends on the time period and utilization of stored hydrogen.

The most discussed methods of hydrogen storage are the following:

1. Underground Hydrogen Storage (UHS) / Geological storage of hydrogen
2. Above Ground Pressurized Gas Storage Systems
3. Vehicular Pressurized Hydrogen Tanks
4. Metal Hydride Storage
5. Novel Hydrogen Storage Methods

Hydrogen can take place of fossil fuels to some extent due to its wide scope and applications in many industries. Our interest is to store hydrogen on a large scale so that it can fulfill the energy demands in the future without any fluctuations. And UHS is the only method by which we can store hydrogen on a very large scale. Extraction of underground hydrogen is also efficient due to very mature industry of UGS.

Besides geologic storage there are many other ways to store hydrogen including standard canister made of steel or composites or Liquefied confinement of H_2, but the methods are more expensive and usually for a particular reason and doesn't serve a more variety of reasons of storage.

Therefore a more inclusive approach is taken and a number of high density storage options are linked with inclusion of hydrogen in metal lattices (as hydrides) or into more complex chemical structures. Even though the method is promising but still the schemes considered have various issues including the sensible rates of getting the hydrogen into and out of the confining structure.

Due to these reasons, methods that are considered as alternative to geologic storage are often considered as other ways of transforming electric power and regaining it without using hydrogen, and hence why the methods are at disadvantage.

The issue is about the long term use of stored hydrogen because at present hydrogen is not well adopted as a fuel for vehicles. In future, if the applications of hydrogen just remain limited to the electricity production or fuel cells and batteries then canisters or compressed air stores would be adequate for storage. Geological storage is much more reasonable in the era when cars and other transportation vehicles use hydrogen as a fuel instead of gasoline or diesel.

At the end, we will discuss in detail the subsurface storage of hydrogen its types and technical aspects related to all the ways of underground hydrogen storage.

2.6 Ways and Mechanisms

On the basis of geological characteristics one can decide which way of UHS is suitable. However, produced formations of petroleum reserves have highest usage of seventy five percent, aquifers have usage of fourteen percent, salt caverns has nine percent and pits or mines has less than one percent usage for storage purposes. (Kruck, Crotogino et al. 2013).

2.6.1 Depleted Oil and Gas Reservoirs for UHS

Depleted oil and gas reservoirs for UHS have got limited attention in the past as compared to salt caverns but depleted reservoirs are very interesting and have a potential to store larger amount of hydrogen (Ganzer, Reitenbach et al. 2013). Hydrogen can be stored in existing production wells and new wells can also be drilled to inject or extract more gas to cover a reservoir of larger extent.

2.6.1.1 Advantages

The major benefit of depleted fields is the well-known geological structure and petrophysical properties from the time of exploration till the production of hydrocarbons. In case of gas fields, the remaining or residual gas can be used as a cushion gas. Subsurface and surface facilities that were installed for exploration and production of hydrocarbons can be reused for storage operations. Hence, conversion can be fulfilled with much less cost and effort if the above mentioned conditions are achievable.

2.6.1.2 Limitations

The majority of the converted fields are gas fields because of the treatment and production issues in case of depleted oil fields. The mixture of oil, residual gas and water cause complex fluid mechanics. Additional wells may also be drilled during conversion because the production scheme of a gas field during exploitation is different from a cyclic withdrawal and injection strategy of underground gas storage.

2.6.1.3 Pilot tests/Pre-requisites

Pilot tests must be performed to validate the feasibility and efficiency of UHS in a particular reservoir. Some of the properties are mentioned below:

1. Good reservoir thickness for expected volume of gas to be stored.
2. To achieve desired injection and withdrawal rates porosity and permeability should be in good range.
3. To check the reactivity of hydrogen gas with the fluids and particles within the rock.
4. Presence of proper sealing to avoid any leakage (cap-rock integrity).
5. Occurrence of biological processes in the presence of bacteria.
6. Fluid transport properties during the storage of H_2.

2.6.1.4 Required Research and Development

There is a need to perform research on several aspects for the efficient geological storage of hydrogen in depleted oil and gas fields (Stolten and Emonts 2012).

- Modeling of the propagation of hydrogen gas in the reservoir rock and its mixing with the residual gas has to be performed.
- Examination of hydrogen reactivity whether the hydrogen could react chemically with the rocks into which it is injected or the overlying seal rock, which could prevent the gas from being recovered and used.
- Migration of hydrogen through water-filled porous media, and how much of the injected hydrogen can actually be recovered from the rock.
- Biotic and abiotic reactions caused by the injection of hydrogen gas in the porous media.
- Evaluation of best injection and storage scenario.

2.6.2 UHS in Aquifers

UHS in aquifers involves first displacement of pore water by injecting hydrogen, and then it can be stored in subsurface under low permeability barrier or tarp. At present, developed countries are storing hydrogen storage in water reservoirs due to the easiness in operations and simultaneous drilling and completion activities. On contrary, there are some cons, i.e. intricacy of H_2 interactions with rock and fluids and risks of contamination of drinking water.

2.6.3 UHS in Salt Caverns

For UHS in salt caverns firstly there is a need to generate a space in salt formation so that hydrogen can be stored. For this purpose, fresh water in injected and then produced with dissolved amount of salt (Tu, 2005; Wu, 2010). A salt cavern is made one hundred and fifty meters deep down the Earth in USA, which has the ability to store nearly hundred million of hydrogen for 2 years. This storage medium is particularly useful in areas where there are no porous mediums present in subsurface. Salt cavern is very much suitable for storage operation due to its unique physical properties and the flexibility in operating conditions. On the other hand, materials of steel and drilling instruments encounter the problems of erosion or corrosion. There are also risks of some safety issues such as leakage and explosion issues.

2.7 Area need to be explored

There is very little work done globally to ensure the feasibility of UHS in reservoirs of fossil fuels. According to latest experimental work there is a need to work on the core flooding of hydrogen gas and find the reactions and fate of hydrogen gas plume after the injection has stopped. Then the simulation is required to cover the geomechanical and geochemical aspects of storage operation to know about the long term safety of storage operation. Some countries such as Germany and USA put their efforts and investments to make UHS an industrial operation but there is not much real field data available to fill the research gaps present in this area. So there is a need to invest in UHS operations worldwide to make it a good contribution to environmental protection schemes.

3 Screening criteria for CO_2 storage in aquifers

3.1 Critical review

Economic development is directly dependent on fossil fuel consumption. However, the application of fossil fuels in fulfilling global energy demands resulting increase in greenhouse gases that leads to pollution in environment, depletion of ozone layer, and causing climate change. Consequently, greenhouse gases methane (CH_4) and nitrous oxide (N_2O) and particularly CO_2 have significantly increased in atmosphere (Raza, Rezaee et al. 2016).

Many ways have been introduced to decrease the amount of carbon dioxide from the atmosphere including carbon capture and storage (CCS). There are three classes of CCS from getting CO_2 from operations of oil and gas fields to no carbon schemes where carbon dioxide produced from biomass is kept. (Chalmers and Gibbins 2010). These types of CCS are shown in Table 1. According to the International Environmental Agency this technology has the ability to mitigate 17% of the atmospheric CO_2 emissions by 2050 and to achieve this every country should have clear policies and implementations about CCS (Edenhofer, Pichs-Madruga et al. 2014). Low-emission techniques will take some years or decades to deploy at industrial level to provide a replacement of conventional fuels and may not do so early as required in countries like India, USA and China, because of huge reserves of fossil fuels especially coal which is sufficient and cheap to fuel economic growth (Blunt 2010) . In this aspect, CCS is the only way to overcome emissions from energy sector and in the meanwhile we can develop energy systems with fewer amounts of carbon emission and without massive disruption in world economics.

Table 1: Classes of CCS **(Blunt 2010, Chalmers and Gibbins 2010)**

Class	Impact on CO_2 emissions	Examples
Carbon positive	Capture and storage of CO_2 from industries of fuel generation. CO_2 is generated in significant quantities by the consumption of fuel, but the redundant CO_2 is collected.	Coal-to-liquids plants producing synthetic fuels. Stripping natural CO_2 from oil or gas production
Near -carbon neutral	Projects that produce energy from systems which emit less amount of carbon such as electric energy, hydrogen and/or steam). These projects limit the CO_2 emissions to a very less amount because the major fraction of CO_2 in the fuel burning	Power plant producing electricity using fossil fuels

	process can be captured and stored. On the other hand, still CO_2 emissions can take place from this process because it burns biomass, but it is near to 100 percent carbon capture project.	
Potentially	Class 3a: direct capture of CO_2 from the air. Class 3b: similar to 2nd class, but in this case biomass is used instead of fossil fuels. When all the CO_2 emitted from biomass is captured and stored to a safe place then carbon emissions can go to negative. This class has the ability to mitigate the amount of emitted CO_2 from project of Class 2 and thus capture CO_2 from the atmosphere on a lifecycle basis.	3b: Power plant using biomass and fitted with CO_2 capture technology.

There are three main ways to store CO_2:

- Geological formations
- Deep Oceans
- Mineral storage

Currently the most flexible and large scale process is the geological storage of CO_2. Large amount of work has been done on the underground storage of CO_2. It can be stored underground in deep saline aquifers, depleted oil and gas reservoirs, un-mined coal beds, basalts and as EOR process in partially depleted oil reservoirs (Tomić, Maričić et al. 2018).

In comparison with depleted reservoirs of fossil fuels, deep saline aquifers are present in wide range around the globe. Benefits of saline aquifers for CCS are their large storage capacity, availability and no other specific use due to their high salinity (BritishGeologicalSurvey(BGS) 2019). Coal beds or coal that is present at high depth or troublesome to mine is known as unminable and it can be used to store CO_2 in adsorbed form. (Tomić, Maričić et al. 2018).

Storage of CO_2 in deep oceans can cause acidification when interacts with H_2O to form H_2CO_3 which is harmful to ocean species.

In mineral storage or mineral carbonation, captured carbon dioxide reacts with magnesium- (Mg) and calcium- (Ca) minerals present in rocks. Nevertheless, these reactions take very much time under normal conditions and to boost it up a sufficient amount of energy is required. According to IPCC if the geological storage sites could be managed and operated in an efficient way then carbon dioxide can be stored for a long period of time without any leakage. Regions like Gulf Coast (USA) and North Sea are believed to contain large potential for geological storage (BritishGeologicalSurvey(BGS) 2019).

3.2 Pilot Projects

In 1977, for the very first time it was suggested that CO_2 could be captured from the coal power plant and injected into suitable geological formations (Marchetti 1977). In the last decade of nineties, the first CO_2 sequestration project with the only purpose to decrease the amount of CO_2 from atmosphere was initiated by Statoil, Norway. IEA states that, there should be an initiation of billions of carbon capture and storage projects within next ten years to ensure the achievement of targeted amount of CO_2 emission reduction. In order to meet the emission targets set up by the IEA within the next decades, there is a need for thousands of plants, storing billion of tons annually (IEA 2009). CCS projects from different industries are playing their role to reduce the CO_2 from atmosphere. Three power plant projects capturing CO_2 are: Boundary Dam in Canada, Kemper County in Mississippi US and Petra Nova CCS project in Texas US (Carbonbrief 2014).

Industrial projects are based on production sites for fertilizer or steel and plants which involve processing of tar or fuel obtained from biomass. Some of industrial CCS projects from fertilizer or steel or plants of tar sands are: Carbon Trunk Line in Canada, Enid Fertilizer in Oklahoma US, Illinois Industrial CCS Project in Illinois US, Coffeyville Gasification plant in Kansas US, and Weyburn project, Quest in Alberta Canada, Abu Dhabi CCS project in UAE (Carbonbrief 2014). Some of the gas processing plants which include CSS activities are: Century Plant in Texas US, In Salah in Algeria, Gorgon Injection, Project in Australia, Sleipner project in Norway, Snøhvit project in Norway, Uthmaniyah Demonstration Project in Saudi Arabia. In

2016, the first large-scale carbon capture and storage operation in the iron and steel industry started operation in Abu Dhabi, which captures almost 8 lac tons per year.

Most of the studies are focused on saline aquifers because of their high storage capacity and feasibility for CO_2 properties. Some of the major works on CCS in deep saline aquifers are listed here: The Sleipner carbon capture and storage project marked 20 years of successful operation in 2016 and stored approximately 17 Mt of carbon dioxide in saline aquifer. In Salah project initiated capturing and storing carbon dioxide from methane gas in 2010 and paused in 2011 as there are some problems of gas leakage. At that time, three and a half million tons of CO_2 had been kept in an aquifer.

Gorgon Injection Project, Australia captures carbon from CH_4 processing plant in Western Australia. It has the ability to capture 3.4-4 million tons. The captured carbon dioxide stored in a saline aquifer. The Snøhvit project captures CO_2 gas at an offshore gas treatment plant. CCS activity initiated in 2008 and the capacity is 0.7 million tons per year. Industry of bioenergy is also getting linked with CCS and the very first example of this is Illinois Industrial CCS Project.

3.3 Storage Potential

As discussed, carbon dioxide can be stored in many ways but the geological storage has the largest storage potential. In conclusion from IPCC estimation, some storage facilities have the ability to store billion or trillion tonnes of injected gas. We can compare the storage capacities of different geological storage options as shown in Table 2.

Table 2: Comparison of different geological sites in terms of storage capacity **(GlobalCCSInstitute 2010)**

Reservoir type	Lower estimate of storage capacity in billions of tonnes of CO_2($GtCO_2$)	Upper estimate of storage capacity in billions of tonnes of CO_2($GtCO_2$)
Depleted Petroleum field	675	$9*10^2$
Deep coal beds	3 to 15	$2*10^2$
Aquifers	10^3	10^4 (uncertain)
Total	1675	11,000

So this comparison shows that geological formations can store billions of carbon dioxide and play their part for clean environment. Deep saline aquifers are the best in terms of storage capacity. In Europe and other regions where there are less depleted oil and gas fields as compared to USA and Arab countries deep saline aquifers can become vital storage sites.

~~3.4~~ CO_2 Storage

3.4.1 Site selection for CO_2 storage

After capturing the carbon dioxide from different fields there is a need to find a suitable site where CO_2 can stored on a large scale. Due to the inefficiency of surface mineral carbonation, deep ocean sinks and many other proposed methods the term CCS is now focused to only capture, transportation and geological storage (Bachu, Hawkes et al. 2009). Then among three geological options coal bed methane is known to be an immature technology and with the least storage potential (IPCC 2005).

Along the various steps of the CCS process, the stage of site selection and characterization is mandatory because any storage site must satisfy three basic requirements (Bachu, Hawkes et al. 2009):

a). Storage capacity in terms of volume which can be stored throughout the life of operation.

b). Injectivity in terms of rate at which CO_2 is injected.

c). Containment or confinement to trap the CO_2 and prevent it from leakage.

All of these requirements are interrelated. There are also other site selection criteria that can be merged into three vast categories: economic, legal regulatory and societal. Operating cost and development cost is the most important to start the project so it lies in the first phase, obtaining the particular license or follow the regulations that allow or interdict CO_2 storage would fall into the second category, and public behavior and approval (or opposition) would fall into the third category (Bachu, Hawkes et al. 2009). At the very first stage we will do the screening criteria at the basin scale and then we check the properties of the geological formations and characterize whether it is feasible and safe to store CO_2 in this site.

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Usually when CO_2 is injected in subsurface at a depth below 800 m its nature becomes supercritical. It simply means to have a density equivalent to liquid and viscosity in the range of gases. A Pressure reduction results in the expansion of CO_2 which then becomes gas which doesn't change its state. The CO_2 density will still be less than water and viscosity will be almost ten times less than that of the salt water present in the rock. CO_2 can interact with rock minerals or formation fluid and causes solid precipitation instead of burning or exploding.

3.4.2 Storage capacity

Storage capacity is usually estimated by total volume of pores (not the bulk volume) of the rock multiplied by an efficiency factor. We subtract the amount of water present in pores for gas reservoirs (Raza, Rezaee et al. 2016). For saline aquifers, the storage efficiency at pore scale is given by (Bachu 2015):

$$E_{pore} = (1 - S_w) \tag{1}$$

Where E_{pore} is storage efficiency at pore scale and S_w is water saturation. There are two main methods used to find storage capacity in deep saline aquifers:

a. CSLF
b. USDOE

CSLF methodology only takes into account the storage or trapping done by structural or stratigraphic traps. And the capacity in terms of equation is given by (Bachu 2015):

$$M_{CO2} = C_c \iiint \phi\,(1 - Swirr)\rho dxdydz \tag{2}$$

$$C_c\,\rho - A_{av}\,H_{av}\,\phi_{av}\,(1\text{-}S_w)_{av} \tag{3}$$

Where A_{av}, H_{av}, ϕ_{av} and ρ are average aquifer area, average thickness, average porosity and density respectively. C_c is an efficiency coefficient. Some modifications have been done by (Gorecki, Sorensen et al. 2009, Bachu 2015). USDOE method of storage capacity calculation takes into account the complete area of the aquifer as shown by the following equation:

$$M_{CO2} = E\rho_{CO2} - A_{av}H_{av}\phi_{av} \tag{4}$$

There is another method to find the storage capacity named as US Geological Survey (USGS). USGS involves assessment of CO_2 from structural and stratigraphic traps and also from residual trapping (Blondes, Brennan et al. 2013) (Bachu 2015). These calculation methods are applicable for both local and regional levels. All of the three methods are volumetric and the storage capacity found by volumetric method is called static storage capacity. Due to the involvement of time element estimation of CO_2 storage capacity by analytical and numerical simulations is known as “dynamic”.

Storage capacity depends on number of factors including aquifer characteristics, storage operation and regulatory constraints (Celia, Bachu et al. 2015). Aquifer characteristics, such as pressure, temperature, water salinity, displacement characteristics of the CO_2/brine system, depositional environment, lithology, porosity and permeability, heterogeneity and anisotropy, compressibility, areal extent, thickness, dip, topography at the top of the aquifer, and aquifer boundaries (open, semi open, or closed) have an influence on fate of injected in aquifer and CO_2 storage capacity (Celia, Bachu et al. 2015).

Supercritical nature of CO_2 is necessary for the efficient storage process because in this way it can occupy more space and can move deep into the rock due to high mobility (Ketzer, Iglesias et al. 2012) (Raza, Rezaee et al. 2016). Feasible pressure and temperature are the key requirements to reach this supercritical state. In the subsurface as we go deep an increase in pressure and temperature is observed so the depth is the deciding factor in normal temperature and pressure conditions. Many studies have shown that depth of the formation should be greater than 800m and less than 2500 m to achieve better storage of CO_2 (Chadwick, Arts et al. 2008). Temperature on the other hand affects the migration of CO_2 plume. If the reservoir temperature is high the upward movement of CO_2 plume is enhanced and it will reach the top of the formation in less time as compared to low reservoir temperatures (Al-Khdheeawi, Vialle et al. 2018). Larger storage capacity can be achieved when rock has higher compressibility (pore compressibility). As the amount of injected CO_2 is increased there is an increase in pore compressibility and as a consequence aquifer pore volume is also increased (Vulin, Kurevija et al. 2012).

Aquifer boundary conditions are very important for the storage potential because it defines the size and type of aquifers. Open, closed and semi-closed aquifers can be used for storage purposes. In an aquifer of small size the migration of CO_2 is limited by aquifer boundaries and injected CO_2 can only occupy the space created by rock and water compressibility. Mathematical form of this storage efficiency is given below (Zhou, Birkholzer et al. 2008) :

$$E = (\beta_m + \beta_w)\,\Delta p_{max} \equiv (\beta m + \beta w)(p_{max} - p_i) \qquad (5)$$

β is the compressibility and p is the pressure and for storage media and water m and w are used respectively. In the case of a laterally open aquifer the accommodation space is mainly created by displacement of water and then by compressibility of both water and rock. Semi-closed aquifer is the one where CO_2 can pass through the boundary or leakage of gas is possible. In this particular case it is difficult to say about storage capacity because there is no linearity in the system. We have to use numerical simulation to find storage capacity of semi-closed aquifer (Zhou, Birkholzer et al. 2008). Different studies on aquifer boundaries have shown that open aquifers, because of their large lateral extent, are capable of storing more CO_2 as compared to closed or semi-closed aquifers (Bachu 2015).

The pore throat size is very critical in the fluid dynamics and for CO_2 storage capacity. Pore throat size affects different reservoir properties such as fluid saturation, porosity and permeability (Lake, 1989) (Raza, Rezaee et al. 2016). Narrow pore throat sizes are advantageous for high storage capacity as compared to wider ones because they direct the flow of wetting phase into pore throats and increase the overall saturation of CO_2 gas in pores. Aquifer top-surface topography is very important in determining the efficiency of storage operation. It includes structural closures, dip, and channels. When compared to structurally open aquifer models, structural closures increase efficiency because they provide a trap necessary to stop the upward migration of CO_2. Channels generally provide an easy way to injected gas which can flow or leak through the storage formation and in this way decrease the storage capacity (Goater, Bijeljic et al. 2013).

The dip angle of storage medium has an impact on CO_2 sequestration operation. As the dip angle is increased, CO_2 storage in gas phase is decreased, but the amount of CO_2 in dissolved form is increased. In a limited time span, the CO_2 amount is less in the dissolved form and a significant amount is in gas-phase. In this aspect, the total CO_2 storage capacity falls down due to more dipping formations (Wang, Jing et al. 2016). CO_2 plume migration is also affected by dip angle of formation. It is observed for the Shiqianfeng group reservoir in China that when the formation dip is high there is significant increase in migration distance even after several years of injection (Wang, Jing et al. 2016).

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Some formations have large differences between vertical and horizontal permeabilites. Information regarding vertical permeability anisotropy is useful to get fair estimate about the storage potential of a particular sink. High vertical permeability anisotropy hinders the upward movement of CO_2 and it will help to prevent the leakage or very sharp reach of CO_2 at the top of geological media (Bachu 2015). In this way a larger storage capacity is achieved for vertical permeability less than the horizontal permeability.

Flow dynamics of carbon dioxide in an aquifer is dependent on buoyancy, viscous and capillary forces. Buoyancy is the result of density difference between CO_2 and saline water and it acts as the driving force for the movement of CO_2, while viscous and capillary forces hinders the flow of injected gas. To simplify the meaning and effect of two terms (buoyancy and viscosity) a new concept is introduced which is named as gravity number (Nordbotten, Celia et al. 2005). Gravity number is the ratio of buoyancy to viscous forces. From the definition, large gravity numbers allow the migration of CO_2 to the top of the formation and hence low storage efficiency is achieved. And the small gravity numbers have high viscous forces which support the lateral movement of carbon dioxide which will increase capacity of storage (Ide, Jessen et al. 2007) (Bachu 2015). Mobility ratio has also the similar effect as of the buoyancy forces. So the lower mobility ratio is better for a good storage operation. Capillary entry pressure changes in direct proportion with IFT and inversely with the pore throat size, introduces capillary barriers in aquifers (Bryant et al., 2006). Capillary pressure causes residual or capillary trapping occurs during drainage and imbibition cycles and consequently traps gas in the pores.

In deep saline aquifers the role of water salinity is very important due to its influence on other mechanisms of storage. Some studies have been done on the effect of salinity and it is concluded that water salinity can affect the storage efficiency in two different ways. For increasing salinity the density and viscosity of brine increase which in turn increase the mobility and buoyancy. And as we discussed before, both of these terms cause less storage capacity. On the other hand, when salinity decreases the solubility of carbon dioxide in the brine and hence the overall amount of gas that can be stored is reduced due to decrease in solubility trapping (Enick and Klara 1990).

In the past, very little attention was given to the effect of wettability of the rock on sequestration process. A proper and systematic investigation was done by (Al-Khdheeawi, Vialle et al. 2018) to investigate the effects of wettability on CO_2 flow at reservoir scale. A number of wettability models were studied from strongly water wet to strong CO_2-wet conditions. The results illustrate that a formation which has highest affinity towards CO_2 marked highest migration of gas, while formations with high affinity towards water can trap more CO_2. In conclusion that the water-wet formations are best to store a large amount of CO_2, and undesired leakage or migration can occur in CO_2-wet reservoirs.

Normally different types of heterogeneities are present in the geological formations. Wettability heterogeneity is common in most of the geological formations and we need to consider its effect for an efficient CCS project. Simulation works have been done on the comparison of homogenous and heterogeneous wettability models in terms of their storage capacity of CO_2 (Al-Khdheeawi, Vialle et al. 2018). From the simulation results it can be concluded that formations with high wettability heterogeneity are more inclined to allow the upward migration of CO_2 and opposite is the case with homogenous formation models.

Caprock thickness and sealing ability is one of the most necessary requirements for underground CO_2 storage operation. Sealing ability of a caprock depends on number of factors such as: **(1)** buoyant force due to difference between the densities of water and CO_2; **(2)** thickness and petrophysical properties, such as capillary pressure, absolute and relative permeability of seals; **(3)** the time taken by the CO_2 plume after which it exceeds the seal capacity (Chen, Zhou et al. 2014). From the simulation results it is shown that thickness of the caprock can counter the leakage of CO_2 if it is permeable to some extent. In conclusion, caprock thickness has an inverse relation with leakage of CO_2 and direct relation with the storage capacity (Chen, Zhou et al. 2014).

Faults are the result of subsurface tectonic activities and are very abundant in geological formations. Fault can be sealing or leaky depends on the transmissivity factor of the fault T_f. Selection criteria of a site for storage purposes must also involve the checking of transmissibility of faults to get better understanding about future storage processes. Pressure transient effects have been checked by performing the sensitivity of different fault models. Results show that for transmittivity factor of the fault (T_f) less than 0.01, high fraction of injected CO_2 is stored and for T_f higher than 0.1 bbl / psi-day the reservoir cannot store high fraction of CO_2 (Alexander and Bryant 2011).

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Formations which are usually considered for storage activities are sedimentary rocks which are mainly composed of quartz, feldspar and mica. The information of characteristics of the brine-CO_2-quartz system is very useful because quartz has an influence on capillary (residual) trapping of CO_2. Core flooding experiments were conducted to monitor the effect of quartz on residual water saturation. Carbon dioxide was injected into the samples at subsurface conditions and after the process of drainage water and water-gas mixtures were gathered and observed. The results of experimentation on core samples show that higher the concentration of quartz in the core sample lesser will be the amount of residual water saturation which will generate high storage capacity (Li, Wu et al. 2015).

3.4.3 Injectivity

Injectivity is considered to be the back bone of CCS operation because without an efficient injection process we cannot achieve a desirable amount of CO_2 storage. For injectivity a number of factors need to be considered such as permeability of aquifer, heterogeneity of the aquifer, pressure build ups, fracture pressure, capillary entry pressure, seal rock properties and integrity, injection rate, number and distribution of wells and types of wells.

Permeability has very strong influence on the injection of gas because it can affect the injectivity in two different ways. On the one hand, low permeability of the formation hinders the lateral migration of CO_2 plume and in this way injectivity and storage capacity is reduced. On the other hand, pressure build up is the factor which is affected by permeability of both storage aquifer and sealing rock (Buscheck, Sun et al. 2012). As we inject the gas beneath the Earth’s surface there is an increase in pressure but this pressure is sufficiently increased by small amount of injection if the permeability of the storage formation is very low and in terms it limits the injectivity and storage capacity. Formation pressure must be less than the fracture limit of the sealing rock to avoid any escape of injected gas. (Raza, Rezaee et al. 2016).

In low permeability reservoirs problem of high pressure build up can be resolved by increasing the number of wells (van der Meer and Yavuz 2009). However, injectivity is not only improved by increasing the number of wells but it also requires the optimum scheme of injection and distribution of wells. Well spacing is very important in this regard because if the wells are not evenly distributed in the field they can cause more severe issue of high pressure build up (Ehlig-Economides and Economides 2010, Bachu 2015). Horizontal wells can mitigate the requirement of drilling more vertical wells and from different studies it is demonstrated that hydraulically fractured horizontal wells are better than vertical ones due to their feasibility both under the economic and technical standpoint (Cinar, Bukhteeva et al. 2008, Raza, Rezaee et al. 2016).

Sealing rock can play its role in the releasing the excessive pressure build-up if its permeability is high or confining aquitards is leaky. High permeability path in sealing rock will provide a path for saline water to escape through it and CO_2 will remain trapped due to higher capillary entry pressure (Birkholzer, Zhou et al. 2009). But if the brine got leaked from the caprock, it should be evaluated that it will not reach to shallow water aquifers which are in use for water supply. Practically the upward migration is very limited due to less permeability and speed of migration but when a fault or high permeability channel is available then according to EPA safety of fresh water aquifer should be of great concern to operating company. Results of simulations done by (Birkholzer, Zhou et al. 2009) suggest that vertical brine leakage becomes important when the seal permeability is higher than 10^{-19} m^2.

Pore compressibility also becomes the cause of variation in injectivity strategies by influencing the pressure buildup during injection. Formation with less pore compressibility causes a higher pressure buildup during injectivity and the pressure transient also affects larger area (Birkholzer, Zhou et al. 2009). While on the other hand formation with high pore compressibility will bear the injection of CO_2 and will not cause large pressure build up and is beneficial for injectivity and storage capacity.

Core experiments and numerical simulations were performed by (André, Peysson et al. 2014, Peysson, André et al. 2014) to investigate the effects of concentration of salinity, capillary forces and the gas injection rates on injectivity. Salinity of the brine present in the aquifer causes the precipitation of salt. Evaporation of water occurs due to continuous injection of gas and the salt is left behind in the form of precipitates which clogs the pores. More is the salinity of brine more will be the precipitation and clogging which will decrease the permeability and porosity of the formation. This reduction in permeability is not only limited to the injection zone but it will propagate far into the rock and in different locations depending on the amount of salt and injection rate of gas (André, Peysson et al. 2014, Bachu 2015). Evaporation of water results in activation of capillary properties of the porous media and the migration of brine will take place from the other end of the reservoir to the injection zone and for the time being precipitation will stop. After sometime, continuous injection of gas causes the evaporation of water initiating the precipitation of salt, which will expand more and more as brine migrates towards the injection zone. Ultimately massive clogging of formation will stop the further injection of gas.

Gas injection rate is a very critical parameter for evaluating the injectivity of gas in saline aquifers. For a fixed concentration of salt in brine, higher injection rates prevent the drying of saline water as compared to the lower ones. Sensitivity analysis has shown that there is a threshold value of injection rate evaluated on the basis of concentration of salinity within each formation and CO_2 should be injected at a rate higher than the estimated threshold value (André, Peysson et al. 2014). Salt precipitation can also occur in rocks with low salinity due to very low injection rates. So threshold injection rate should be evaluated for the particular amount of salt present in water to get better injectivity operation.

1. Trapping Mechanisms

Once CO_2 is entered in the formation it will try to go to the top of the formation due to its less density or buoyancy effect. To sustain the CO_2 storage for a longer period i.e. for centuries, it is obligatory that the leakage of CO_2 shouldn't occur. There are four main mechanisms through which the CO_2 is trapped in underground formations.

Injected CO_2 migrates upward in the aquifer until it finds some caprock or barrier of low permeability; this trapping mechanism is named as structural or stratigraphic trapping. It works on the same principle of trapping of natural oil and gas. It is not mandatory for the caprocks to be completely impermeable. Their pore size should be small enough so that high pressure is required to enter in the formation. Examples of some common caprocks are layers of salt, shale and clays. The storage mechanism in the world famous Sleipner project is the caprock trapping which is still very much efficient after 23 years (Blunt 2010).

Capillary trapping occurs when capillary forces within the rock pores trap some of the injected CO_2. Capillary trapping is the most rapid and secure mechanism among other schemes of storage (Kimbrel, Herring et al. 2015). Displacement of water occurs and potentially traps CO_2 when there is local movement of formation water or when carbon dioxide moves to the top of the aquifer. Recent research has shown that brine can be produced out from the saline formation and then re-injecting would increase this natural phenomenon (Juanes, Spiteri et al. 2006).

Afterwards work has been done on it and the proposal of an injection scheme is presented where both carbon dioxide and saline water are injected simultaneously followed by brine. (Qi, LaForce et al. 2009).

CO_2 has ability to get dissolve in saline water and as a result produce a high density phase. Solubility of CO_2 increases with the increase in pressure but as the salinity of water increases it decreases the solubility. The dissolution of CO_2 is not a quick process, arbitrated by diffusion of molecules and the movement of dense saline water. It requires several numbers of years or even a century to dissolve CO_2 on large scale in geological formations. (Ennis-King and Paterson 2002).

Geochemical trapping comes into play when dissolved CO_2 interacts with the residing pore liquid and/or the minerals composing the formation. CO_2 dissolves in brine and forms an acidic solution which then reacts with the rock minerals and produce solid carbonate and aqueous complexes. It is also called ionic trapping due to the presence of bicarbonate anions. Precipitation of solid carbonates decrease the pore volume and permeability but opposite can also happen when acidic solution of brine dissolves part of the rock. (Blunt 2010).

3.4.4 Containment

Once the gas is injected in the storage aquifer then containment is the significant aspect that comes into play. Gas is contained in the storage formation due to the presence of a caprock or any sealing fault. If proper sealing or containment is not present then the injected gas can be leaked out into other formations which can cause contamination of drinking water or escaping of CO_2 back into the atmosphere (Raza, Gholami et al. 2018). Escaping of CO_2 can only be possible in the presence of highly permeable faults or flow channels otherwise in normal conditions permeability of seal is very low and migration velocity is very less. Capillary entry pressure should always be greater than buoyancy forces of CO_2 to trap the injected gas.

Top surface topography and caprock thickness also have a prevailing influence on the containment ability of the sealing rock. As discussed before top surface topography includes structural closures, channeling and dipping (Goater, Bijeljic et al. 2013). Structural closures provide a lot of support to trap CO_2, while channeling provide a path to injected gas to migrate or escape from the sealing rock. If we talk about dipping formations they also enhance the upward migration of CO_2 and thus cause the leakage of stored gas. Caprock thickness is a very essential parameter for storage of gas because if the caprock is not sufficiently thick it can also easy leak out of CO_2 (Chen, Zhou et al. 2014).

Different types of dissolution reactions occur in the caprocks and some of them provide further containment and some act opposite to the trapping ability. Dissolution of dolomite, K-feldspar and dehydration reactions of shale and slate mitigate the capability of the sealing rock to contain CO_2 (Rochelle, Czernichowski-Lauriol et al. 2004) . Oppositely precipitation can take place due to dissolution of carbonates of calcium, magnesium and iron which will decrease the porosity and permeability of the rock avoiding the migration of CO_2 (Rochelle, Czernichowski-Lauriol et al. 2004).

Presence of gypsum also produces clogging of pores that increase the containing ability but on the other reduce injectivity of gas which is not much suitable. In the region of 30m within injection zone precipitation of gypsum causes greater than 1 percent reduction in pore volume but if precipitation takes place within 10m of injection zone then the reduction in porosity would reach till 10 percent (Brehme, Nowak et al. 2019). To avoid the clogging of pores by gypsum precipitation calcium polyphosphonate can be added in the formation but the addition of calcium polyphosphonate also causes the clogging of pore throats by the process of fibrous precipitation. At the end borehole condition can also affect the injection and containment abilities of CCS operation so there is a need of proper evaluation of the integrity and strength of borehole (Raza, Rezaee et al. 2016). Any borehole problem must be avoided during CCS process for better containment and injectivity.

3.5 Area need to be explored

In the last decade carbon capture and storage was the new trend so huge amount of research has been done on this subject. Deep saline storage aquifers and depleted oil and gas fields were the most focused and appealing areas for researchers due to their large scale storage capacity and compatibility with the well-known and developed technology of oil and gas industry. Deep saline storage aquifers are still the most enchanting and captivating storage sites for research works because of their largest storage capacity among other storage sinks and plentiful occurrence in the regions with high awareness towards sustainable environment such as Europe.

Different aspects of CO_2 injection and storage such as geochemical reactions with rock minerals, geo-mechanical effects, hydrodynamic behavior of CO_2-brine system and pre and post injection processes have been discussed in literature. Yet a substantial amount of work is required to be done on the development of a preliminary process for identifying a suitable aquifer for CCS operation. Site selection and characterization is very essential part of CCS operation (Chadwick, Arts et al. 2008, Bachu, Hawkes et al. 2009). For the very first time in 2008, Chadwick, Arts et al. (2008) worked on the selection process for CO_2 storage in aquifers but at that time very limited research had been done on the factors affecting CCS operation in aquifers.

In 2016, a screening criteria for CO_2 storage in gas reservoirs was presented by (Raza, Rezaee et al. 2016) which is very much extensive and based on strong literature review but again no example was available for aquifers. So there is a need of development of an up to date and extended screening criteria on the basis of which one can decide the most suitable aquifer for CO_2 storage among different available options. One aspect to be investigated is the effects of aquifer heterogeneity. A simulation stud can be done on the effect of various types of heterogeneities in aquifers on CO_2 storage capacity and injectivity.

3.6 Proposed screening criteria

Screening criteria proposed by (Chadwick, Arts et al. 2008) was the first one to distinguish between different aquifers for storage purposes. It is shown below:

Table 3: Screening criteria for CO_2 storage in aquifers **(Chadwick, Arts et al. 2008)**

Parameters	Feasible conditions	Negative Indicators
Total storage capacity	Volume of CO_2 is less than the total capacity of storage medium	Volume of CO_2 obtained from the source is higher than the total capacity
Depth	1000-2500	<800m and >2500m
Thickness (aquifer)	>50m	<20m
Porosity	>20%	<10%
Permeability	>300mD	<100mD
Salinity	>100g/l	<30g/l

Capillary entry pressure	Higher than buoyancy force of CO_2 column	Buoyancy force equal to or lower than capillary entry pressure

It was very useful and many research workers have taken guideline from Chadwick et al. work but at present there is a need to present new and more extensive screening criteria which will provide a solid basis for the industry personals and researchers. These updated criteria cover most of the parameters based on literature review and it is shown in Table 4.

Table 4: Updated screening criteria for CO_2 storage in aquifers

Parameters	Feasible conditions	Negative Indicators
Total storage capacity	Volume of CO_2 is less than the total capacity of storage medium	Total capacity similar or less than the total amount produced from the source
Depth	1000-2500	<800m and >2500m
Thickness (aquifer)	>50m	<20m
Porosity	>20%	<10%
Permeability	>300mD	<100mD
Salinity	>100g/l	<30g/l
Temperature	Lower reservoir temperatures	Higher reservoir temperatures drastically accelerated the vertical CO_2 migration
Capillary entry pressure	Higher than buoyancy force of CO_2 column	Buoyancy force equal to or lower than capillary entry pressure
Cap-rock thickness	>100 m	<20 m
Top surface topography:		
a)Top surface channels	Absence of channeling (smooth topography)	Presence of local channels
b)Structural closure	Presence of structural closure	Absence of any structural closure
c)Dip	Lower dipping surfaces	Higher dipping surfaces
Residual water	Less	High

saturation		
Gravity number	Less	High
Pore throat size	Narrow pore throat size	Wide pore throats
Anisotropy	High anisotropy restricts upward migration of CO_2	Low vertical permeability anisotropy results in more concave vertical shape of CO_2 plume
Compressibility of aquifer (pore compressibility)	High compressibilities of pores result in larger storage capacity at corresponding pressures	Lower pore compressibility
Aquifer heterogeneity	Homogenous aquifer is better for storage of CO_2	Heterogeneity reduces storage efficiency
Wettability	Formations having high affinity towards water (water-wet)	Undesired movement can occur in non-water-wet formations
Wettability heterogeneity	Homogeneous aquifers w.r.t wettability can retain more carbon.	Heterogeneous aquifer w.r.t wettability can cause upward movement of carbon dioxide.
Boundary conditions	Laterally open aquifers	Closed aquifers in lateral extent
Transmittivity of faults	Aquifer having transmittivity factor less than 0.01 has the high capability to store injected gas	Aquifers having T_f greater than 0.1 bbl/psi-day is not much fit for storage
Quartz Content	High quartz content	Low quartz content
Concentration of $CaCO_3$	High $CaCO_3$	Low $CaCO_3$

4 Modeling of CO_2 storage in aquifer

4.1 Simulation Approach

The purpose of this project is to calculate the different levels of heterogeneity through Lorenz coefficient and investigate the influence of it on CO_2 storage capacity and injectivity. CO2STORE dynamic numerical modeling which is a part of Schlumberger Eclipse300 Simulator is used to carry out this study. CO2STORE module is specifically designed for CO_2 operation and it takes into account the trapping mechanisms to investigate the storage capacity of a porous medium. Solubility trapping, capillary or residual trapping and fraction of CO_2 in mobile phase are the important and unique features of this simulation approach.

4.2 Synthetic aquifer model

The built aquifer model is a 3D model. The aquifer is assumed to be anticline model with no-flow boundaries. It consists of five layers of equal thicknesses of 5 meters. The aquifer is composed of 2660 cells, 19 in X direction, 28 in Y direction and 5 in Z direction. In each cell DX = DY = 100 meters and DZ = 5 meters. Top of the aquifer is at 2000 m to achieve the supercritical condition of carbon dioxide. Each layer has same porosity but different values of permeability. To make a realistic model specific for storage operation and injection process all other properties of the aquifer are taken from a real field model. Injection well is located in the middle of the aquifer model. The temperature of the aquifer is 100^0 F. Initial pressure of the aquifer at the datum depth of 2020 meters is 278 bars. Carbon dioxide is injected in the aquifer for a period of thirty years at the initial rate of 5663369 Sm^3/day. The aquifer model used in this study has compressibility of $5 \times 10^{-4} bar^{-1}$. All the inputs of the dataset are presented in **Appendix I, II and III**.

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Table 5: Water saturation function

Water saturation (S_w)	**Relative Permeability (K_{rw})**
0.3	0
0.38	0.000152
0.46	0.002439
0.53	0.012346
0.61	0.039018
0.69	0.09526
0.77	0.197531
0.84	0.36595
0.92	0.624295
1	1

Table 6: Gas saturation function

Gas Saturation (S_g)	**Relative permeability K_{rg}**	**Capillary pressure P_c**
0	0	0
0.08	0	0.6
0.16	0.000407	0.78
0.23	0.005831	0.93
0.31	0.024131	1.09
0.39	0.064892	1.26
0.47	0.140566	1.49
0.54	0.269314	1.84
0.62	0.484797	2.53
0.7	1	10
0	0	0

4.3 Methodology

Permeability heterogeneity is added in the aquifer starting from homogenous system to highly heterogeneous system. Level of heterogeneity is depicted by the values of Lorenz coefficients in each case which is 0.1 for least heterogeneous aquifer, 0.5 for intermediate one and 0.78 for highly heterogeneous system. For three aquifer models Lorenz coefficients have been calculated to find the degree of heterogeneity. After the calculation of Lorenz coefficients simulation of aquifer model has been done for three cases of heterogeneities.

This simulation study is repeated for three different cases of porosities i.e. 0.1, 0.2 and 0.3. For each value of porosity three Lorenz coefficients (0.1, 0.5 and 0.78) have been calculated and then the simulation has been done for each single case. So there are total nine cases of simulation study. Comparison of the storage capacity and fraction of trapped or dissolved CO_2 will reveal the best suitable conditions for carbon dioxide storage and trapping in aquifers with different level of heterogeneities and porosity values. Variations in gas in place, gas injection rate and pressure buildup is observed for total injection operation and compared for three levels of permeability heterogeneities and then for three different porosity models.

4.4 Lorenz coefficient

Permeability heterogeneity can be found by a dimensionless factor named as Lorenz coefficient (Schmalz and Rahme). First of all, permeability values for different layers of subsurface formation need to be arranged in a descending order. Then the product of permeability and thickness of each layer is calculated which is known as flow capacity kh. Similarly volume capacity is calculated which is the product of porosity and thickness. A plot of normalized cumulative flow capacity (kh) and normalized cumulative volume capacity (ϕh) is plotted on Cartesian plot. There is a line of equality and a line of Lorenz curve on the plot. The area between the two lines shows the value of Lorenz coefficient. Lorenz coefficient ranges from 0, for a completely homogeneous system, to 1 for a completely heterogeneous system (Ahmed 2018). The tables for the calculation of Lorenz coefficients are shown in the APPENDIX. Plots of Lorenz curves for three degrees of heterogeneities are presented below.

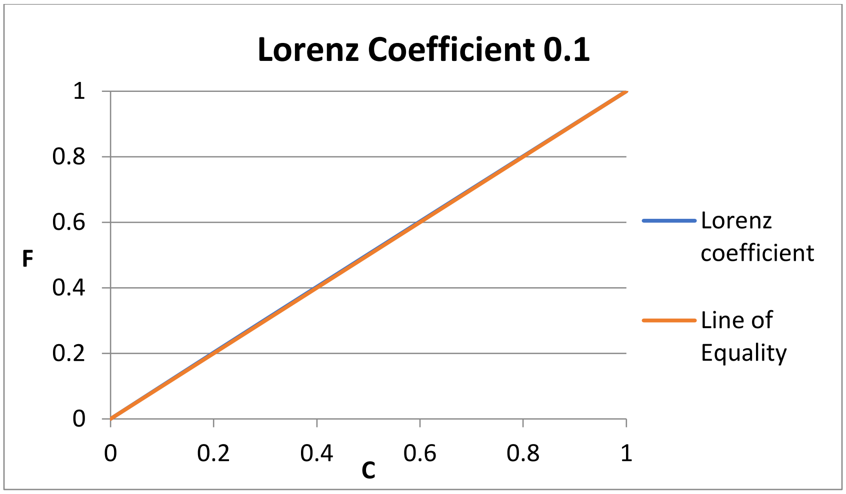

Figure 2: Plot of Lorenz coefficient 0.1 showing medium level of permeability heterogeneity

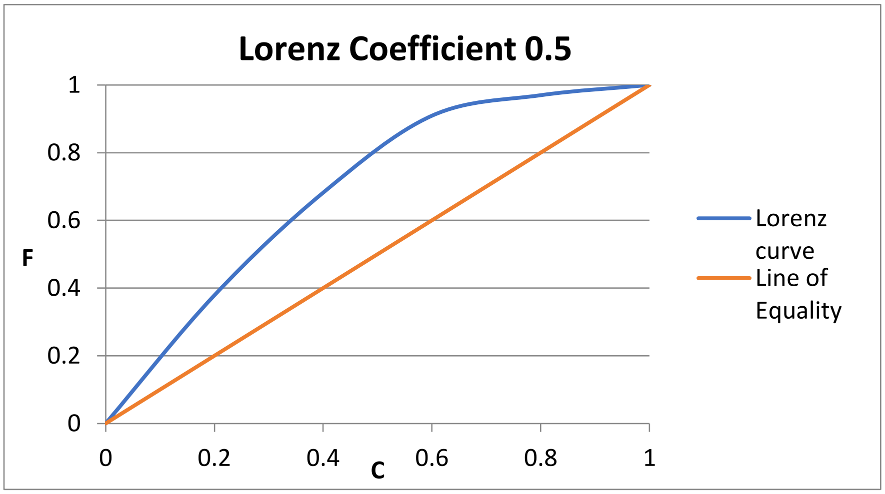

Figure 3: Plot of Lorenz coefficient 0.1 showing low level of permeability heterogeneity.

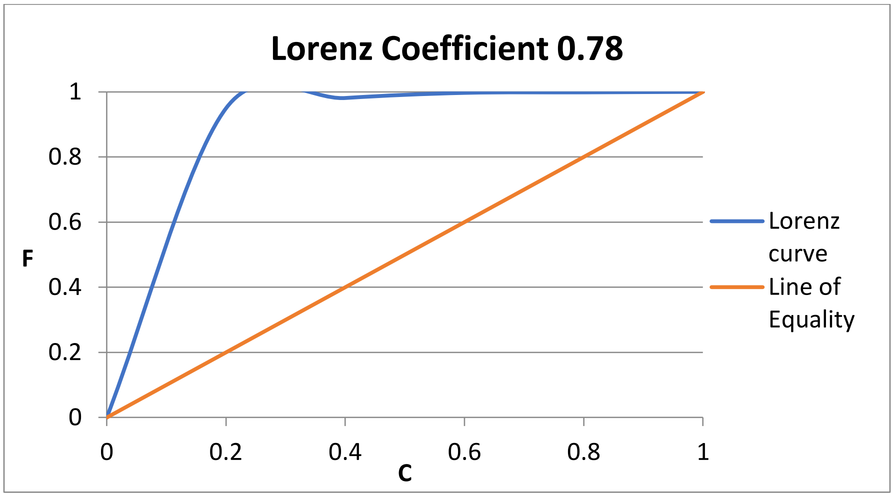

Figure 4: Lorenz coefficient 0.78 showing high level of permeability heterogeneity.

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4.5 Results and Discussion

4.5.1 CASE A: Simulation results for aquifer model with porosity 0.3

The fraction of injected CO_2 trapped by different mechanisms and gas in place for Lorenz coefficients 0.1 and porosity 0.3 has been calculated and plotted in the figure-5. The trend shows that in the first year of injection FGIP (gas in place) starts to increase from 1500 million Sm^3 and as the injection proceeds it goes on increasing till 22 years of injection and then stabilized at the value of 5200 million Sm^3. Capillary or residual trapping plays very key role in the storage of CO_2 in any medium. In this case the fraction of trapped carbon dioxide in gas phase starts from 20 million kg-mole and gradually increased for 30 years and reaches a value of 95 million kg-mole.

Solubility trapping in gas phase is much more than the residual trapping and therefore is of high worth in the storage of CO_2 in saline aquifers. At the end of injection it reaches the maximum value of 350 million kg-mole. On the other hand if we talk about the fraction of free gas i.e. mobile in the gas phase, at the start of injection it follows an increasing trend and reaches a maximum value of 130 million kg-mole of gas. After five years of injection there is a continuous decline and it ended up with 50 million kg-mole of gas. It can be concluded that in this particular scenario the most of the storage capacity is achieved by solubility trapping.

Figure-6 shows the variation of gas injection rate and pressure build up for the total injection period. It is very clear from the figure that injection rate is dropped sharply just after 4 years of injection and reaches at almost zero value. Field reservoir pressure increases for four years of injection and stabilized at a value of 480 bars. Then gas injection rate drops and pressure builds up which adversely affects the injectivity of CO_2.

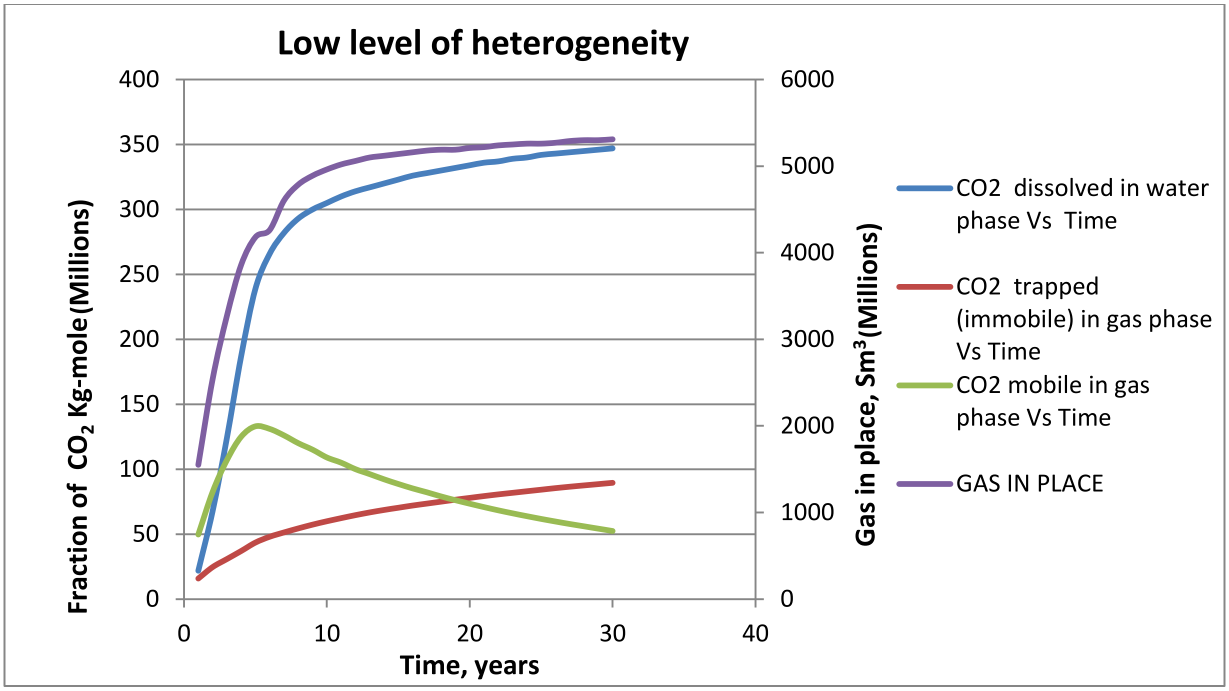

Figure 5 Fraction of injected CO_2 trapped by residual trapping/immobile (FGCDI) and solubility trapping (FWCD) and fraction as free gas (FGCDM) for 30 years of injection in aquifer with Lorenz coefficients 0.1 and porosity 0.3.

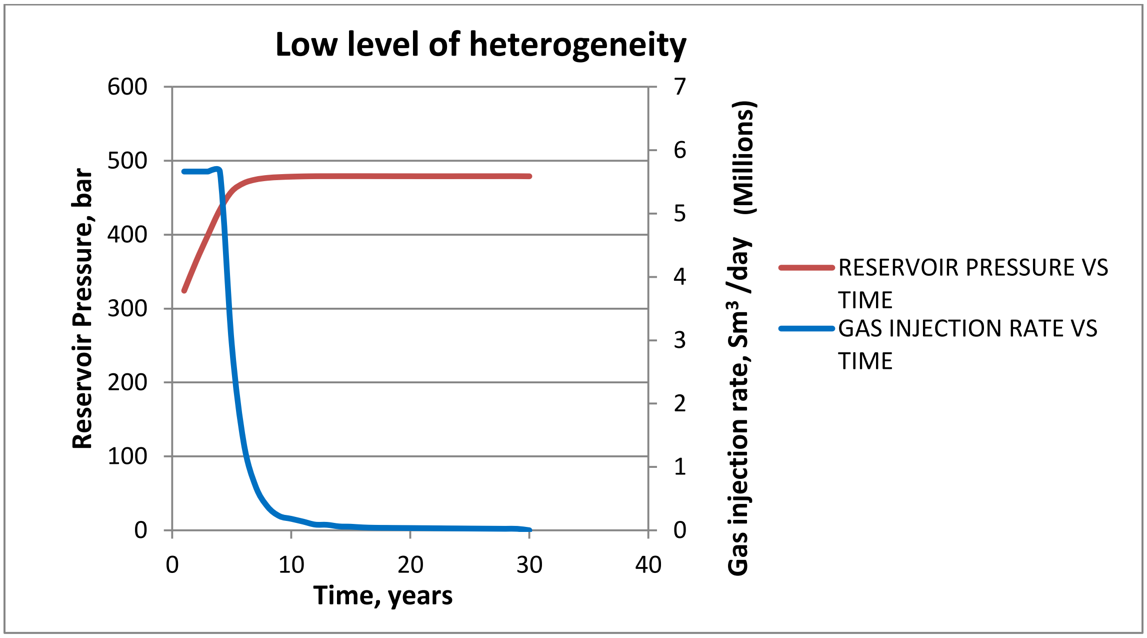

Figure 6 Field gas injection rate (FGIR) and Field reservoir pressure (FPR) for 30 years of injection in aquifer with LC 0.1 and porosity 0.3.

Figure-7 shows the trends of trapping mechanisms and gas in place for the aquifer having intermediate level of heterogeneity (LC 0.5). CO_2 dissolved in water phase (FWCD) has the highest contribution towards the storage of injected gas in aquifer. It is shown by a sharp increase at the very start of injection period and at the end it reaches a maximum value of 360 million kg-mole. When the injection of gas initiated, residual trapping (FGCDI) is the one whose contribution to the storage capacity was the least. But over time the fraction of capillary trapped CO_2 increases and reaches a value of 78 million kg-mole.

Conversely, fraction of free gas has increased to the fraction of 105 million kg-mole at the beginning of injection period but it started to decline with further injection and stopped at the value of 51 million kg-mole. It means that there is a lower amount of free gas present at the end of injection process which is a positive indication for long term storage. One of the reasons of the lower amount of mobile gas is the conditions which favors the trapping mechanisms instead of plume migration.

On the y-axis of figure-7 gas in place increased sharply with the injection process and reached a value of 4500 million Sm^3 just after seven years of injection. After completion of injection process gas in place reached a value of 5200 million Sm^3.

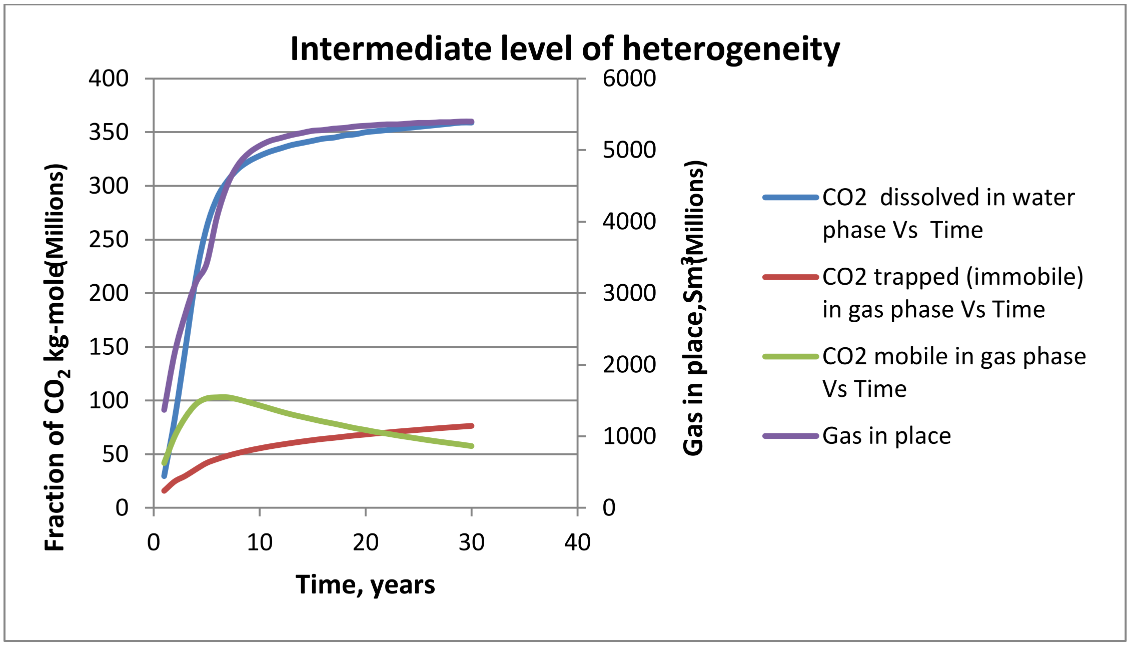

Figure 7: Fraction of injected CO_2 trapped by residual trapping/immobile (FGCDI) and solubility trapping (FWCD) and fraction as free gas (FGCDM) for 30 years of injection in aquifer with Lorenz coefficients 0.5 and porosity 0.3.

Figure-8 shows the graph containing the trends for reservoir pressure and gas injection rate. Gas injection rate stabilized for a three years of injection and then suddenly declined to zero within 15 years. Reservoir pressure shows a sudden increase as the injection started and stabilized after 10 years of injection.

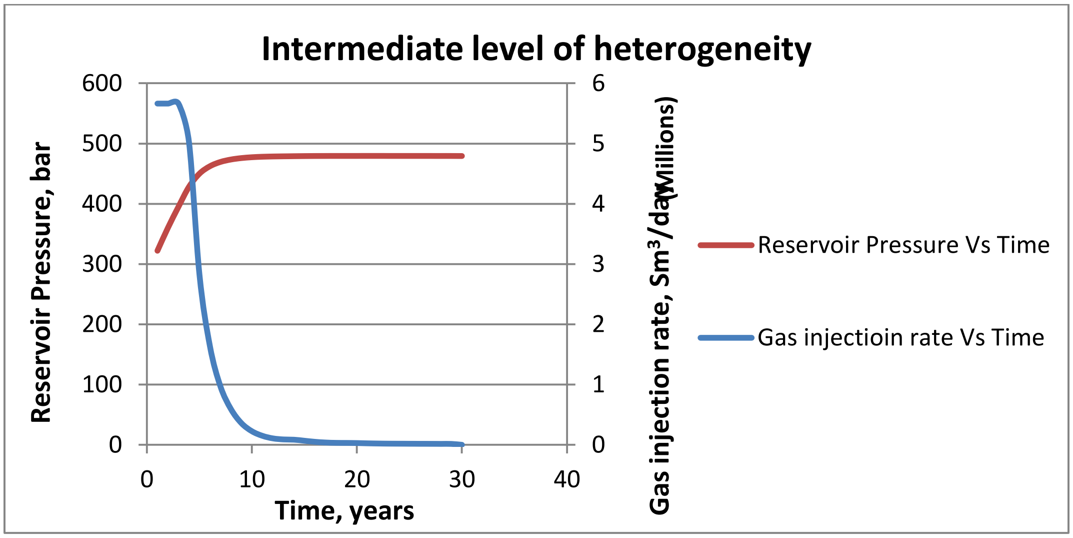

Figure 8 Field gas injection rate (FGIR) and Field reservoir pressure (FPR) for 30 years of injection in aquifer with LC 0.5 and porosity 0.3**.**

Figure-9 shows the trapping mechanisms for the high level of heterogeneity in the aquifer with Lorenz coefficient 0.78. Residual or capillary trapping contributed negligibly to the storage capacity and reached only a value of 50 million kg-mole during the whole injection process. There is also no considerable increase in the amount of free gas in the injection period. On the contrary, fraction of CO_2 dissolved in water phase followed an increasing trend and within three and half years touched the value of 260 million kg-mole. After that its value elevated till 355 million in thirty years. Gas in place also have a similar kind of trend and increased to a value of 4400 million Sm^3 when the injection process ends.

Figure-10 is showing the variation of reservoir pressure and gas injection rate with the passage of time. As the gas is injected reservoir pressure builds up sharply and ended up with 5.5 bars. Oppositely the gas injection rate declined rapidly from 5.6 million Sm^3 to 0.5 million Sm^3 in three and a half years and then gradually dropped to zero.

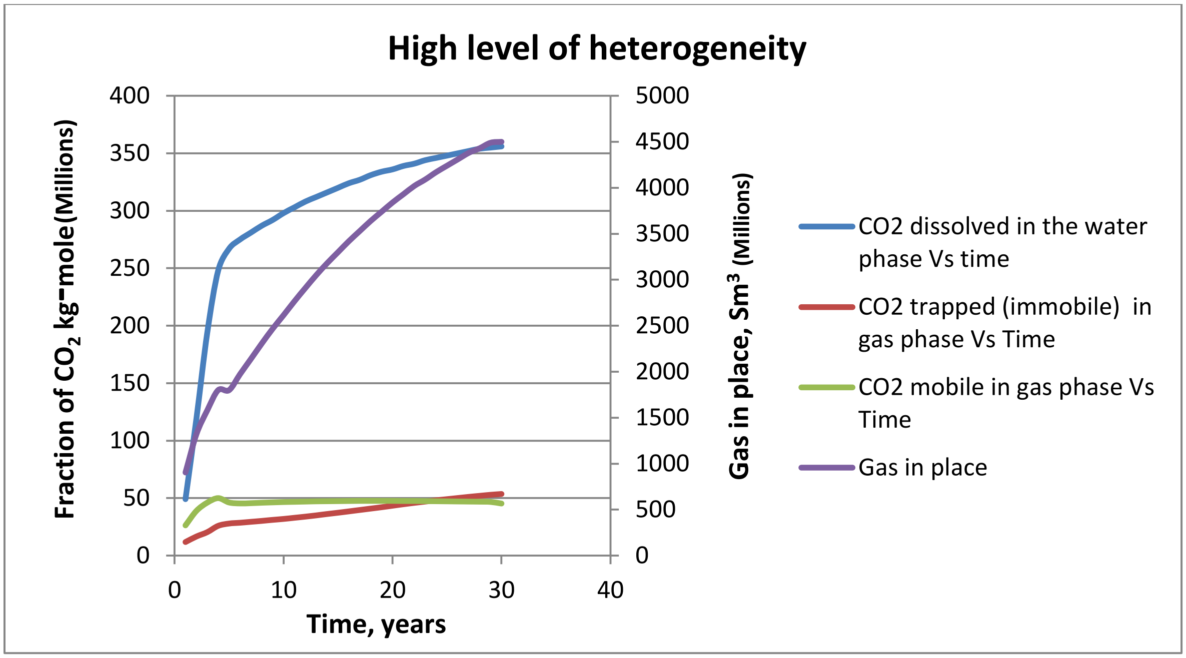

Figure 9 Fraction of injected CO_2 trapped by residual trapping/immobile (FGCDI) and solubility trapping (FWCD) and fraction as free gas (FGCDM) for 30 years of injection in aquifer with Lorenz coefficients 0.78 and porosity 0.3.

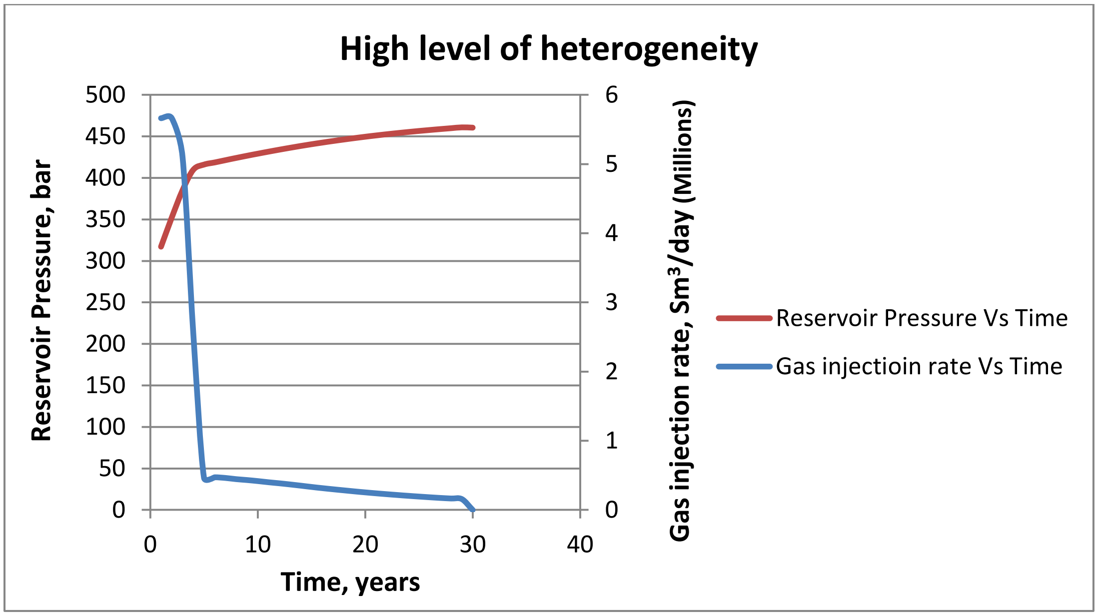

Figure 10 Field gas injection rate (FGIR) and Field reservoir pressure (FPR) for 30 years of injection in aquifer with LC 0.78 and porosity 0.3.

4.5.2 Comparison of trapping mechanism and other features of injectivity and storage for different levels of heterogeneities

Figure-11 presents the comparison of trapping mechanisms for all three cases of heterogeneities added in the aquifer model. Fractions of CO_2 dissolved in water phase (FWCD) for Lorenz coefficients 0.1, 0.5 and 0.78 exhibit that the best case for solubility trapping is the one with intermediate level of heterogeneity in the aquifer. It has increased very sharply and reached a fraction of 325 million kg-mole in first seven years of injection. Then there was gradual rise in the FWCD and at the end of injection process 360 million kg-mole of CO_2 is dissolved in water phase. FWCD for LC 0.1 follows the same trend but the solubility trapping is less in this particular case by reaching a fraction of 349 million kg-mole. But the FWCD for LC 0.78 presented different scenario because its fraction continued to increase more rapidly after five years and reached at a fraction of 358 million kg-mole which is almost equal to FWCD of LC 0.5. So it can be inferred that the most suitable case for achieving highest fraction of solubility trapping is the one in which the aquifer has intermediate level of heterogeneity and then the one with high level of heterogeneity.

If we talk about the capillary or residual trapping (FGCDI) then the trends show that the aquifer with the lowest level of heterogeneity (LC 0.1) has the highest value for the fraction of residually trapped CO_2. FGCDI for LC 0.1 ended up with a value of 85 million kg-mole. The aquifer which has the highest level of heterogeneity has the minimum fraction of residually trapped carbon dioxide in it. The fraction of trapped carbon dioxide for the aquifer with intermediate level of heterogeneity followed the trend of FGCDI for LC 0.1. But at the end it deviated and reached a lower value of 75 million kg-mole. All in all, the contribution of capillary or residual trapping mechanism is relatively higher for the storage medium which has the least level of heterogeneity in it.

FGCDM shows the fraction of CO_2 left as a free gas or mobile gas during the injection period. As the gas is injected into the aquifer there was an increase in the amount of free gas but the aquifer which is almost homogenous has the highest peak of mobile gas/ free gas in it as compared to other types of storage mediums. The peak of free gas for Lorenz coefficient 0.1 reached the value of 130 million kg-mole. On the other hand FGCDM for Lorenz coefficient 0.78 has the minimum peak of free gas with the value of 50 million kg-mole. The aquifer whose level of heterogeneity is intermediate has the peak of fraction of mobile gas in the middle of the other two cases. At the end all the cases declined to a same value of mobile or free gas in the storage medium.

Figure-12 compares the gas in place in the aquifer models with high, low and medium heterogeneities. Trends of gas in place for LC 0.1 and LC 0.5 are almost similar and the both the aquifers contain same approximately same amount of gas at the injection process which is 5350 million Sm^3. The simulation of aquifer model with intermediate heterogeneity has the lowest value of gas in place 4500 million Sm^3 among the three models.

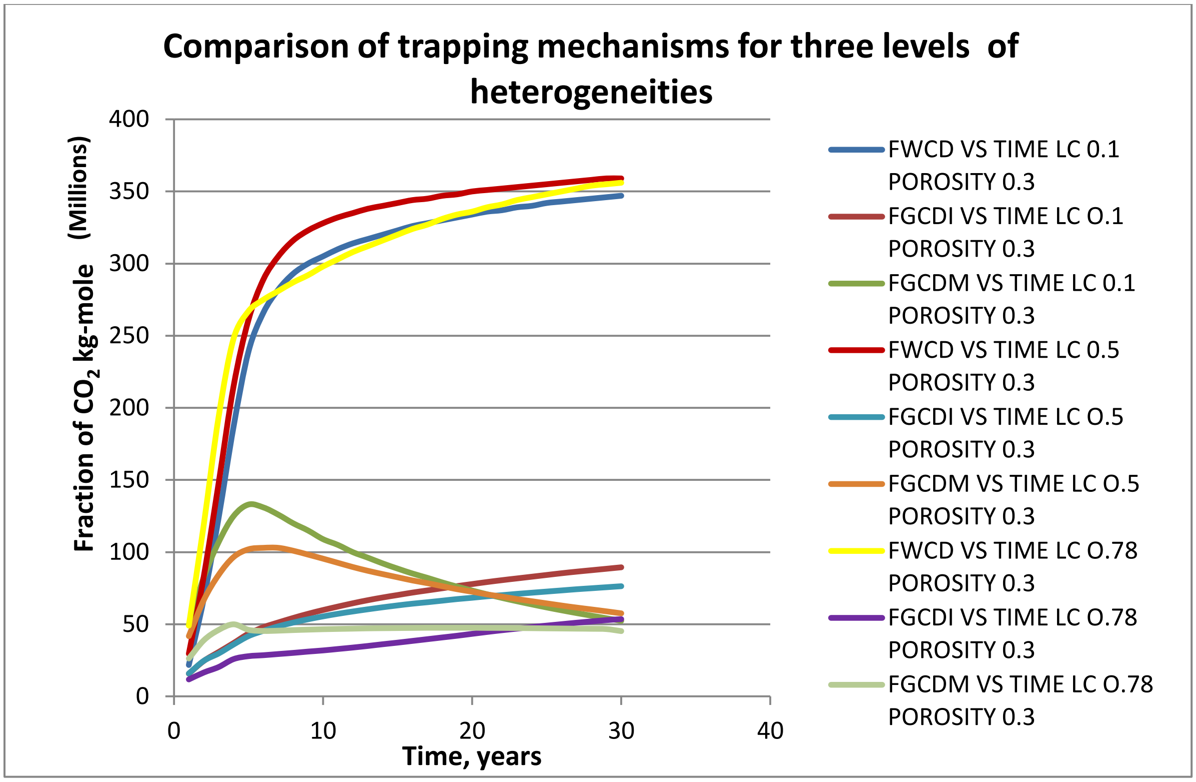

Figure 11 Comparison of trapping mechanisms of the aquifer with porosity 0.3 for three different levels of heterogeneities shown by Lorenz coefficients 0.1, 0.5 and 0.78.

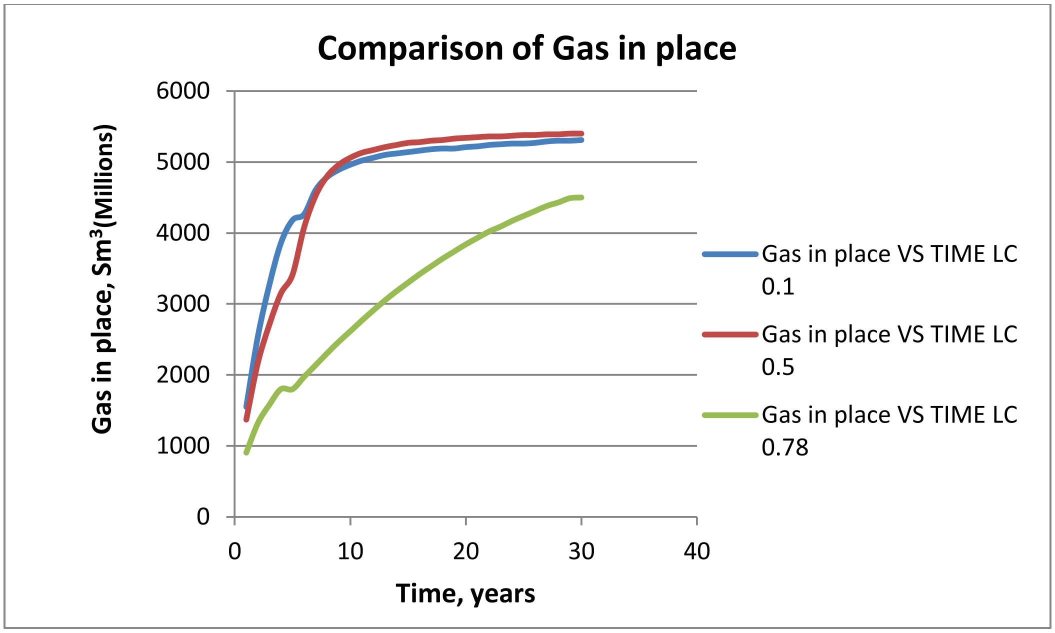

Figure 12 Gas in place for three different levels of heterogeneities in aquifer with porosity 0.3.

4.5.3 Case B: Comparison of trapping mechanism and other features of injectivity for different levels of heterogeneities in aquifer of porosity 0.2

In case (A), individual trends have been discussed for Lorenz coefficients of 0.1, 0.5, and 0.78. Individual graphs of case (B) and case (C) also exhibits similar information so in these two cases our focus is on the comparison between the aquifer models of different heterogeneities. Figure-13 Comparison of trapping mechanisms of the aquifer with porosity 0.2 for three different levels of heterogeneities showed by Lorenz coefficients 0.1, 0.5 and 0.78. In all three cases solubility trapping played very vital role in the storage of injected gas. For approximately homogenous aquifer FWCD has the least value but the other cases have higher amount of trapped CO_2 in solution with water phase. But there is very less difference between the three cases.

Oppositely, capillary trapped CO_2 has the highest fraction in case of aquifer with least heterogeneity and the highly heterogeneous aquifer has comparatively minimum amount of immobile gas. Aquifer having intermediate level of heterogeneity has the trend line of FGCDI in the middle of other two cases. For Lorenz coefficient 0.1 the fraction of trapped carbon dioxide is 70 million kg-mole and for Lorenz coefficient 0.78 the fraction is 45 million kg-mole. So there is a difference of a fraction of 25 million kg-mole which clearly depicts that homogenous aquifer is the best suitable option to achieve the highest storage capacity.

Amount of free gas is a very important parameter to evaluate the fate of CO_2 plume after the injection has stopped. The more is the mobile gas present in the storage medium less is the storage capacity. From the figure it is clear that aquifer heterogeneity has an impact on the fraction of free gas because as the injection initiated relatively homogeneous aquifer has the highest peak of FGCDM and the highly heterogeneous aquifer has the lowest peak for mobile gas fraction. And similar to the trends of other trapping mechanisms aquifer with Lorenz coefficient 0.5 has the intermediate fraction of mobile gas. As the injection starts there is a sharp increase in the amount of free gas for all three cases and after few years the fraction of gas declined.

In conclusion, from the above results we can say that the aquifer has the highest storage capacity for Lorenz coefficient 0.1 because in this case aquifer has the highest amount of CO_2 by capillary or residual trapping mechanism as compared to other two scenarios. For solubility trapping there is only a small difference between the three aquifers with different heterogeneities levels. Fraction of mobile gas is different but as the years of injection passed the FGCDM declined gradually for all three cases. Figure-14 exhibits the trends of gas in place for three values of Lorenz coefficients 0.1, 0.5, 0.78. Aquifer models of Lorenz coefficients 0.1 and 0.5 have similar trend lines throughout the injection period and have equal value of 3600 million Sm^3 at the end of injection of gas. While the gas in place for LC 0.78 increased gradually and followed different path. At the end gas in place reached a value of 340 million Sm^3.

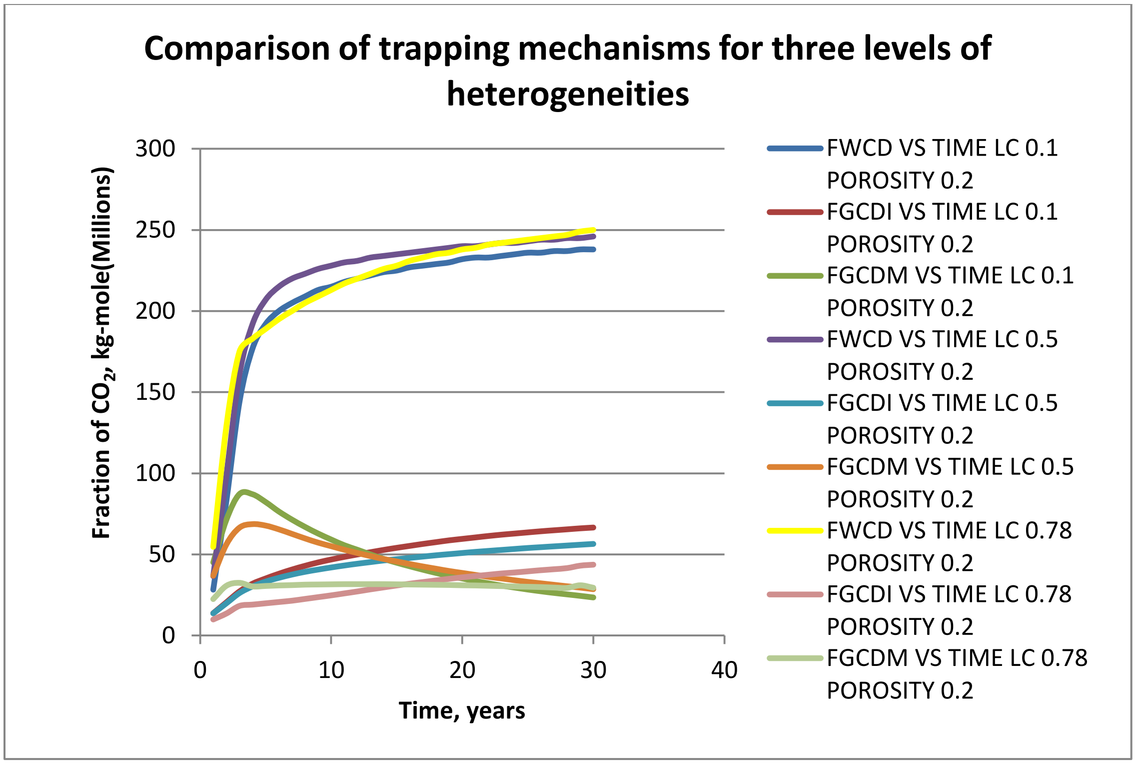

Figure 13 Comparison of trapping mechanisms of the aquifer with porosity 0.2 for three different levels of heterogeneities shown by Lorenz coefficients 0.1, 0.5 and 0.78.

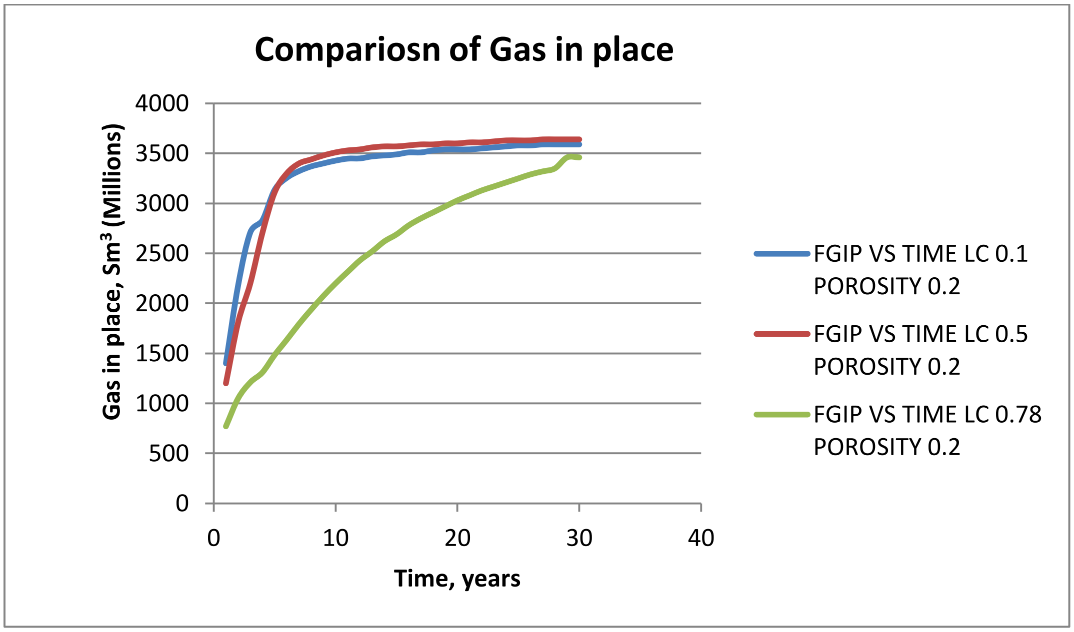

Figure 14 Gas in place for three different levels of heterogeneities in aquifer with porosity 0.2.

4.5.4 CASE C: Comparison of trapping mechanism and other features of injectivity for different levels of heterogeneities in aquifer of porosity 0.1

Trends of trapping mechanisms for three aquifer models having different permeability heterogeneities are shown in figure 15. Like previous two cases FWCD for highly heterogeneous aquifer is highest among others and the lowest one is of LC 0.1. Capillary or residual trapping is highest for least heterogeneous system and lowest for highly heterogeneous aquifer. In the previous cases the amount of free gas is more for homogenous system and less for heterogeneous system. But in this case as the injection started FGCDM is higher for LC 0.1 but as the injection proceeded further the FGCDM of LC 0.1 became lesser than FGCDM of LC 0.78. It means that for aquifer model of porosity 0.1 least heterogeneous system has lesser amount of mobile or free gas at the end of injection process. So the simulation study of this case indicates that aquifer model with the least level of heterogeneity is better for storage operation among all.

Gas in place (FGIP) is an important parameter to know about the efficiency of storage operation. FGIP for aquifer model having porosity 0.1 is calculated for three values of Lorenz coefficient. The results are shown in figure 16. FGIP of Lorenz coefficients 0.1 and 0.5 followed the same line and ended up with the same values. Gas in place of LC 0.78 started from a lower value but in the end of injection period its value is a little bit more than the other two models.

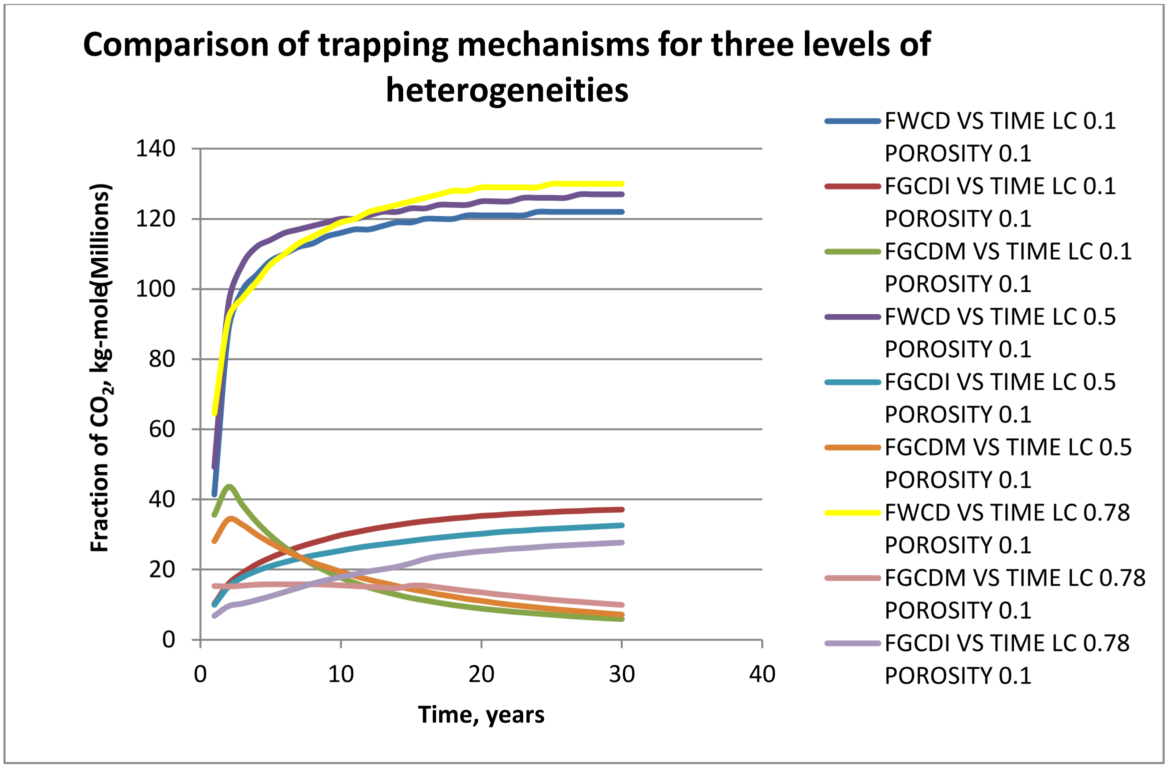

Figure 15 Comparison of trapping mechanisms of the aquifer with porosity 0.1 for three different levels of heterogeneities shown by Lorenz coefficients 0.1, 0.5 and 0.78.

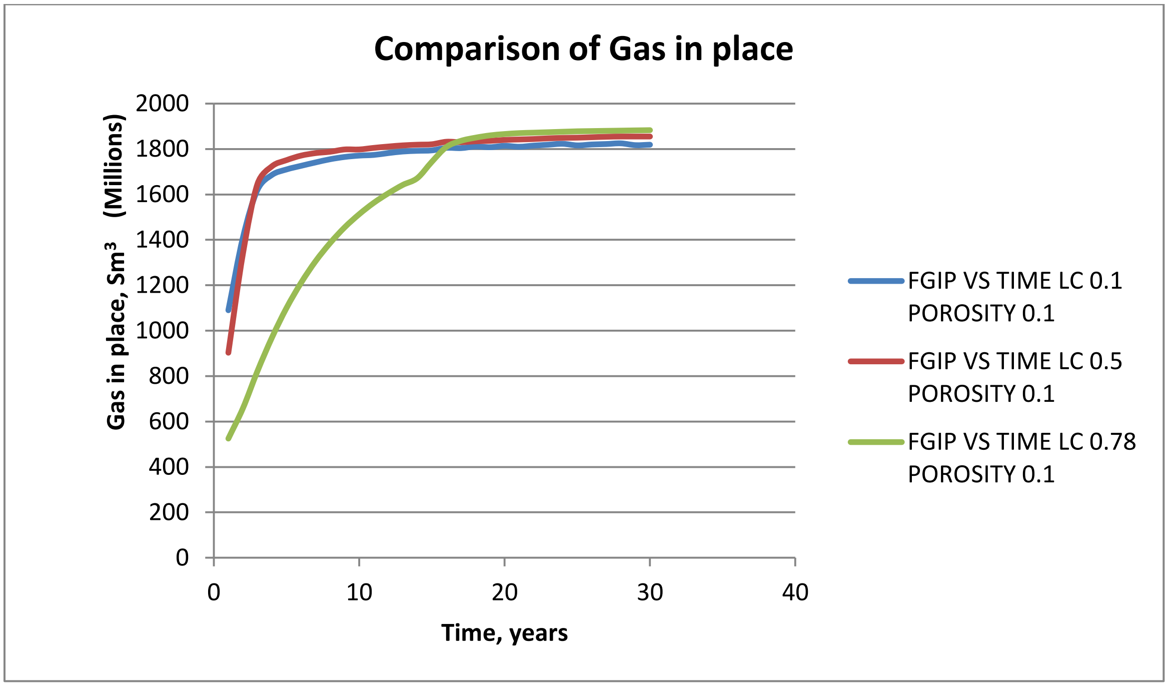

Figure 16 Gas in place for three different levels of heterogeneities in aquifer with porosity 0.1.

5 Conclusions

Greenhouse gases are increasing in the atmosphere and they are creating many health and environmental issues. In this alarming situation there is a need to mitigate these emissions, particularly CO_2 emissions, and to find an alternative to fossil fuels so that we can live in a sustainable environment. Hydrogen storage and its use in future is a new. Hydrogen has many applications in different industries but the main focus is the use of hydrogen as a fuel for vehicles. Like underground gas storage and carbon dioxide storage operation, hydrogen can be stored underground but the feasibility and long term storage capacity is the concern. Recent studies showed that there are no significant geochemical reactions of H_2 occurring with sandstone and carbonate rocks.

CO_2 storage in underground aquifers is very useful and efficient technique to get rid of a huge amount of carbon dioxide gas. A critical review has been done to discuss different aspects of CO_2 storage operation. Factors affecting storage capacity, injectivity and containment have been discussed in detail to get a thorough understanding of positive and negative indicators of carbon capture and storage process, such as aquifer characteristics, caprock integrity, fluid dynamics and geochemical reactions affect the CCS operation. So a screening criterion should be available in order to choose the best aquifer for safe and large scale storage of CO_2. In this regard, a contribution to the screening criteria which must be consider before selecting an aquifer as a storage site is presented in this project.

The degree of heterogeneities of the aquifer has an impact on the storage capacity. Structural trapping, capillary trapping, solubility trapping and mineral trapping are the four main mechanisms to trap CO_2. Permeability heterogeneity affects these trapping mechanisms and a simulation study was performed to discover the variation in the fraction of the trapped CO_2 for different levels of permeability heterogeneities. Heterogeneity calculation was done by the use of Lorenz coefficient. Three levels of heterogeneities (low, intermediate and high) expressed by Lorenz coefficients equal to 0.1, 0.5 and 0.78 were investigated.

Capillary or residual trapping, solubility trapping and mineral trapping are the trapping mechanisms. Modeling is done for three aquifer models with porosity values 0.1, 0.2, 0.3 for three different levels of permeability heterogeneity. Comparison of these results showed that solubility trapping (FWCD) is high for highly heterogeneous aquifer but the difference in the storage capacity is limited for three cases of porosities. Capillary or residual trapping has highest amount of CO_2 for least heterogeneous aquifer and the lowest for aquifer with high level of permeability heterogeneity. The difference between the fractions of CO_2 for capillary trapping for two cases of LC 0.1 and LC 0.78 is much more as compared to solubility trapping differences.

Fraction of mobile gas also plays a role on the fate of plume migration when the injection stops. At the start of injection process the amount of mobile gas is high for highly heterogeneous aquifers; and low for homogeneous aquifers but at the end all the cases reached to same value. All in all permeability heterogeneity causes the aquifer to have a lower storage capacity compared to homogeneous aquifers. So it is preferred to choose a homogenous site for CCS operation.

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APPENDIX I: TABLES FOR CALCULATION OF LORENZ COEFFICIENTS

CASE A: POROSITY 0.3 LC 0.1

h (ft)	k (md)	ϕ	kh	ϕh	Sum kh	F Sum kh/total kh	sum ϕh	C Sumϕh/ total ϕh	Bar width	Bar height	Bar Area
0			0		0	0	0	0	0	0	0
5	1000	0.3	5000	1.5	5000	0.20255216	1.5	0.2	0.2	0.3028155	0.060563
5	990	0.3	4950	1.5	9950	0.40307879	3	0.4	0.2	0.5028357	0.100567
5	985	0.3	4925	1.5	14875	0.60259267	4.5	0.6	0.2	0.7020458	0.140409
5	982	0.3	4910	1.5	19785	0.80149889	6	0.8	0.2	0.9007494	0.18015
5	980	0.3	4900	1.5	24685	1	7.5	1	0.2	0.5	0.1
			Total 24685	7.5							Total Area 0.581689

Lorenz Coefficient 0.5

h (ft)	k (md)	ϕ	kh	ϕh	Sum kh	F sum kh/total kh	sum ϕh	C Sum ϕh/ total ϕh	Bar width	Bar height	Bar Area
0	0		0		0	0	0	0	0	0	0
5	1000	0.3	5000	1.5	5000	0.37878788	1.5	0.2	0.2	0.530303	0.106061
5	800	0.3	4000	1.5	9000	0.68181818	3	0.4	0.2	0.7954545	0.159091
5	600	0.3	3000	1.5	12000	0.90909091	4.5	0.6	0.2	0.9393939	0.187879
5	160	0.3	800	1.5	12800	0.96969697	6	0.8	0.2	0.9848485	0.19697
5	80	0.3	400	1.5	13200	1	7.5	1	0.2	0.5	0.1
			Total 13200	7.5							Total Area 0.75

Lorenz coefficient 0.78

h (ft)	k (md)	ϕ	kh	ϕh	Sum kh	F Sum kh/total kh	sum ϕh	C Sum ϕh/ total ϕh	Bar width	Bar height	Bar Area
0			0		0	0	0	0	0	0	0
5	1200	0.3	6000	1.5	6000	0.94936709	1.5	0.2	0.2	0.9651899	0.193038
5	40	0.3	200	1.5	6200	0.98101266	3	0.4	0.2	0.9889241	0.197785
5	20	0.3	100	1.5	6300	0.99683544	4.5	0.6	0.2	0.9976266	0.199525
5	2	0.3	10	1.5	6310	0.99841772	6	0.8	0.2	0.9992089	0.199842
5	2	0.3	10	1.5	6320	1	7.5	1	0.2	0.5	0.1
			Total 6320	7.5							**Total Area** 0.89019

CASE B: POROSITY 0.2 LC 0.1

h (ft)	k (md)	ϕ	kh	ϕh	Sum kh	F Sum kh/total kh	Sum ϕh	C Sum ϕh/ total ϕh	Bar width	Bar height	Bar Area
0			0		0	0	0	0	0	0	0
5	1000	0.2	5000	1	5000	0.20255216	1	0.2	0.2	0.3028155	0.060563
5	990	0.2	4950	1	9950	0.40307879	2	0.4	0.2	0.5028357	0.100567
5	985	0.2	4925	1	14875	0.60259267	3	0.6	0.2	0.7020458	0.140409
5	982	0.2	4910	1	19785	0.80149889	4	0.8	0.2	0.9007494	0.18015
5	980	0.2	4900	1	24685	1	5	1	0.2	0.5	0.1
			Total 24685	5							**Total area** 0.581689

Zain Rasheed

LC 0.5

h (ft)	k (md)	ϕ	kh	ϕh	Sum kh	F Sum kh/total kh	Sum ϕh	C Sum ϕh/ total ϕh	Bar width	Bar height	Bar Area
0	0	0	0	0	0	0	0	0	0	0	0
5	1000	0.2	5000	1	5000	0.37878788	1	0.2	0.2	0.530303	0.106061
5	800	0.2	4000	1	9000	0.68181818	2	0.4	0.2	0.7954545	0.159091
5	600	0.2	3000	1	12000	0.90909091	3	0.6	0.2	0.9393939	0.187879
5	160	0.2	800	1	12800	0.96969697	4	0.8	0.2	0.9848485	0.19697
5	80	0.2	400	1	13200	1	5	1	0.2	0.5	0.1
			Total 13200	5							**Total Area** 0.75

LC 0.78

h (ft)	k (md)	ϕ	kh	ϕh	Sum kh	F Sum kh/total kh	Sum ϕh	C Sum ϕh/ total ϕh	Bar width	Bar height	Bar Area
0			0		0	0	0	0	0	0	0
5	1200	0.2	6000	1	6000	0.94936709	1	0.2	0.2	0.9651899	0.193038
5	40	0.2	200	1	6200	0.98101266	2	0.4	0.2	0.9889241	0.197785
5	20	0.2	100	1	6300	0.99683544	3	0.6	0.2	0.9976266	0.199525
5	2	0.2	10	1	6310	0.99841772	4	0.8	0.2	0.9992089	0.199842
5	2	0.2	10	1	6320	1	5	1	0.2	0.5	0.1
			Total 6320	5							**Total Area** 0.89019

CASE C: POROSITY 0.1 **LC 0.1**

h (ft)	k (md)	ϕ	kh	ϕh	Sum kh	F Sum kh/total kh	Sum ϕh	C Sum ϕh/ total ϕh	Bar width	Bar height	Bar Area
0			0		0	0	0	0	0	0	0
5	1000	0.1	5000	0.5	5000	0.20255216	0.5	0.2	0.2	0.3028155	0.060563
5	990	0.1	4950	0.5	9950	0.40307879	1	0.4	0.2	0.5028357	0.100567
5	985	0.1	4925	0.5	14875	0.60259267	1.5	0.6	0.2	0.7020458	0.140409
5	982	0.1	4910	0.5	19785	0.80149889	2	0.8	0.2	0.9007494	0.18015
5	980	0.1	4900	0.5	24685	1	2.5	1	0.2	0.5	0.1
			Total 24685	2.5							**Total Area** 0.581689

LC 0.5

h (ft)	k (md)	ϕ	kh	ϕh	Sum kh	F Sum kh/total kh	Sum ϕh	C Sum ϕh/ total ϕh	Bar width	Bar height	Bar Area
0			0		0	0	0	0	0	0	0
5	1000	0.1	5000	0.5	5000	0.37878788	0.5	0.2	0.2	0.530303	0.106061
5	800	0.1	4000	0.5	9000	0.68181818	1	0.4	0.2	0.7954545	0.159091
5	600	0.1	3000	0.5	12000	0.90909091	1.5	0.6	0.2	0.9393939	0.187879
5	160	0.1	800	0.5	12800	0.96969697	2	0.8	0.2	0.9848485	0.19697
5	80	0.1	400	0.5	13200	1	2.5	1	0.2	0.5	0.1
			Total 13200	2.5							**Total Area** 0.75

LC 0.78

h (ft)	k (md)	ϕ	kh	ϕh	Sum kh	F Sum kh/total kh	Sum ϕh	C Sum ϕh/ total ϕh	Bar width	Bar height	Bar Area
0			0		0	0	0	0	0	0	0
5	1200	0.1	6000	0.5	6000	0.94936709	0.5	0.2	0.2	0.9651899	0.193038
5	40	0.1	200	0.5	6200	0.98101266	1	0.4	0.2	0.9889241	0.197785
5	20	0.1	100	0.5	6300	0.99683544	1.5	0.6	0.2	0.9976266	0.199525
5	2	0.1	10	0.5	6310	0.99841772	2	0.8	0.2	0.9992089	0.199842
5	2	0.1	10	0.5	6320	1	2.5	1	0.2	0.5	0.1
			Total 6320	2.5							**Total Area** 0.89019

APPENDIX II

Trends for Lorenz Coefficients

Input data for Case A

```
------------------------------------------------------------------------

-->    CO2 storage example

------------------------------------------------------------------------

RUNSPEC

METRIC
```

```
-- Capillary pressure mode
-- PW = P - PC
-- PG = P
OPTIONS3
  7* 1 /
-- Include diffusion
DIFFUSE
--Four components in study.
COMPS
 4 /
DIMENS
19 28 5/
TABDIMS
 1 1 40 40 /
ROCKCOMP
REVERS 2/
CO2STORE
FULLIMP
SOLID
START
 1 JAN 2015 /
UNIFOUT
UNIFIN
--Grid section-------------------------------------------------------
-----------------------------------------------------------------------
```

```
-- 2. Grid (Required)
--The GRID section determines the basic geometry of the simulation grid and
--various rock properties (porosity, absolute permeability, net-to-gross
--ratios) in each grid cell. From this information, the program calculates the
--grid block pore volumes, mid-point depths and inter-block
--transmissibilities.
-------------------------------------------------------------------------
GRID
DX
2660*100 /
DY
2660*100 /
DZ
2660*5 /
EQUALS
--    ARRAY    VALUE      ------ BOX ------
    'DZ'      5         1 19 1 28 1 1  /  LAYER 1
    'PERMX'   1000   /
    'PORO'    0.3   /
     TOPS     2000/
    'DZ'      5         1 19 1 28 2 2  /  LAYER 2
    'PERMX'   990    /
    'PORO'    0.3    /
     TOPS     2010/
    'DZ'      5         1 19 1 28 3 3  /  LAYER 3
```

```
      'PERMX'   985    /
      'PORO'    0.3    /
       TOPS     2015/
      'DZ'      5         1 19 1 28 4 4  /  LAYER 4
      'PERMX'   982    /
      'PORO'    0.3    /
       TOPS    2020/


      'DZ'      5         1 19 1 28 5 5  /  LAYER 5
      'PERMX'   980     /
      'PORO'    0.3    /
       TOPS    2025/
/ EQUALS IS TERMINATED BY A NULL RECORD
-- THE Y AND Z DIRECTION PERMEABILITIES ARE COPIED FROM PERMX
-- SOURCE DESTINATION      ------- BOX --------
COPY
      'PERMX'  'PERMZ'     1 19 1 28 1 5  /
      'PERMX'  'PERMY'     /
/
ACTNUM
/
--Depth of cell centres
--MIDS
--2660*840/
--Depth of cell centres
```

```
-- request init and grid file, necessary for post processing
INIT
GRIDFILE
1 /
------------------------------------------------------------------------
-- 3. EDIT (Optional) Instructions for modifying the pore volumes, block
--center depths, transmissibilities, diffusivities (for the Molecular
--Diffusion option), and nonneighbor connections (NNCs) computed by the
--program from the data entered in the GRID section.
------------------------------------------------------------------------
EDIT
-- Modify pore volumes of boundary blocks to simulate constant-pressure
MULTIPLY
-- Array Constant Box
  PORV  1000    19 19  2  2  1  1 /
  PORV  1000    18 18  3  6  1  1 /
  PORV  1000    19 19  7 22  1  1 /
  PORV  1000    18 18 23 24  1  1 /
  PORV  1000    16 17 25 25  1  1 /
  PORV  1000    14 15 26 26  1  1 /
  PORV  1000    12 13 27 27  1  1 /
  PORV  1000     4 11 28 28  1  1 /
  PORV  1000     3  3 27 27  1  1 /
  PORV  1000     2  2 26 27  1  1 /
  PORV  1000     1  1 23 25  1  1 /
```

```
  PORV  1000    2  2 16 22  1  1 /
  PORV  1000    3  3 15 15  1  1 /
  PORV  1000    4  4 13 14  1  1 /
  PORV  1000    5  5 10 12  1  1 /
  PORV  1000    6  6  8  9  1  1 /
  PORV  1000    7  7  7  7  1  1 /
  PORV  1000    8  8  6  6  1  1 /
  PORV  1000    9  9  5  5  1  1 /
  PORV  1000   10 10  4  4  1  1 /
  PORV  1000   11 13  3  3  1  1 /
  PORV  1000   14 14  2  2  1  1 /
  PORV  1000   15 18  1  1  1  1 /
/

--Properties section-----------------------------------------------
PROPS
CNAMES
  'H2O' 'CO2' 'NACL'  'CACL2' /
ZMFVD
-- depth  h20  co2  nacl  cacl2
 2000       0.9109 0.0  0.0741     0.015
 2500       0.9109 0.0  0.0741     0.015 /
-- Solid component NACL_S referece density
SDREF
 3* 135 1* /
```

```
-- Mobility multiplier
SOLIDMMS
-- SS   Mult
   0.0    1.0
   0.1    0.5
   0.8    0.0 /--
-- Set diffusion constants (example)
--DIFFCWAT
-- h2o   co2   nacl         cacl2
  0.0001  0.0001  0.0001     0.0001 /


DIFFCGAS
--  h2o  co2
   0.001 0.001  /
-- Temp in deg F
RTEMP
 100 /
-- Water saturation functions
WSF
--   Sw        Krw
--  -----     -----
    0.3       0.0
    0.38      0.000152
    0.46      0.002439
    0.53      0.012346
```

```
   0.61      0.039018
   0.69      0.09526
   0.77      0.197531
   0.84      0.36595
   0.92      0.624295
   1.0       1.0     /



-- Gas saturation functions
GSF
--   Sg        Krg      Drain Pcog
--  -----      ------    ----------
   0.0       0.0        0.
   0.08      0.0        0.6
   0.16      0.000407    0.78
   0.23      0.005831    0.93
   0.31      0.024131    1.09
   0.39      0.064892    1.26
   0.47      0.140566    1.49
   0.54      0.269314    1.84
   0.62      0.484797    2.53
   0.7       1.0        10.0   /
/
--G 0.97---
--OVERBURD
```

```
--2000 720
--2010 780
--2020 832
--/

--ROCKOPTS
--STRESS NOSTORE/
--/
--ROCKTAB
--300 .86 .90
--420 0.89. 0.96 /
/
--Rock data
--Solution section------------------------------------------------------
SOLUTION
--Equilibration data
EQUIL
 2020 278 0.0 0 0.0 0 2 2 0  /
RPTRST
 RESTART PRESSURE SGAS SWAT DENG DENW VGAS VWAT XMF AQSP AQPH SSOLID /
RPTSOL
 PRESSURE SGAS SWAT DENG DENW VGAS VWAT XMF AQSP AQPH SSOLID /
FIELDSEP
 1 41 50 /
/
```

```
SUMMARY    ============================================================
RUNSUM
FPR
FGIPL
FGIPG
FGIR
FPRP
FWCD
FGCDI
FGCDM
WBHP
 CO2_INJ /
/
RUNSUM
--Schedule section------------------------------------------------------
RPTONLY
SCHEDULE
-- Lower throughput target and solution change target for aim selection
-- and increase implicitness, do eval every time step.
RPTSCHED
 PRESSURE SGAS SWAT DENG DENW VGAS VWAT XMF AQPH SSOLID /
--Define injection well
WELSPECS
 'CO2_INJ' FIELD 10 10 2024 GAS /
```

```
/

COMPDAT

 'CO2_INJ' 10 10 1 4 1* 1* 1* 0.1524 10000 2* 'Z' /

/

WELLSTRE

 'SeqCO2' 0.0 1.0 /

/

WINJGAS

 'CO2_INJ' STREAM 'SeqCO2' /

/

--

-- BHP LIMIT 482.6 BARS

--

WCONINJE

 'CO2_INJ' GAS OPEN RATE 5663369 1* 482.6 /

/

DATES

1 JAN 2016 /

1 JAN 2017 /

1 JAN 2018 /

1 JAN 2019 /

1 JAN 2020 /

1 JAN 2021 /

1 JAN 2022 /

1 JAN 2023 /
```

```
1 JAN 2024 /
1 JAN 2025 /
1 JAN 2026 /
1 JAN 2027 /
1 JAN 2028 /
1 JAN 2029 /
1 JAN 2030 /
1 JAN 2031 /
1 JAN 2032 /
1 JAN 2033 /
1 JAN 2034 /
1 JAN 2035 /
1 JAN 2036 /
1 JAN 2037 /
1 JAN 2038 /
1 JAN 2039 /
1 JAN 2040 /
1 JAN 2041 /
1 JAN 2042 /
1 JAN 2043 /
1 JAN 2044 /
/
WELLSHUT
'CO2_INJ' /
/
```

```
DATES

 1 JAN 2045 /

/

END
```

APPENDIX III:

Input data for Case B (LORENZ COEFFICIENT 0.5)

```
----------------------------------------------------------------------

-->    CO2 storage example

-----------------------------------------------------------------------

RUNSPEC

METRIC

-- Capillary pressure mode

-- PW = P - PC

-- PG = P

OPTIONS3

  7* 1 /

-- Include diffusion

DIFFUSE

--Four components in study.

COMPS

 4 /

DIMENS

19 28 5/
```

```
TABDIMS

 1 1 40 40 /

ROCKCOMP

REVERS 2/



CO2STORE

FULLIMP

SOLID

START

 1 JAN 2015 /

UNIFOUT

UNIFIN

--Grid section----------------------------------------------------------

---------------------------------------------------------------------------

-- 2. Grid (Required)

--The GRID section determines the basic geometry of the simulation grid and

--various rock properties (porosity, absolute permeability, net-to-gross

--ratios) in each grid cell. From this information, the program calculates the

--grid block pore volumes, mid-point depths and inter-block

--transmissibilities.

---------------------------------------------------------------------------

GRID

DX

2660*100 /

DY
```

```
2660*100 /

DZ

2660*5 /

EQUALS

--    ARRAY    VALUE      ------ BOX ------

      'DZ'      5         1 19 1 28 1 1  /  LAYER 1

      'PERMX'   1000   /

      'PORO'    0.3   /

       TOPS     2000/



      'DZ'      5         1 19 1 28 2 2  /  LAYER 2

      'PERMX'   800    /

      'PORO'    0.3    /

       TOPS     2010/

      'DZ'      5         1 19 1 28 3 3  /  LAYER 3

      'PERMX'   600    /

      'PORO'    0.3    /

       TOPS     2015/

      'DZ'      5         1 19 1 28 4 4  /  LAYER 4

      'PERMX'   160    /

      'PORO'    0.3    /

       TOPS    2020/

      'DZ'      5         1 19 1 28 5 5  /  LAYER 5

      'PERMX'   80    /

      'PORO'    0.3    /
```

```
    TOPS    2025/

/ EQUALS IS TERMINATED BY A NULL RECORD



-- THE Y AND Z DIRECTION PERMEABILITIES ARE COPIED FROM PERMX

-- SOURCE DESTINATION      ------- BOX --------

COPY

   'PERMX'  'PERMZ'     1 19 1 28 1 5  /

   'PERMX'  'PERMY'     /

/

ACTNUM




 /

--Depth of cell centres

--MIDS

--2660*840/

--Depth of cell centres

-- request init and grid file, necessary for post processing

INIT

GRIDFILE

1 /

-------------------------------------------------------------------------

-- 3. EDIT (Optional) Instructions for modifying the pore volumes, block

--center depths, transmissibilities, diffusivities (for the Molecular
```

```
--Diffusion option), and nonneighbor connections (NNCs) computed by the

--program from the data entered in the GRID section.

-----------------------------------------------------------------------

EDIT



-- Modify pore volumes of boundary blocks to simulate constant-pressure

MULTIPLY

-- Array Constant Box

  PORV  1000    19 19  2  2  1  1 /

  PORV  1000    18 18  3  6  1  1 /

  PORV  1000    19 19  7 22  1  1 /

  PORV  1000    18 18 23 24  1  1 /

  PORV  1000    16 17 25 25  1  1 /

  PORV  1000    14 15 26 26  1  1 /

  PORV  1000    12 13 27 27  1  1 /

  PORV  1000     4 11 28 28  1  1 /

  PORV  1000     3  3 27 27  1  1 /

  PORV  1000     2  2 26 27  1  1 /

  PORV  1000     1  1 23 25  1  1 /

  PORV  1000     2  2 16 22  1  1 /

  PORV  1000     3  3 15 15  1  1 /

  PORV  1000     4  4 13 14  1  1 /

  PORV  1000     5  5 10 12  1  1 /

  PORV  1000     6  6  8  9  1  1 /

  PORV  1000     7  7  7  7  1  1 /
```

```
  PORV  1000    8  8  6  6  1  1 /
  PORV  1000    9  9  5  5  1  1 /
  PORV  1000   10 10  4  4  1  1 /
  PORV  1000   11 13  3  3  1  1 /
  PORV  1000   14 14  2  2  1  1 /
  PORV  1000   15 18  1  1  1  1 /
/


--Properties section---------------------------------------------


PROPS


CNAMES
  'H2O' 'CO2' 'NACL'  'CACL2' /


ZMFVD
-- depth  h20  co2  nacl  cacl2
 2000       0.9109 0.0  0.0741     0.015
 2500       0.9109 0.0  0.0741     0.015 /


-- Solid component NACL_S referece density
SDREF
 3* 135 1* /


-- Mobility multiplier
```

```
SOLIDMMS
-- SS   Mult
   0.0    1.0
   0.1    0.5
   0.8    0.0 /
--
-- Set diffusion constants (example)
--
DIFFCWAT
-- h2o   co2   nacl         cacl2
  0.0001  0.0001  0.0001     0.0001 /

DIFFCGAS
--  h2o  co2
   0.001 0.001  /

-- Temp in deg F
RTEMP
 100 /

-- Water saturation functions
WSF
--   Sw        Krw
--  -----     -----
    0.3       0.0
```

```
   0.38      0.000152
   0.46      0.002439
   0.53      0.012346
   0.61      0.039018
   0.69      0.09526
   0.77      0.197531
   0.84      0.36595
   0.92      0.624295
   1.0       1.0     /
-- Gas saturation functions
GSF
--   Sg        Krg      Drain Pcog
--  -----     ------    ----------
   0.0       0.0        0.
   0.08      0.0         0.6
   0.16      0.000407    0.78
   0.23      0.005831    0.93
   0.31      0.024131    1.09
   0.39      0.064892    1.26
   0.47      0.140566    1.49
   0.54      0.269314    1.84
   0.62      0.484797    2.53
   0.7       1.0        10.0   /
/
--G 0.97---
```

```
--OVERBURD
--2000 720
--2010 780
--2020 832
--/

--ROCKOPTS
--STRESS NOSTORE/
--/
--ROCKTAB
--300 .86 .90
--420 0.89. 0.96 /
/
--Rock data
--Solution section-----------------------------------------------------
SOLUTION
--Equilibration data
EQUIL
 2020 278 0.0 0 0.0 0 2 2 0  /
RPTRST
 RESTART PRESSURE SGAS SWAT DENG DENW VGAS VWAT XMF AQSP AQPH SSOLID /
RPTSOL
 PRESSURE SGAS SWAT DENG DENW VGAS VWAT XMF AQSP AQPH SSOLID /
FIELDSEP
 1 41 50 /
```

```
/
SUMMARY    ============================================================
FPR
FGIPL--
FGIPG--
FGIR
FPRP
FWCD--soluble
FGCDI--
FGCDM--
  --field gas in place
WBHP
 CO2_INJ /
/
RUNSUM
--Schedule section-------------------------------------------------------
RPTONLY
SCHEDULE
-- Lower throughput target and solution change target for aim selection
-- and increase implicitness, do eval every time step.
RPTSCHED
 PRESSURE SGAS SWAT DENG DENW VGAS VWAT XMF AQPH SSOLID /
--Define injection well
WELSPECS
 'CO2_INJ' FIELD 10 10 2024 GAS /
```

```
/
COMPDAT
 'CO2_INJ' 10 10 1 4 1* 1* 1* 0.1524 10000 2* 'Z' /
/
WELLSTRE
 'SeqCO2' 0.0 1.0 /
/
WINJGAS
 'CO2_INJ' STREAM 'SeqCO2' /
/
--
-- BHP LIMIT 482.6 BARS
--
WCONINJE
 'CO2_INJ' GAS OPEN RATE 5663369 1* 482.6 /
/
DATES
1 JAN 2016 /
1 JAN 2017 /
1 JAN 2018 /
1 JAN 2019 /
1 JAN 2020 /
1 JAN 2021 /
1 JAN 2022 /
1 JAN 2023 /
```

```
1 JAN 2024 /
1 JAN 2025 /
1 JAN 2026 /
1 JAN 2027 /
1 JAN 2028 /
1 JAN 2029 /
1 JAN 2030 /
1 JAN 2031 /
1 JAN 2032 /
1 JAN 2033 /
1 JAN 2034 /
1 JAN 2035 /
1 JAN 2036 /
1 JAN 2037 /
1 JAN 2038 /
1 JAN 2039 /
1 JAN 2040 /
1 JAN 2041 /
1 JAN 2042 /
1 JAN 2043 /
1 JAN 2044 /
/
WELLSHUT
'CO2_INJ' /
/
```

```
DATES
 1 JAN 2045 /
/
END
```

APPENDIX IV

Input data for CASE C (LORENZ COEFFICIENT 0.78):

```
------------------------------------------------------------------------
-->    CO2 storage example
-------------------------------------------------------------------------
RUNSPEC
METRIC
-- Capillary pressure mode
-- PW = P - PC
-- PG = P
OPTIONS3
  7* 1 /
-- Include diffusion
DIFFUSE
--Four components in study.
COMPS
 4 /

DIMENS
19 28 5/
```

```
TABDIMS

 1 1 40 40 /

ROCKCOMP

REVERS 2/

CO2STORE

FULLIMP

SOLID

START

 1 JAN 2015 /


UNIFOUT

UNIFIN


--Grid section-----------------------------------------------------------


--------------------------------------------------------------------------

-- 2. Grid (Required)

--The GRID section determines the basic geometry of the simulation grid and

--various rock properties (porosity, absolute permeability, net-to-gross

--ratios) in each grid cell. From this information, the program calculates the

--grid block pore volumes, mid-point depths and inter-block

--transmissibilities.

--------------------------------------------------------------------------

GRID

DX
```

```
2660*100 /
DY
2660*100 /
DZ
2660*5 /

EQUALS
--     ARRAY    VALUE       ------ BOX ------

      'DZ'      5         1 19 1 28 1 1  /  LAYER 1
      'PERMX'   1200   /
      'PORO'    0.3   /
       TOPS     2000/

      'DZ'      5         1 19 1 28 2 2  /  LAYER 2
      'PERMX'   40    /
      'PORO'    0.3    /
       TOPS     2010/

      'DZ'      5         1 19 1 28 3 3  /  LAYER 3
      'PERMX'   20    /
      'PORO'    0.3    /
       TOPS     2015/

      'DZ'      5         1 19 1 28 4 4  /  LAYER 4
```

```
      'PERMX'   2    /

      'PORO'    0.3    /

       TOPS    2020/

      'DZ'      5         1 19 1 28 5 5  /  LAYER 5

      'PERMX'   2     /

      'PORO'    0.3    /

       TOPS    2025/

/ EQUALS IS TERMINATED BY A NULL RECORD

-- THE Y AND Z DIRECTION PERMEABILITIES ARE COPIED FROM PERMX

-- SOURCE DESTINATION      ------- BOX --------

COPY

      'PERMX'  'PERMZ'     1 19 1 28 1 5  /

      'PERMX'  'PERMY'     /

/

ACTNUM




 /

--Depth of cell centres

--MIDS

--2660*840/

--Depth of cell centres

-- request init and grid file, necessary for post processing

INIT

GRIDFILE
```

```
1 /
--------------------------------------------------------------------------
-- 3. EDIT (Optional) Instructions for modifying the pore volumes, block
--center depths, transmissibilities, diffusivities (for the Molecular
--Diffusion option), and nonneighbor connections (NNCs) computed by the
--program from the data entered in the GRID section.
--------------------------------------------------------------------------
EDIT

-- Modify pore volumes of boundary blocks to simulate constant-pressure

MULTIPLY
-- Array Constant Box
  PORV  1000    19 19  2  2  1  1 /
  PORV  1000    18 18  3  6  1  1 /
  PORV  1000    19 19  7 22  1  1 /
  PORV  1000    18 18 23 24  1  1 /
  PORV  1000    16 17 25 25  1  1 /
  PORV  1000    14 15 26 26  1  1 /
  PORV  1000    12 13 27 27  1  1 /
  PORV  1000     4 11 28 28  1  1 /
  PORV  1000     3  3 27 27  1  1 /
  PORV  1000     2  2 26 27  1  1 /
  PORV  1000     1  1 23 25  1  1 /
  PORV  1000     2  2 16 22  1  1 /
```

```
  PORV  1000    3  3 15 15  1  1 /
  PORV  1000    4  4 13 14  1  1 /
  PORV  1000    5  5 10 12  1  1 /
  PORV  1000    6  6  8  9  1  1 /
  PORV  1000    7  7  7  7  1  1 /
  PORV  1000    8  8  6  6  1  1 /
  PORV  1000    9  9  5  5  1  1 /
  PORV  1000   10 10  4  4  1  1 /
  PORV  1000   11 13  3  3  1  1 /
  PORV  1000   14 14  2  2  1  1 /
  PORV  1000   15 18  1  1  1  1 /
/
--Properties section-----------------------------------------------
PROPS
CNAMES
 'H2O' 'CO2' 'NACL'  'CACL2' /


ZMFVD
-- depth  h20  co2  nacl  cacl2
 2000       0.9109 0.0  0.0741     0.015
 2500       0.9109 0.0  0.0741     0.015 /


-- Solid component NACL_S referece density
SDREF
 3* 135 1* /
```

```
-- Mobility multiplier
SOLIDMMS
-- SS   Mult
   0.0    1.0
   0.1    0.5
   0.8    0.0 /
--
-- Set diffusion constants (example)
--
DIFFCWAT
-- h2o   co2   nacl         cacl2
  0.0001  0.0001  0.0001     0.0001 /

DIFFCGAS
--  h2o  co2
   0.001 0.001  /

-- Temp in deg F
RTEMP
 100 /

-- Water saturation functions
WSF
--   Sw        Krw
```

```
--  -----     -----

   0.3       0.0

   0.38      0.000152

   0.46      0.002439

   0.53      0.012346

   0.61      0.039018

   0.69      0.09526

   0.77      0.197531

   0.84      0.36595

   0.92      0.624295

   1.0       1.0     /




-- Gas saturation functions

GSF

--   Sg        Krg     Drain Pcog

--  -----     ------    ----------

   0.0       0.0        0.

   0.08      0.0        0.6

   0.16      0.000407    0.78

   0.23      0.005831    0.93

   0.31      0.024131    1.09

   0.39      0.064892    1.26

   0.47      0.140566    1.49

   0.54      0.269314    1.84
```

```
   0.62      0.484797    2.53
   0.7       1.0         10.0   /
/
--G 0.97---
--OVERBURD
--2000 720
--2010 780
--2020 832
--/

--ROCKOPTS
--STRESS NOSTORE/
--/
--ROCKTAB
--300 .86 .90
--420 0.89. 0.96 /
/
--Rock data

--Solution section-----------------------------------------------------

SOLUTION

--Equilibration data
EQUIL
```

```
 2020 278 0.0 0 0.0 0 2 2 0  /

RPTRST

 RESTART PRESSURE SGAS SWAT DENG DENW VGAS VWAT XMF AQSP AQPH SSOLID /

RPTSOL

 PRESSURE SGAS SWAT DENG DENW VGAS VWAT XMF AQSP AQPH SSOLID /

FIELDSEP

 1 41 50 /

/

SUMMARY    ==============================================================

FPR

FGIPL--

FGIPG--

FGIR

FPRP

FWCD--soluble

FGCDI--

FGCDM--

  --field gas in place

WBHP

 CO2_INJ /



/



RUNSUM
```

```
--Schedule section-----------------------------------------------------


RPTONLY
SCHEDULE
-- Lower throughput target and solution change target for aim selection
-- and increase implicitness, do eval every time step.
RPTSCHED
 PRESSURE SGAS SWAT DENG DENW VGAS VWAT XMF AQPH SSOLID /
--Define injection well
WELSPECS
 'CO2_INJ' FIELD 10 10 2024 GAS /
/
COMPDAT
 'CO2_INJ' 10 10 1 4 1* 1* 1* 0.1524 10000 2* 'Z' /
/
WELLSTRE
 'SeqCO2' 0.0 1.0 /
/

WINJGAS
 'CO2_INJ' STREAM 'SeqCO2' /
/

--
-- BHP LIMIT 482.6 BARS
```

```
--
WCONINJE
 'CO2_INJ' GAS OPEN RATE 5663369 1* 482.6 /
/
DATES
1 JAN 2016 /
1 JAN 2017 /
1 JAN 2018 /
1 JAN 2019 /
1 JAN 2020 /
1 JAN 2021 /
1 JAN 2022 /
1 JAN 2023 /
1 JAN 2024 /
1 JAN 2025 /
1 JAN 2026 /
1 JAN 2027 /
1 JAN 2028 /
1 JAN 2029 /
1 JAN 2030 /
1 JAN 2031 /
1 JAN 2032 /
1 JAN 2033 /
1 JAN 2034 /
1 JAN 2035 /
```

```
1 JAN 2036 /
1 JAN 2037 /
1 JAN 2038 /
1 JAN 2039 /
1 JAN 2040 /
1 JAN 2041 /
1 JAN 2042 /
1 JAN 2043 /
1 JAN 2044 /
/
WELLSHUT
'CO2_INJ' /
/
DATES
 1 JAN 2045 /
/
END
```