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Effect of Capillary Heterogeneity on Buoyant Plumes: New Trapping Mechanism in Carbon Sequestration

by

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Effect of Capillary Heterogeneity on Buoyant Plumes: New Trapping Mechanism in Carbon Sequestration

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______________________________________________
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Dedication

To the Lord,
all glory and honor to whom

To my parents,
Parvin and Reza
for their unconditional support
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This research project would not be possible without the support of many people. I am deeply indebted to my supervisor, Dr. Steven L. Bryant for being an outstanding advisor and excellent professor. I personally believe that his constant encouragement, invaluable support and endless patience were the principal keys to my success. He has been everything that one could want in an advisor. I would also like to express my sincere gratitude to my co-supervisor, Dr. Kamy Sepehrnoori who was abundantly helpful and offered assistance, support and guidance for many research problems.

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Abstract

Effect of Capillary Heterogeneity on Buoyant Plumes: New Trapping Mechanism in Carbon Sequestration

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The modes of geologic storage of CO$_2$ are usually categorized as structural, dissolution, residual, and mineral trapping. Here we argue that the heterogeneity intrinsic to sedimentary rocks gives rise to a fifth category of storage, which we call local capillary trapping. Capillary trapping occurs during buoyancy-driven migration of bulk phase CO$_2$ within a saline aquifer. When the rising CO$_2$ plume encounters a region ($10^2$ to $10^5$ m) where capillary entry pressure is locally larger than average, CO$_2$ accumulates beneath the region. This form of storage differs from structural trapping in that much of the accumulated saturation will not escape, should the integrity of the seal overlying the aquifer be compromised. Capillary trapping differs from residual trapping in that the accumulated saturation can be much larger than the residual saturation for the rock.
We examine local capillary trapping in a series of numerical simulations. The essential feature is that drainage curves (capillary pressure versus saturation for CO$_2$ displacing brine) are required to be consistent with permeabilities in a heterogeneous domain. In this work we accomplish this with the Leverett $J$-function, so that each grid block has its own drainage curve, scaled from a reference curve to the permeability and porosity in that block.

We find that capillary heterogeneity controls the path taken by rising CO$_2$. The displacement front is much more ramified than in a homogeneous domain, or in a heterogeneous domain with a single drainage curve. Consequently residual trapping is overestimated in simulations that ignore capillary heterogeneity. In the cases studied here, the reduction in residual trapping is compensated by local capillary trapping, which yields larger saturations held in a smaller volume of pore space. Moreover, the amount of CO$_2$ phase remaining mobile after a leak develops in the caprock is smaller. Therefore the extent of immobilization in a heterogeneous formation exceeds that reported in previous studies of buoyancy-driven plume movement.
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Chapter 1: Introduction

1.1 **Problem Statement**

The world’s climate varies naturally as a result of:

- the way the ocean and the atmosphere interact,
- changes in energy received from the sun and volcanic eruptions,
- changes in the earth’s orbit.

However, there is now strong evidence and almost universal agreement that significant global warming can’t be explained just by natural variations. The changes seen over recent years, and those predicted over the next 100 years, are thought to be mainly a result of human behavior.

1.1.1 **The greenhouse effect: global warming**

The Earth is surrounded by a layer of gases which act like the glass walls of a greenhouse. These gases allow the sun’s rays enter, but stop much of the heat from escaping. This is a natural process which has been going on for millions of years, and it is water vapor and these “greenhouse gases” (mainly carbon dioxide and methane) that keep the planet warm enough to sustain life. About 85% of total global warming on the earth’s surface is related to water vapor and about 12% to greenhouse gases. Figure 1-1 illustrates the greenhouse effect on the earth’s surface.

However, as humans cause more greenhouse gases to be released into the atmosphere, the greenhouse effect becomes stronger. More heat is trapped and the earth's climate begins to change unnaturally. Nowadays the atmospheric concentration of carbon dioxide has reached levels the planet has not experienced for 800,000 years, and as a
Figure 1-1: The greenhouse effect on the earth’s surface. This graphic explains how solar energy is absorbed by the earth’s surface, causing the earth to warm and to emit infrared radiation. The greenhouse gases then trap the infrared radiation, thus warming the atmosphere. (Figure from UNEP/GRID-Arendal)

result the global mean temperature has risen for more than a century. The international Intergovernmental Panel on Climate Change, the National Academies of Science in the United States and scientific academies in 10 other nations have all stated that human activity, especially the burning of fossil fuels in cars and power plants, is a major driver of this warming trend since 1950. Figure 1-2 shows world greenhouse gas emissions by
sector. Global warming is a profound threat to both humanity and the natural world, and one of the most serious challenges humankind has ever faced.

Figure 1-2: World greenhouse gas emissions by sector. All data is for year 2000. All calculations are based on CO₂ equivalents, using 100-year global warming potentials from the IPCC (1996), based on a total global estimate of 41,755 Mton CO₂ equivalent. Land use change includes both emissions and absorptions. Dotted lines represent flows of less than 0.1% percent of total GHG emissions. (Figure from UNEP/GRID-Arendal)
Since the industrial revolution in the 18th century, consumption of fossil fuel (natural gas, petroleum and coal) has increased the total load of carbon dioxide in the atmosphere from pre-industrial levels of 280 ppm to present levels of 375 ppm, an increase of about 35 per cent according to the US Department of Energy’s Office of Science. Predictions of global energy use in the next century suggest a continued increase in carbon emissions and rising concentrations of CO₂ in the atmosphere. For instance, the US Energy Information Administration predicts that, if no action is taken, the United States will emit 8,800 million tons of CO₂ by 2030, a 33 percent increase above 2005 emission levels.

The 2007 report of the Intergovernmental Panel on Climate Change unequivocally concluded that our climate is warming, stating with at least 90 percent certainty that the warming of the last several decades is primarily due to human activities. Global average temperatures have already risen about 0.7°C (1.3°F) over the last 100 years, and impacts are now being observed worldwide. Figure 1-3 shows increases in annual temperatures for five-year period of 2001-2005, relative to 1951-1980. Human-caused emissions to date have locked in further changes including sea-level rise that will intensify coastal flooding, and dramatic reductions in snowpack that are likely to disrupt water supplies in the western United States. If emissions continue unabated, our nation and the world will face more sea level rise, heat waves, droughts, wildfires, snowmelt, flood risk, and public health threats, as well as increased rates of plant and animal species extinctions.

Scientists are aware that the window for reducing global warming emissions to reasonably safe levels is closing quickly. Several recent analyses have concluded that, to avoid dangerous climate change, the United States and industrialized nations will need to reduce emissions at least 80 percent by mid-century, compared with 2000 levels, and that
national and international policies must be in place within the next 5 to 10 years to achieve this ambitious outcome.

Figure 1-3: Increases in annual temperatures for five-year period of 2001-2005, relative to 1951-1980. Warming is widespread, generally greater over land than over oceans, and the largest gains in temperatures for the planet are over the North American Arctic, north central Siberia, and on the Antarctic Peninsula. (Figure from UNEP/GRID-Arendal)

1.1.2 Impacts of global warming

Human-induced warming over recent decades is already affecting many physical and biological processes on every continent (IPCC, 2007). Several researches have revealed changes consistent with the expected response to global warming, and the observed physical and biological responses have been greatest in the regions that warmed the most. Challenges remain over the influence of other factors such as local pollution, invasive species, and land-use change.
Additional substantial effects on human society and natural environments are expected around the world. One reason is that 0.7 degree Celsius (°C), or 1.3 degree Fahrenheit (°F) of additional warming is already unavoidable due to past emissions. Further emissions would cause additional warming and thus additional impacts. So the magnitude and timing of these consequences are not often predicted because they depend on the amount and rate of warming and, in some cases, on society’s ability to adapt. Figure 1-4 shows a summary of projected impacts of climate change. Some of these impacts are discussed in more details in following pages.

![Projected impact of climate change](image)

Figure 1-4: Future climate change and projected impacts (Figure from UNEP/GRID-Arendal)
1.1.2.1 *Changes in water resources*

Hundreds of millions of people face water shortages that will worsen as temperatures rise. Most at risk are current drought-affected regions, areas with heavily used water resources, and areas that get their water from glaciers and snowpack (including the western United States).

The land area affected by drought is expected to increase and water resources in affected areas could decline as much as 30 percent by mid-century. U.S. crops that are already near the upper end of their temperature tolerance range or depend on heavily used water resources could suffer with further warming.

More than one-sixth of the world’s population currently lives near rivers that derive their water from glaciers and snow cover; these communities can expect to see their water resources decline over this century. The Intergovernmental Panel on Climate Change (IPCC) expects many Latin American glaciers to disappear entirely over the next couple of decades, and water resource competition to increase in western North America when decreased snowpack in the mountains reduces summer river flow. Many rivers that derive their water from melting glaciers or snow will have earlier peak runoff in spring and an overall increase in runoff, at least in the short term. Such a temporary increase in water flow would not always be welcome; for example, melting glaciers in the Himalayas would increase flooding and rockslide risks, while flash flood risks could increase in Northern, Central, and Eastern Europe.

1.1.2.2 *Changes in food production*

Food production is expected to decline in low-latitude regions (near the equator), particularly in the seasonally dry tropics, as even small temperature increases decrease crop yields in these areas.
The projections show drought-prone areas of Africa to be particularly vulnerable to food shortages due to a reduction in the land area suitable for agriculture; some rain-fed crop yields could decline as much as 50 percent by 2020. Rising lake temperatures in Africa combined with overfishing may also decrease fish supplies.

Under local average temperature increases of 1 to 3°C (about 2 to 5°F), regions such as Northern Europe, North America, New Zealand, and parts of Latin America could benefit from increased growing season length, more precipitation, and/or less frost. However, these regions can also expect more flooding, and if local average temperatures rise beyond this range, crop yields could decline in some of these areas. Note that these higher-latitude regions warm at a faster rate than the global average.

1.1.2.3 Extinction of species

Up to 30 percent of plant and animal species could face extinction if the global average temperature rises more than 1.5 to 2.5°C (about 3 to 5°F) relative to the 1980–1999 period. Many projections suggest the low end of this temperature range could be reached by mid-century.

Many species have already shifted their ranges to higher latitudes (toward the poles) and higher elevations over the past several decades. Spring has been arriving earlier during this time, influencing the timing of bird and fish migration, egg laying, leaf unfolding, and spring planting for agriculture and forestry in the high northern latitudes. Satellite records since the early 1980s confirm that increased temperatures have produced longer growing seasons.

Scientists expect the magnitude of these changes to increase along with temperatures over this century. Many species and ecosystems may not be able to adapt as the effects of global warming and its associated disturbances (including floods, drought,
wildfire, and insects) are compounded by other stresses such as pollution and resource exploitation. Polar and alpine species are especially vulnerable to the effects of climate change, as their unique habitats could shrink due to warming.

Acidification of the oceans due to increasing atmospheric carbon dioxide negatively affects marine shell-forming organisms such as corals and some plankton (and the species that depend upon them). Warming ocean waters represent another threat to corals; if they are unable to adapt to projected sea surface temperature increases of 1 to 3°C (about 2 to 5°F), corals could lose the algae that nourish and give them color, and many would die.

Some areas, such as the national parks of Australia and New Zealand and many parts of tropical Latin America are likely to experience a significant loss of biodiversity. By mid-century, tropical forests in the eastern Amazon Basin could be gradually replaced by less species-rich savanna because of rising temperatures and decreasing soil moisture.

1.1.2.4 Escalating hazards for coasts

Figure 1-5 shows the causes of sea level rise from climate change. Flooding caused by sea-level rise is expected to affect millions of additional people every year by the end of this century, with small islands and the crowded delta regions around large Asian rivers (such as the Ganges-Brahmaputra) facing the highest risk.
Sea-level rise exposes coasts to higher risks of flooding and erosion, which would be exacerbated by growing population, increased human infrastructure within flood-prone areas, and human activities that increase erosion or local subsidence. Regions especially at risk are low-lying areas of North America, Latin America, Africa, populous coastal cities of Europe, crowded delta regions of Asia that face flood risks from both large rivers and ocean storms, and many small islands whose very existence is threatened by rising seas. In North America, current preparedness for rising seas, more frequent severe weather, and higher storm surges is low.

The Greenland and West Antarctic ice sheets face substantial melting if the global average temperature rises more than 1 to 4°C (about 2 to 7°F) relative to the period 1990–2000, eventually contributing to an additional sea-level rise of about 13 to 20 feet.
(4 to 6 meters) or more. This would result in the inundation of low-lying coastal areas, including parts of many major cities.

1.1.2.5 More extreme weather

The IPCC expects extreme weather and weather-related events to become more frequent and/or intense, with serious consequences for human health and well-being.

Scientists expect heat waves, droughts, wildfires, floods, severe storms, and dust transported between continents to cause locally severe economic damage and substantial social and cultural disruption. The IPCC projects an extended fire season for North America as well as increased threats from pests and disease (which could significantly enlarge the area burned in a fire). Moreover, because fires release the carbon stored in trees, an increase in wildfires would further worsen global warming.

Increases in the frequency of droughts and floods would negatively affect local food production, and communities in mountain regions would face an increased risk of floods caused by melting glaciers. In addition, the risk of flood-induced illness and death from diseases could rise.

1.1.2.6 Threats to human health

The IPCC expects heat waves, floods, storms, fires, and droughts related to global warming to contribute to increased rates of death, disease, and injuries for millions around the world.

U.S. cities that currently experience heat waves can expect increases in the number, intensity, and duration of heat waves over the course of the century. Some
infectious diseases, such as those carried by insects and rodents, may become more common in regions where those diseases are not currently prevalent.

Developing countries, many of which are already under stress, could experience increases in the incidence of diseases and malnutrition and consequent disorders, affecting child growth and development. The populations most vulnerable to harsh living conditions in any nation (the elderly, children, and poor) may be unable to cope with further climate change.

1.2 POSSIBLE SOLUTIONS

We need adaptation strategies to cope with those consequences of global warming that are already unavoidable due to past emissions. Many additional consequences can be avoided, minimized, or delayed by reducing our emissions.

Many of the unavoidable near-term consequences of global warming can be addressed through adaptation strategies such as building levees and restoring wetlands to protect coasts, altering farm practices to grow crops that can survive higher temperatures, building infrastructure that can withstand extreme weather, and implementing public health programs to help people in cities survive brutal heat waves. However, the options for successful adaptation diminish and the associated costs increase as temperatures continue to rise. One of the IPCC’s fundamental conclusions is that both adaptation and mitigation (in the form of emission reductions) are required to cope with climate change over the short and long term. Strategic options for climate change mitigation are shown in Figure 1-6. The graphic is global cost curve for greenhouse gas abatement measures. It attempts to show all in one: the various measures for greenhouse gas reduction with both reduction (in CO₂ equivalent) and cost (in Euros) quantified.
The following solutions are available today and can have an enormous impact on the problem CO₂ remains in the atmosphere for about 100 years. Some of these common sense solutions will not only reduce global warming, but will save us money and create new business opportunities.
1.2.1 Build better cars

The technology exists to build cars, minivans, and SUVs that are just as powerful and safe as vehicles on the road today, but get 40 miles per gallon (mpg) or more. Better transmissions and engines, more aerodynamic designs, and stronger yet lighter material for chassis and bodies can cost-effectively increase the average fuel economy of today’s automotive fleet from 24 mpg to 40 mpg over 10 years. This would be equivalent to taking 44 million cars off the road, and it would save individual drivers thousands of dollars in fuel costs over the life of a vehicle.

Because transportation accounts for nearly 30 percent of U.S. annual CO₂ emissions (Figure 1-7), raising fuel economy is one of the most important things we can do to slow climate change.

Figure 1-7: Sources of U.S. CO₂ emissions
1.2.2 Modernize the electricity system

More than half of America’s electricity is produced from outdated, coal-burning power plants that dump pollutants and heat-trapping gases into the atmosphere. In fact, power plants are the single largest source of CO₂ (one-third of the U.S. total).

However, cost effective, clean energy sources do exist. By increasing our use of clean renewable energy, investing in energy efficiency, and reducing pollution from fossil fuel plants we can save money for consumers, reduce heat-trapping emissions, and lessen the need for new coal or gas power plants.

A study by the Union of Concerned Scientists (UCS) found that we could reduce power plant CO₂ emissions by 60 percent compared with government forecasts for 2020.

1.2.3 Increase energy efficiency

Like better technology for transportation and power generation, the technology for more efficient motors, appliances, windows, homes, and manufacturing processes is here today. These simple solutions save consumers money and can have an enormous impact on climate change at the same time. For instance, in the past two decades, energy-efficiency standards for household appliances kept 53 million tons of heat-trapping gases out of the air each year.

1.2.4 Protect threatened forests

In addition to sheltering more than half of the planet’s species and providing benefits such as clean drinking water, forests play a critical role in climate change: they store carbon, the base of CO₂. When forests are burned, cleared, or otherwise degraded,
their stored carbon is released into the atmosphere. Tropical deforestation now accounts for about 20 percent of all human-caused CO₂ emissions each year (Figure 1-8).

Figure 1-8: Comparison of mean annual global emissions from deforestation (1989-1995) and fossil fuels (1990-1999).

1.2.5 Storing carbon underground (geologic sequestration)

Slowing the growth in greenhouse gas emissions, while ensuring availability of the plentiful energy essential to economic vitality is an important concern. The Carbon Sequestration contributes significantly to the goal of developing technologies to substantially reduce greenhouse gas emissions. Sequestration is capturing gasses after combustion and injecting them into subsurface formations where they will be retained for geological periods of time.

Of course natural carbon sequestration is a cycle that has been happening on this planet for billions of years. It is simply the process by which nature has achieved a balance of carbon dioxide in our atmosphere suitable for sustaining life. Nature provided trees, the oceans, earth and the animals as carbon sinks, or sponges. All organic life on
this planet is carbon based and when plants and animals die, much of the carbon goes back into the ground where it has little impact on contributing to global warming.

Other types of carbon sequestration are ocean sequestration and geologic sequestration. In the former, carbon is stored in oceans through direct injection or fertilization. In the latter, natural pore space in geologic formations serve as reservoirs for long term carbon dioxide storage. This includes depleted oil and gas reservoirs, unmineable coal seams, deep saline aquifers, and unconventional reservoirs like tight gas sands or salt domes or large underground cavities. Figure 1-9 shows some of the carbon dioxide sequestration options.

![Figure 1-9: Some of the CO$_2$ sequestration options. (Figure from CSIRO)](image-url)
Many power plants and other large emitters of CO$_2$ are located near geologic formations that are amenable to CO$_2$ sequestration. Further, in many cases, injection of CO$_2$ into a geologic formation can enhance the recovery of hydrocarbons, providing value-added byproducts that can offset the cost of CO$_2$ capture and sequestration.

Saline formations do not contain oil and gas resources and thus do not offer the value-added benefit of enhanced hydrocarbon production. However, the potential CO$_2$ storage capacity of saline formations is huge; e.g. US Department of Energy has estimated that deep saline formations in the United States could potentially store up to 500 billion tons of CO$_2$ which is in the order of several hundred years of CO$_2$ emissions. As a practical example, the Norwegian oil company, Statoil, is injecting approximately one million tons per year of recovered CO$_2$ into the Utsira Sand, a saline formation under the sea associated with the Sleipner West Heimdel gas reservoir. The amount being sequestered is equivalent to the output of a 150 MWatt coal-fired power plant.

The main goal of research in this area is to understand the behavior of CO$_2$ when stored in geologic formations so that CO$_2$ can be stored in a manner that is secure and environmentally acceptable. Determining that CO$_2$ will not escape from formations and either migrate up to the earth’s surface or contaminate drinking water supplies is a key aspect of sequestration research.

1.3 **RESEARCH OBJECTIVES**

There are three known modes of sequestration that decrease the risk of leakage:

- Immobilization of CO$_2$ as a residual disconnected phase trapped by capillary forces (residual trapping),
- Immobilization of CO$_2$ as aqueous species dissolved in brine (dissolution trapping),
- Immobilization of CO$_2$ as a solid phase through precipitation or adsorption.
• Immobilization of CO$_2$ as precipitated carbonate anions and metal cations (mineral trapping)

Previous works have studied the effectiveness of residual phase trapping. When CO$_2$ is injected in deeper parts of aquifer, buoyancy forces drive the injected CO$_2$ upward, since CO$_2$ is less dense than brine under typical storage conditions. As it rises, a residual phase trapped by capillary forces remains in the rock previously occupied by large CO$_2$ saturation. The intrinsically unstable character of buoyancy-driven flow does not govern the displacement; instead, the CO$_2$ follows preferential flow paths determined by the spatial correlation of permeability in the aquifer (Bryant et al., 2006). The behavior is then better referred to as channeling, not fingering.

CO$_2$ also dissolves in previously uncontacted brine on its way up. The dissolved CO$_2$ then reacts with the other species present in the aqueous phase and also with the rock minerals. As a result, precipitation or dissolution of minerals occurs leading to storage of some part of the injected CO$_2$ as minerals. Ozah et al. (2005) conclude that CO$_2$ trapped in minerals even after thousands of years is small compared to the other forms of storage.

Thus we neglect the effect of mineral trapping in this work and focus on other modes of secure storage of CO$_2$.

Simulations of the “inject low and let rise” scenario using a single $p_c$-$S_w$ curve in a heterogeneous permeability field indicate that capillary pressure always smooths a rising CO$_2$ front. A uniform displacement front allows a large volume of CO$_2$ to rise but not reach the top of the formation, thereby maximizing the amount of trapped CO$_2$. In this situation, capillarity increases the security of CO$_2$ storage.

However, capillary entry pressure of a rock is correlated with its permeability (Leverett, 1941), and the use of a single drainage curve in a heterogeneous formation is physically inconsistent. Moreover, heterogeneity that leads to a small decrease in
permeability in the vertical direction would cause the capillary entry pressure to increase in that direction. This can be sufficient to block the rising CO₂, which must instead accumulate or move laterally.

On one hand, this phenomenon can amplify the influence of preferential flow paths on the displacement front. On the other hand, the same phenomenon applies even within a region of large permeabilities. This leads to an opposing effect of capillarity, namely that it can disrupt the buoyant front within a preferential flow path. Hence, using a correct model that considers the heterogeneity in capillary pressure could result in a qualitatively different rising front and different amount of stored CO₂ in two favorable modes.

In this work, we examine this possibility by means of simulations that account for heterogeneity in the capillary properties of the domain. We show the completely changed qualitative behavior of buoyant movement under the effect of heterogeneous capillary pressure field. Once buoyancy-driven flow stops, we impose a simulated leak in the top seal of the aquifer and observe the response. This leads to the identification of a new mode of trapping, termed “local capillary trapping” as it is associated with contiguous regions of larger-than-average capillary entry pressure.

Chapter 2 gives a literature review of the CO₂ storage in geologic formations and some of its aspects related to this work. Chapter 3 introduces the simulator (GEM) used in this work. Then the aquifer model is presented and implementation of such model in GEM is described. All of the model properties, including capillary pressure scaling, are discussed separately. A new model for leak in the aquifer is also presented in this chapter. Chapter 4 gives the results of simulation of buoyancy-driven flow in previously described model and compares the results of using a scaled capillary pressure field with simple capillary pressure models, like single capillary pressure. Effect of capillary pressure
scaling on both front behavior and gas trapping is discussed. Chapter 5 focuses on leak simulation in order to analyze the risk involved in sequestration process. The new mode of trapping in CO$_2$ sequestration is introduced in this chapter. Chapter 6 is a summary of conclusions and gives some recommendations for future works.
Chapter 2: Literature Survey

2.1 Storage of CO₂ in Geologic Formations

Hoffert et al. (2002) discuss that meeting the challenge of stabilizing CO₂ concentrations requires development of new technologies beside more efficient use of energy. They conclude that one technology that can contribute to meeting that challenge is the capture and storage of CO₂ that would otherwise be emitted to the atmosphere. Orr (2004) reviews options for capturing and storing CO₂ in geologic formations and discusses the advantages and limitations of each approach. He states that at least three options exist for geologic storage of CO₂: oil and gas reservoirs, deep saline aquifers, and unmineable coalbeds. Table 2-1 summarizes estimates of the capacity of the three storage options made by Parson and Keith (1998) and by the International Energy Agency (IEA) Greenhouse R&D program (Gale, 2004). These IEA estimates were those expected at storage costs of $20 per tonne or less (excluding the cost of separating the CO₂ from combustion gases, compression, or transportation to the storage site).

Table 2-1: Estimated CO₂ storage capacities of geologic formations (Gt CO₂)

<table>
<thead>
<tr>
<th>Storage Option</th>
<th>Parson and Keith</th>
<th>Gale</th>
</tr>
</thead>
<tbody>
<tr>
<td>Oil and gas reservoirs</td>
<td>740 to 1850</td>
<td>920</td>
</tr>
<tr>
<td>Deep saline aquifers</td>
<td>370 to 3700</td>
<td>400 to 10,000</td>
</tr>
<tr>
<td>Coalbeds</td>
<td>370 to 1100</td>
<td>40</td>
</tr>
</tbody>
</table>

Orr (2004) argues that while these estimates involve significant uncertainties as the differences between estimates show, the amounts shown are large enough compared
with current and estimated future emission rates to suggest that there is potential for storing sufficient quantities of CO₂ to have an effect on overall emissions if remaining research questions can be resolved and if costs can be reduced sufficiently.

2.1.1 Oil reservoirs

Orr (2004) suggests that because oil reservoirs have known seals and because there is a regulatory structure that has experience in permitting gas injection operations, existing oil fields will likely be the first places to undertake CO₂ sequestration, if it is done on a large scale.

Significant experience with CO₂ injection into oil reservoirs has been obtained during the last three decades. SACROC (Hawkins et al., 1996) and North Cross (Mizenko, 1992) projects are among the first CO₂ injection projects in which CO₂ that otherwise would have been vented to the atmosphere was separated from natural gas in southwest Texas and then injected. Most CO₂ injection projects have used naturally occurring CO₂ likewise. Commercial CO₂ injection operations in the Permian Basin of west Texas began in 1970s and 1980s (Stein et al., 1992; Lambert et al., 1996). These projects use CO₂ transported by pipelines from Colorado and New Mexico where large natural sources of CO₂ exist.

The motivation for most of these projects is enhanced oil recovery (EOR), not CO₂ sequestration, because the injected CO₂ would not have been emitted to the atmosphere. Taber et al. (1997) conclude that if CO₂ were widely available, either because the cost of capture was reduced or because incentives for CO₂ storage were in place, many oil reservoirs would be candidates for CO₂ injection. Screening criteria for oil reservoirs that might be candidates for CO₂ storage have been suggested by Kovscek (2002) and by Shaw and Bachu (2002).
Considerable engineering effort has gone into minimizing the amount of CO₂ required to recover oil in EOR projects. Jessen et al. (2005) discuss that if the objective is also to increase storage of CO₂, then changing injection horizons, injection of CO₂ into an aquifer below the reservoir, or injection into the capillary transition zone may also be useful. While many of the specific actions taken to increase CO₂ storage will depend on the details of the particular reservoir setting, it is apparent that many opportunities exist for developing the design of CO₂ injection projects in a way that increases storage substantially over the amounts stored in EOR projects. Kovscek and Cakici (2005) discuss that modifications of the commonly used water-alternating-gas (WAG) injection schemes may allow greater CO₂ storage while at the same time controlling cycling of injected CO₂.

The first project specifically aimed at CO₂ sequestration in an oil reservoir is being conducted at the Weyburn field in Saskatchewan (Malik and Islam, 2000). The CO₂ generated at a coal-gasification plant in North Dakota is transported by pipeline to Weyburn, where a combined EOR and CO₂ sequestration project is under way. Moberg et al. (2003) describe the extensive monitoring program aimed at detecting leakage of injected CO₂.

Orr (2004) concludes that while there is a considerable experience from CO₂ EOR projects to guide future CO₂ storage projects, there is a need to extend the range of reservoirs investigated and to develop the design considerations that will allow efficient CO₂ storage in addition to EOR.

2.1.2 Gas reservoirs

Oldenburg and Benson (2002) and Oldenburg et al. (2004) has proposed and studied CO₂ injection into gas reservoirs. CO₂ could be used for pressure maintenance or
for condensate vaporization, but the cost of purchasing CO₂ has made these applications uneconomical in the absence of incentives for CO₂ storage.

Orr (2004) believes that if CO₂ sequestration were undertaken in a substantial way, gas reservoirs would be candidates for storage, again with a known geologic seal capable of holding gas indefinitely. He says that the main advantage of CO₂ storage in a gas reservoir is that all CO₂ from the oxidation of CH₄ produced from the reservoir could be stored in the same reservoir, at the same temperature and pressure, with additional volume available for storage of more CO₂. One mole of CO₂ is produced for each mole of CH₄ oxidized, and the molar density of CO₂ is larger than that of CH₄ at a given temperature and pressure. He also discusses that if CO₂ injection is used to store CO₂ and maintain pressure in a gas reservoir, a key issue will be the mixing of the injected CO₂ with the CH₄ in the reservoir and the resulting concentration in the produced gas. Significant breakthrough of the injected CO₂ would require separation of CH₄ and CO₂. Oldenburg and Benson (2002) suggest that in reservoirs with good vertical communication, it may be possible to take advantage of the higher density of CO₂ to design injection strategies and well completions that place CO₂ low in the reservoir, with production taken from the top. Oldenburg (2004) gives a comparison of diffusion models of gas mixing in subsurface reservoirs and suggests that slow diffusional mixing may also be a concern in long-lived projects, although diffusion is very slow compared with typical reservoir flow velocities.

2.1.3 Deep saline aquifers

While anthropogenic CO₂ is generated in many locations which are not close to potential storage sites in oil or gas reservoirs, deep formations containing salt water are widely distributed geographically.
Pope et al. (2003) performed a simulation study of CO$_2$ storage in deep saline aquifers. Their study suggests that injected CO$_2$ will flow more easily through high permeability paths, but the flow will not be dominated by the pressure gradients imposed by injection and production wells. Gravity segregation caused by the density difference between the injected CO$_2$ and brine will cause preferential flow at the top of the aquifer, though injection of the CO$_2$ well below the top of the aquifer can mitigate this gravity segregation to some extent. Aquifers with large volume, reasonable permeability and thickness, and good pressure communication over long distances will be most attractive such that large volumes could be injected without raising aquifer pressure significantly. The injected CO$_2$ will dissolve in brine and the resulting brine/CO$_2$ mixture will be slightly denser than the brine alone. Slow vertical flow of denser brine will cause further dissolution, as fresh brine is brought in contact with the CO$_2$ phase. Trapping of a separate CO$_2$ phase by brine also can immobilize CO$_2$ as a residual phase. Relatively slow chemical reactions, depending on the chemical composition of the brine and minerals in the aquifer, may then sequester some of the CO$_2$ as minerals.

The largest aquifer storage project is being conducted in the North Sea at the Sleipner gas field (Torp and Gale, 2003). About 1M tonnes of CO$_2$, separated from produced natural gas is injected each year into an overlying aquifer. An extensive time-lapse seismic monitoring effort accompanies the injection. The injected CO$_2$ appears to be contained within the sand in which the CO$_2$ is injected, although there is evidence of vertical migration within the aquifer. Injected CO$_2$ flowed horizontally under thin shales, migrating upward toward the caprock at breaks in the shales, behavior that also is common in gas injection projects in oil reservoirs.
2.1.4 Coalbeds

In oil and gas reservoirs and aquifers, injected CO\textsubscript{2} occupies the pore space as a separate phase or is dissolved in water or oil. Deep unmineable coalbeds offer a different storage mechanism, the same mechanism that is the source of coalbed methane. Gases such as CH\textsubscript{4} or CO\textsubscript{2} adsorb on the surface of coal particles at high pressure. Significantly more CO\textsubscript{2} adsorbs on coal at a given pressure and temperature than does CH\textsubscript{4} or N\textsubscript{2}. In addition, the adsorption curve hysteresis suggests that once CO\textsubscript{2} is adsorbed, much of it will remain adsorbed even if the pressure decreased at a later time. Ohga et al. (2003) report results of adsorption experiments in which approximately three times as much CO\textsubscript{2} adsorbed on a coal sample as did CH\textsubscript{4} at a given pressure.

Ohga et al. (2003) perform fundamental tests on CO\textsubscript{2} sequestration into coalbeds and report that flow in coalbedes will occur primarily in the fracture network (cleats in coal). Injected CO\textsubscript{2} will flow through the cleats, diffusing into matrix blocks and replacing adsorbed CH\textsubscript{4}. Thus they conclude that CO\textsubscript{2} can be used to enhance CH\textsubscript{4} recovery. This displacement process is said to be similar to adsorption chromatography. According to Pekot and Reeves (2002) there is evidence that coal permeability changes with the amount of adsorbed gas. Typically, as CH\textsubscript{4} is removed from coal, permeability increases, and as CO\textsubscript{2} adsorbs, permeability decreases. Thus, displacement process in coalbeds will involve a complex interplay of flow in the cleat system, changes in permeability, diffusion and adsorption.

Stevens et al. (1998) say that field experience with CO\textsubscript{2} injection into coalbeds is limited, although field tests are being conducted in the U.S., Canada, Poland, Australia and Japan. In the Allison Unit in the San Juan basin, CO\textsubscript{2} from a pipeline delivering natural CO\textsubscript{2} to the Permian Basin is being injected. Again, the motivation is enhance recovery of coalbed methane. They report that production of CH\textsubscript{4} showed clear response
to CO₂ injection, an observation that is consistent with the idea that CO₂ can replace adsorbed CH₄ and make it available for production. They also conclude that minimal breakthrough of injected CO₂ is consistent with the idea that the injected CO₂ is being absorbed on the coal.

Orr (2004) believes that the complex physical mechanisms and flows will offer challenges as well as opportunities. The combination of physical mechanisms and the potential for offsetting costs of CO₂ storage by CH₄ recovery suggest that more investigation of this approach is warranted.

2.2 Feasibility of Aquifer Disposal

Gunter et al. (1996) did a three year study of the technical and economic feasibility of aquifer disposal of CO₂ in the low permeability sedimentary rocks of the Alberta Basin. Their study has revealed several new generic concepts. They conclude that high permeability aquifers are not necessarily required for CO₂ disposal. Injectivity of CO₂ can be maximized by locating disposal wells in targeted zones of locally high permeability surrounded by the generally low permeability aquifer, as also was suggested by Bachu et al. (1994) and Law and Bachu (1996). This method prevents near-well pressure buildups above the maximum levels imposed by regulatory agencies in low permeability rocks and precludes possible rock fracturing which may lead to CO₂ escape through vertical conduits.

The low regional permeability forms a “hydrodynamic” or “time” trap for CO₂, where the residence time of CO₂ in the aquifer is of the order of 10⁵ to 10⁶ years. Bachu (1995) shows another type of hydrodynamic trapping in sedimentary basins which is produced by the “sink” effect of rebounding shales. Perkins and Gunter (1995) also show that on a smaller time scale, over hundreds of years, “mineral” trapping by reaction of the
CO$_2$ with basic aluminosilicate minerals will occur in siliciclastic aquifers. Consequently, stratigraphic traps may not be necessary for safe disposal of CO$_2$ in the subsurface.

Gunter et al. (1996) conclude that hydraulic, hydrodynamic and mineral traps may be found in any deep sedimentary aquifer with low permeability and low regional heads. They are alternatives to stratigraphic traps which may not be available. Sedimentary basins around the world provide hydrodynamic traps, hydraulic sinks and mineral traps that are operable and are ideal candidates for CO$_2$ disposal in aquifers.

Pruess et al. (2003) give the following as the main issues for disposal of CO$_2$ in aquifers from an engineering perspective:

- The feasible rate of CO$_2$ disposal,
- The available storage capacity,
- The presence of a low permeability cap rock and the possibility of leakage through it,
- Identification of suitable aquifers and cap rocks,
- Uncertainty and possible failure caused by incomplete knowledge of subsurface phenomena,
- Corrosion resistance of materials that are used in injection facilities.

Gunter et al. (1998) categorize the carbon dioxide sinks into three broad classes based on the nature, location and ultimate fate of CO$_2$ as depicted in Figure 2-1. The groupings are:

- Biosphere sinks, which are environmentally sensitive, active, natural reservoirs for CO$_2$. The oceans, forests, and agricultural ecosystems are members of this class.
• Geosphere sinks, which are natural reservoirs for CO₂, but require anthropogenic intervention in order to make use of the sink. This class includes oil reservoirs suitable for enhanced oil recovery (EOR), depleted oil and gas reservoirs, coal beds and deep saline aquifers.

• Material sinks, which are anthropogenically created pools of carbon. They include chemicals, durable wood products and plastics.

They evaluated the use of different sinks as emission-reduction mechanisms, considering different factors including: environmental impact of the sink; CO₂ capacity of the sink; retention/residence time of CO₂ in the sink; potential for accelerated leakage of CO₂; rate of CO₂ uptake by the sink; validation of sequestration in the sink; suitability of the sink/match to the emission source and type; and cost of utilization of the sink mechanism. Table 2-2 and Table 2-3 show the assessment of these factors related to the use of geosphere sinks for carbon sequestration.

As they discussed, deep aquifers contain high salinity water and can host large amounts of CO₂ trapped by the formation pressure. The pressure and temperature of the reservoir are determining factors. At reservoir depths of 800 m and more, the temperature and pressure of the CO₂ would be above the supercritical condition, which is desirable for
storage. On the other hand, CO₂ storage in aquifers has the following environmental and safety problems:

- CO₂ escape,
- Dissolution of host rock,
- Devaluation of mineral resources,
- Effects on groundwater.

However, the implications may not be as serious as those for biosphere sinks.

Table 2-2: Assessment of environmental impact, security and verifiability related to the use of biological and geologic sinks for carbon sequestration. (From Gunter et al., 1998)

<table>
<thead>
<tr>
<th>Sink</th>
<th>Environmental impact</th>
<th>Stability/security</th>
<th>Verifiability</th>
</tr>
</thead>
<tbody>
<tr>
<td>Biological sinks</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Ocean</td>
<td>Negative</td>
<td>L</td>
<td>M</td>
</tr>
<tr>
<td>Forests</td>
<td>Positive</td>
<td>L–M</td>
<td>L</td>
</tr>
<tr>
<td>Agriculture</td>
<td>Positive</td>
<td>L–M</td>
<td>L</td>
</tr>
<tr>
<td>Geologic Sinks</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Enhanced oil recovery</td>
<td>Neutral</td>
<td>M</td>
<td>H</td>
</tr>
<tr>
<td>Coal beds</td>
<td>Neutral</td>
<td>H</td>
<td>H</td>
</tr>
<tr>
<td>Depleted oil and gas reservoirs</td>
<td>Neutral</td>
<td>H</td>
<td>H</td>
</tr>
<tr>
<td>Deep aquifers</td>
<td>Neutral</td>
<td>H</td>
<td>H</td>
</tr>
</tbody>
</table>

*Note: L = Low, M = Medium, H = High.*
Table 2-3: Assessment of capacities, retention times and cost related to the use of geosphere sinks for carbon sequestration. (From Gunter et al., 1998)

<table>
<thead>
<tr>
<th>Sink</th>
<th>Capacities</th>
<th>Retention (yr)</th>
<th>Rate</th>
<th>Costs ($ US/tC)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Global (Gt C)</td>
<td>Canada (Mt C)</td>
<td>Alberta (Mt C)</td>
<td></td>
</tr>
<tr>
<td>Enhanced oil recovery</td>
<td>&gt; 20 (1)</td>
<td>90 (3)</td>
<td>60 (3)</td>
<td>10a</td>
</tr>
<tr>
<td>Coal beds</td>
<td>82 - 263 (4)</td>
<td>4,000 - 7,500 (5)</td>
<td>5,000 (6)</td>
<td>100,000s - 1,000,000s</td>
</tr>
<tr>
<td>Depleted oil and gas reservoirs</td>
<td>150 (1)</td>
<td>5,000 (7)</td>
<td>3,500 (7)</td>
<td>100,000s to 1,000,000s</td>
</tr>
<tr>
<td></td>
<td>100 (7)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>500 (8)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>172 (11)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Deep aquifers</td>
<td>90 (1)</td>
<td></td>
<td>5,400 (10)</td>
<td>100,000s to 1,000,000s</td>
</tr>
<tr>
<td></td>
<td>30 - 14,000 (8)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>27 - 650 (11)</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Data sources:
(2) IEA, 1995 [17]
(3) Taber, 1994 [18]; Alberta is 70% of Canada total
(4) Kaushik et al., 1992 [22]
(5) Canadian Gas Potential Committee, 1997 [23]
(6) Gunter et al., 1997 [21]
(7) IEA OE15, 1993 [26]; Alberta is 70% of Canada total
(8) Hendris, 1994 [27]; 100 Gt C oil fields, 400 Gt C gas fields
(9) Bambhart et al., 1995 [28], at a delivered price of $ Cdn 22 / t CO2
(10) Gunter et al., 1996 [32], $ Cdn 52 / t CO2
(11) Ribeiro and Henry, 1995 [8], 1.95 ECU / t CO2

Overall, Gunter et al. (1998) conclude that although agricultural sinks and forestry are by far the lowest cost sink available, the more expensive use of geological storage might be needed to reach the targets for reduction of CO2 emissions. The biosphere sinks are limited by the CO2 uptake rate and the residence time of the sequestered carbon compared to geologic sinks. Also both verifiability of the sequestered amount and security against upsets which release the sequestered carbon tend to favor geological storage over agricultural sinks.

Bachu et al. (1994) specify the following general conditions that must be satisfied to make an aquifer suitable for CO2 disposal:
- The top of the aquifer must be greater than 800 m below ground level,
- The aquifer should be capped by a regional aquitard (sealing unit),
The aquifer should have enough porosity and adequate permeability, and
The injection site should be close to the CO2 emitting source.

Orr (2004) believes that the Sleipner project has demonstrated that large scale CO2 injection in a saline aquifer is feasible. Because it is a high permeability aquifer with relatively high porosity at the source of the CO2, it is an especially favorable application of aquifer injection. He also implies that additional field tests are needed to investigate a range of other aquifer settings.

2.3 AFFECTING PARAMETERS IN AQUIFER DISPOSAL

Gunter et al. (1996) state the effect of different petrophysical properties in CO2 sequestration based on numerical simulations. Their findings suggest:

- The porosity of aquifer has little impact on CO2 injectivity.
- The permeability is the parameter that effectively controls the injectivity, pressure distribution, flow velocity, and CO2 travel distance.
- The thickness of the aquifer directly affects the volume of injected CO2.
- Other properties, such as formation water salinity and temperature were found to have very little effect on CO2 injection for the range of values characterizing the studied aquifers.

Law and Bachu (1996) have generalized the results for prediction of the CO2 injectivity as a function of CO2 mobility for homogeneous aquifers:

\[
\frac{Q}{D(p_i - p_o)} = 5.38 \times 10^{-4} \rho \left(\frac{kk_r}{\mu}\right) \ln\left(\frac{r}{r_w}\right)
\]  

(2-1)
where mass injection rate $Q$ (ton/day) is a function of aquifer thickness $D$ (m), absolute permeability $k$ (md), CO$_2$ relative permeability $k_r$, CO$_2$ density $\rho$ (kg/m$^3$), dynamic viscosity $\mu$ (mPa.s), and the radii of the injection well $r_w$ and of injection influence $r_e$.

For heterogeneous aquifers, they generalized the results by calculating an enhancement factor in CO$_2$ injectivity due to injection in a local high permeability zone as a function of the permeability of the sweet zone and of the low permeability aquifer. Their results are shown in Figure 2-2.

![Figure 2-2: Effect of a high permeability zone on CO$_2$ injection into selected aquifers in the Alberta sedimentary basin generalized as an enhancement factor. (Figure from Law and Bachu, 1996)](image-url)
The results of numerical simulations by Pruess et al. (2003) show that based on the ratio of vertical to horizontal permeability, CO\textsubscript{2} has a tendency to migrate toward the top of the aquifer which leads to partially segregated flow with considerable gravity override. This is related to density of CO\textsubscript{2}-rich gas-like phase which is less than water at the temperature and pressure conditions of interest. They conclude that partial segregation of flow from buoyancy effects has one large favorable effect, although it reduces the available CO\textsubscript{2} storage capacity, and that is less interference between liquid and gas phases which leads to a significant reduction in CO\textsubscript{2} injection pressures for a given rate of flow.

They also say that under favorable conditions, the amount of CO\textsubscript{2} that may be sequestered by precipitation is comparable to the amount of dissolution trapping. In contrast, Ozah et al. (2005) report that three-dimensional simulations of coupled flow and reactive transport show that the amount of CO\textsubscript{2} sequestered as minerals is small relative to gas trapping and dissolution into brine and it does not contribute significantly to the permanent storage of CO\textsubscript{2}, however, the mineralization further reduces the already small amount of mobile gas over long periods of time. Also, the possibility of porosity and permeability reduction resulting from mineralization is said to be small.

Ozah et al. (2005) have studied strategies for optimizing several phenomena beneficial to subsurface storage of waste gases by numerical simulations using a compositional reservoir simulator. They argue that hysteresis in relative permeability curve results in substantial volumes of gas trapping. In other words, the phenomenon of capillary trapping plays a big role in determining how the CO\textsubscript{2} is stored in aquifers. Large volumes of CO\textsubscript{2} can be stored for very long time periods without the need for ensuring long-term seal integrity since the CO\textsubscript{2} never reaches the seal. They conclude that this is
by far the most significant mechanism for permanent storage and should be carefully evaluated with a field pilot.

According to Ozah et al. (2005), buoyancy driven vertical flow of CO2-rich gas is an unstable displacement process and it needs careful examination. As the density and viscosity are smaller for CO2-rich gas than for brine, hydrodynamic instabilities (buoyancy-driven and viscous fingering) may occur. Their simulations with local grid refinement show that fingering due to buoyancy is mitigated by natural heterogeneity in the aquifer petrophysical properties. Capillary pressure is also significant in its effect to mitigate the fingers. This effect is captured in their simulations by using six rock types with different capillary pressure tables. They suggest scaling the capillary pressure for each individual grid block to have a more physically accurate model and results. Other observed factor is \( k_v/k_h \). They say that when this parameter is small, flow up dip within a layer can dominate vertical flow, even for small dip angles and this indirectly mitigates the tendency to finger. Overall, they conclude that these effects causes the amount of gas trapping observed in coarse-grid simulations to be likely a reasonable estimate of what can be obtained in the field. Both Kumar (2004) and Ozah (2005) show extensive results of pure CO2 injection over a wide range of conditions including key parameters such as heterogeneity and vertical to horizontal permeability ratio.

Also, Bryant et al. (2006) discuss that in a dipping aquifer the buoyancy force has a non-zero component in the direction of the bedding plane and is therefore aligned with regions of correlated permeability. In conclusion, for isotropic formations \((k_v/k_h = 1)\) and small dip angles \((\alpha < 5^\circ)\) the preferential flow paths followed by CO2 are similar to those in non-dipping formations, i.e. primarily in the vertical direction. For anisotropic formations \((k_v/k_h < 1)\), the preferential flow paths are much more strongly aligned with the bedding plane.
The opportunity for escape of the gases from the aquifer can be minimized by careful design of injection strategies. One such strategy is proposed by Ozah et al. (2005) as using horizontal wells low in the formation so that all of the injected gases are trapped, dissolved or precipitated before they reach geological seals or faults. They argue that horizontal wells have two advantages over vertical wells for geological storage of greenhouse gases:

- A larger volume of CO₂ could be stored without CO₂ reaching the top of the aquifer.
- A higher injection rate might be expected.

They report that under their base case conditions it is possible to store seven times more CO₂ in the aquifer without it reaching the top seal with a horizontal well compared to a vertical well. Bryant et al. (2006) further investigate this strategy of storing CO₂ in deep saline aquifers, i.e. “inject low and let rise” strategy as they call it. They introduce some threshold value of injected volume at which the CO₂ will just reach the upper seal of the aquifer. This threshold volume will depend on several factors, two of which has been discussed by them: the uniformity of the displacement front, and the saturation of CO₂ below the front.

Bryant et al. (2006) simulation results show that the two phases arrange themselves so that water falls where no CO₂ is rising, and CO₂ rises where no water is falling. Thus the displacement is counter-current only in a global sense. This implies that fractional flow theory affords a convenient means of evaluating the effect of relative permeability curves on CO₂ storage, even though the displacement is not cocurrent. They discuss that a mass balance shows that the larger the shock saturations, the smaller the distance that a given volume of CO₂ rises, and because relative permeability is hysteretic,
larger shock saturations will also leave larger residual CO$_2$ saturations, thus increasing capillary trapping.

Based on their simulation results, Bryant et al. (2006) suggest that the first order influence on buoyancy driven CO$_2$ displacement is heterogeneity, not instability of the interface. They also report that capillarity and anisotropy tend to increase the uniformity of a buoyancy-driven immiscible displacement in a heterogeneous domain. They conclude that two important considerations for assessing the vertical distance that CO$_2$ could travel are:

- characterizing the structure of the permeability field within an aquifer,
- accounting for capillarity.
Chapter 3: Modeling the Sequestration Process

Every sequestration project consists of three main phases:

- Capture and surface processing: This phase consists of capturing CO₂ from different sources and its processing, like mixing with water, to prepare the fluid stream for injection.
- Injection: Injection of fluid stream into underground geological structure.
- Storage: After injection phase, the injected CO₂ propagates through the reservoir. In fact, the density of the CO₂ vapor in typical conditions encountered in geological storage is less than the density of the brine. Due to buoyancy effect, an upward migration of CO₂ occurs. During this migration different mechanisms may help it to store inside the reservoir. This could be temporary or permanent storage.

As discussed in previous sections, the main objective of geological sequestration is to increase the permanent storage of CO₂ inside the underground reservoirs. This decreases the risk of leakage of CO₂ back to the atmosphere which is a major concern in long term storage of CO₂. To be able to assess the risk of CO₂ leakage we need to understand the dynamic behavior of CO₂ when moving inside the underground storage site.

In this project, we just consider the third phase of the sequestration to study the dynamics of the CO₂ buoyant movement after injection in most common type of geological storage formations, which are deep saline aquifers. A simplified model of the injected CO₂ in a deep saline aquifer is considered. This would be an idealization of what
happens during injection phase. The principal focus will be the effect of heterogeneity on this phenomenon. In this chapter, we explain the model we used in our study and discuss the implementation of this model using a commercial simulator.

3.1 GEM SIMULATOR

Our study is based on simulations performed with Computer Modeling Group’s simulator. GEM (General Equation of state Model) is CMG’s general equation of state (EOS)-based compositional reservoir simulator for modeling the flow of three-phase, multicomponent fluids. GEM is a robust, fully compositional simulator used to model any type of reservoir where the importance of the fluid composition and their interactions are essential to the understanding of the process. So it is a proper tool in this project where our main discussion is about heterogeneity and its effect on capillary pressure. GEM has all the features required to implement our simplified model in a simulator. The main features used in this study are reviewed in the following sections.

3.2 AQUIFER MODEL AND INITIALIZATION

We do not model any particular aquifer or consider the strategy for the injection phase. Instead we idealize the distribution of CO₂ after injection phase as a large CO₂ saturation in the few bottom layers of a two dimensional aquifer, shown schematically in Figure 3-1. This is intended to approximate the result of high-rate injection into the bottom part of the aquifer. The boundaries of the domain are closed, which leads to countercurrent flow inside the aquifer as brine falls to replace upward moving CO₂.
Figure 3-1: Schematic of the initial condition for the buoyancy-driven flow simulations (base case). A large saturation of CO$_2$ is placed in the bottom 12 ft of the heterogeneous aquifer. This is intended to approximate the result of high-rate injection into the bottom part of the aquifer. The boundaries of the domain are closed.

Simulations are performed on a 100 ft high, 400 ft wide domain with grid blocks of 1 ft by 1 ft length, thus involving 40,000 grid blocks. The aquifer is assumed to be located 5,300 ft below the surface, with initial pressure of 2,265 psi at constant temperature of 140°F which are typical of a deep saline aquifer.

To study the accumulation of CO$_2$ beneath the top seal, we consider several initial volumes of CO$_2$ other than the base case. The heterogeneous part of the domain remains unchanged. New layers are added to the bottom of the domain to hold additional CO$_2$, as indicated in Figure 3-2. The new layers are homogeneous, with permeability and porosity equal respectively to the average permeability and porosity of the aquifer.

Figure 3-2: Schematic of the initial condition used to study the accumulation of CO$_2$ beneath the top seal. The heterogeneous part of the domain ($H_1$) remains unchanged. New homogeneous layers are added to the bottom of the domain ($h_2$) to hold additional CO$_2$. 

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3.3 **Fluid Properties**

In compositional simulators all hydrocarbon phase properties are calculated using an equation of state (EOS). GEM utilizes either the Peng-Robinson or the Soave-Redlich-Kwong equation of state to predict the phase equilibrium compositions and densities of the oil and gas phases, and supports various schemes for computing related properties such as oil and gas viscosities.

Two methods can be used in GEM to model the solubility of CO$_2$ in brine:

1. Modeling brine as the “oil” phase and tuning an equation of state to experimental data on solubility.
2. Modeling brine as the “aqueous” phase and using Henry’s law and an equation of state.

The first method is used in this study and described here. In this case, $S_w$ is assumed to be zero and the EOS is used for flash calculations. The basic properties needed for EOS calculations are the critical properties of each component and the interaction coefficients of each component pair in the conditions of process. Kumar *et al.* (2004) tuned the Peng-Robinson equation of state (PREOS) using experimental data for density and solubility over a wide range of pressures, temperatures and salinities related to aquifer conditions. Solubility determines how much CO$_2$ goes into solution in brine and density determines how fast the buoyant forces sequester the injected gases.

### 3.3.1 BIC: effect of CO$_2$ solubility

The binary interaction coefficient (BIC) for H$_2$O-CO$_2$ pair was tuned by Kumar (2004) to match the experimental values of CO$_2$ solubility in brine. He developed the following correlation for BIC of H$_2$O-CO$_2$ pair in PR equation of state:
\[
BIC_{H_2O-CO_2} = -0.093625 + (4.861 \times 10^{-4} (T - 113)) + (2.29 \times 10^{-7} \times S) 
\]

(3-1)

where:

\[BIC_{H_2O-CO_2} = \text{Binary interaction coefficient for H}_2\text{O-CO}_2 \text{ pair} \]

\[T = \text{Temperature, °F} \]

\[S = \text{Salinity, ppm} \]

So the effect of temperature and brine salinity on CO\textsubscript{2} solubility is considered implicitly in calculation of the BIC which is introduced to simulator.

In this study, we used the typical reservoir temperature of \[T=140 \text{ °F} \] and salinity of \[S=100,000 \text{ ppm} \] which gives \[BIC_{H_2O-CO_2} = -0.0576003 \]. The corresponding keyword in GEM is *BIN.

3.3.2 VSP: effect of phase density

The volume shift parameter (VSP) for brine was tuned by Kumar (2004) to match the brine density data. The following correlation was developed for VSP of brine on a wide range of temperature, pressure and salinity in PR equation of state:

\[
VSP_{H_2O} = 0.179 + (2.2222 \times 10^{-4} (T - 113)) + (4.9867 \times 10^{-7} \times S) 
\]

(3-2)

where:

\[VSP_{H_2O} = \text{Volume shift parameter for H}_2\text{O} \]

\[T = \text{Temperature, °F} \]

\[S = \text{Salinity, ppm} \]
According to Kumar this correlation gives a good match for pure brine density values, but uncertain predictions for CO₂-saturated brine because of lack of sufficient experimental data points.

Using the typical reservoir temperature of $T=140 \, ^\circ\text{F}$ and salinity of $S=100,000$ ppm in this study leads to $VSP_{H_2O} = 0.2348669$. The constant value of 0.024668 is used as $VSP_{CO_2}$ which is the value for pure CO₂. The keyword for VSP in GEM is *VSHIFT.

### 3.3.3 Viscosity

There are five methods to calculate the oil and gas phase viscosities in GEM. We use the corresponding states correlation given in Pedersen et al. (1984). This option is set by keyword: *VISCOR *PEDERSEN.

Under this option the hydrocarbon phase viscosities are functions of fluid composition, pressure and temperature. The viscosity of a mixture calculated using the Pedersen model depends strongly on the critical pressures, critical temperatures and molecular weights of the components, as well as the coefficient values.

The viscosity of the mixture is computed according to the following formula:

$$
\frac{\mu_{\text{mix}}(P, T)}{\mu_0(P_0, T_0)} = \left(\frac{T_{c,\text{mix}}}{T_{c,0}}\right)^{\frac{1}{6}} \left(\frac{P_{c,\text{mix}}}{P_{c,0}}\right)^{\frac{2}{3}} \left(\frac{MW_{\text{mix}}}{MW_0}\right)^{\frac{1}{2}} \left(\frac{\alpha_{\text{mix}}}{\alpha_0}\right)
$$

(3-3)

where:

- $\mu$ = Viscosity
- $T_c$ = Critical temperature
- $P_c$ = Critical pressure
- $MW$ = Molecular weight
- $\alpha$ = Rotational coupling coefficient
The subscript “mix” refers to the mixture property, and the subscript “0” refers to the reference substance property. The reference substance for the Pedersen model is methane.

The mixture critical temperature and pressure are calculated using mixing rules that are a function of the component critical temperatures and pressures, and mole fractions. The molecular weight of the mixture is determined from:

\[ MW_{mix} = coef(1) \times (MW_w^{coef(2)} - MW_n^{coef(2)}) + MW_n \]  \hspace{1cm} (3-4)

where \( MW_w \) is the weight fraction averaged molecular weight, and \( MW_n \) is the mole fraction averaged molecular weight.

The rotational coupling coefficient is calculated as follows:

\[ \alpha = 1 + coef(3) \times \rho_r^{coef(4)} MW^{coef(5)} \]  \hspace{1cm} (3-5)

where \( \rho_r \) is the reduced density of the reference substance.

The coefficients are introduced to GEM using the keyword *VISCOEFF in order from 1 to 5. Coefficients used for Pedersen correlation and other fluid properties used in this work are given in Table 3-1, Table 3-2 and Table 3-3.

Table 3-1: Coefficients used for Pedersen correlation

<table>
<thead>
<tr>
<th>Coefficient No.</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.291</td>
</tr>
<tr>
<td>2</td>
<td>1.4</td>
</tr>
<tr>
<td>3</td>
<td>0.0005747</td>
</tr>
<tr>
<td>4</td>
<td>4.265</td>
</tr>
<tr>
<td>5</td>
<td>1.0579</td>
</tr>
</tbody>
</table>

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Table 3-2: Component properties of the model

<table>
<thead>
<tr>
<th>Property</th>
<th>CO₂</th>
<th>H₂O</th>
</tr>
</thead>
<tbody>
<tr>
<td>Critical pressure, atm</td>
<td>72.8090</td>
<td>217.7546</td>
</tr>
<tr>
<td>Critical temperature, K</td>
<td>304.1278</td>
<td>647.0944</td>
</tr>
<tr>
<td>Critical volume, m³/k.mol</td>
<td>0.094</td>
<td>0.056</td>
</tr>
<tr>
<td>Molecular weight, g/g.mol</td>
<td>44.01</td>
<td>18.015</td>
</tr>
<tr>
<td>Acentric factor</td>
<td>0.22394</td>
<td>0.344</td>
</tr>
<tr>
<td>Parachor</td>
<td>78</td>
<td>52</td>
</tr>
<tr>
<td>Boiling point, °F</td>
<td>-109.21</td>
<td>212</td>
</tr>
</tbody>
</table>

Table 3-3: Tuning parameters of the model

<table>
<thead>
<tr>
<th>Property</th>
<th>CO₂</th>
<th>H₂O</th>
</tr>
</thead>
<tbody>
<tr>
<td>Volume shift parameter</td>
<td>0.024668</td>
<td>0.234867</td>
</tr>
<tr>
<td>Binary interaction coefficient with respect to H₂O</td>
<td>-0.0576003</td>
<td>-0.0576003</td>
</tr>
</tbody>
</table>

3.3.4 Phase identity

When the EOS calculation determines that the hydrocarbon fluid exists as a single phase, the simulator alone cannot determine whether a phase should be called “oil” or “gas” without tedious critical point calculations. Nevertheless, phase identity is important in reservoir simulation, as the oil and gas phases use different relative permeabilities and capillary pressure data. In GEM, the identity of a single phase appearing during the simulation can be determined by four approaches. In this study, phase is classified by whether its mass density is closer to a reference gas density or a reference oil density. If necessary, these reference densities are taken from the unstable phases found during stability testing. This method is invoked with the following keyword: *PHASEID *DEN
3.4 PETROPHYSICAL PROPERTIES

Permeability values were generated for all 40,000 grid blocks to simulate different degrees of heterogeneity, rather than using homogeneous or layered description. The synthetic permeability field is generated using “FFT Simulation” code from Jennings (2000). This software produces required number of values in a specific range based on provided statistical properties like probability distribution function and Dykstra-Parson’s coefficient (a quantitative measure of heterogeneity). The generated values should be post processed by a simple program such that they could be used as actual permeability values.

Two realizations of permeability field were used in the simulations:

- 5 ft correlation length in the horizontal direction
- 50 ft correlation length in the horizontal direction

Both are uncorrelated in the vertical direction. Stochastic parameters used to generate the permeability fields are given in Table 3-4 below. Figure 3-3 shows the two different realizations of permeability field. The aquifer was considered to be isotropic. Probability distribution of permeability field is shown in Figure 3-4.
Table 3-4: Stochastic parameters for permeability field generation

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Correlation length in x direction, ft</td>
<td>5 or 50</td>
</tr>
<tr>
<td>Correlation length in y direction, ft</td>
<td>1</td>
</tr>
<tr>
<td>Correlation length in z direction, ft</td>
<td>1</td>
</tr>
<tr>
<td>Mean, md</td>
<td>194</td>
</tr>
<tr>
<td>Standard deviation of Ln($k$)</td>
<td>1.2</td>
</tr>
<tr>
<td>Dykstra-Parson’s coefficient</td>
<td>0.7</td>
</tr>
</tbody>
</table>
Figure 3-3: Geostatistical realizations of permeability (in mD) at a 1 ft by 1 ft scale used in this work. The vertical scale is exaggerated by a factor of two. The fields have (a) 5 ft correlation length in horizontal direction, (b) 50 ft correlation length in horizontal direction. Both are uncorrelated in the vertical direction.
Holtz (2002) has developed correlations relating porosity, permeability, maximum residual gas saturation and residual water saturation for sandstones. The equation:

\[ k = 7 \times 10^7 \phi^{9.61} \]  

(3-6)

is used to calculate the porosity of each grid block from its stochastically generated permeability value. Also the equation:

\[ S_{wir} = 5.159 \left( \frac{\log k}{\phi} \right)^{-1.559} \]  

(3-7)

is used for calculating irreducible water saturation based on average porosity and permeability of the field. In these equations:

\[ k = \text{permeability, md} \]

\[ \phi = \text{porosity, fraction} \]
3.5 ROCK-FLUID PROPERTIES

3.5.1 Relative permeability

The relative permeability curve is defined based on a smooth theoretical model which is commonly fitted to experimental curves. The model is as follows:

\[ k_{rg} = \begin{cases} 
0, & S_g < S_{gcr} \\
\frac{k_{rg}^0}{ \left(\frac{S_g - S_{gcr}}{1 - S_{wr} - S_{gcr}}\right)^{N_g}}, & S_g > S_{gcr} \end{cases}, \quad (3-8) \]

\[ k_{rw} = \begin{cases} 
0, & S_w < S_{wr} \\
\frac{k_{rw}^0}{ \left(\frac{S_w - S_{wr}}{1 - S_{gcon} - S_{wr}}\right)^{N_w}}, & S_w > S_{wr} \end{cases}, \quad (3-9) \]

where:
- \( k_{rg}^0 \) = Gas end point relative permeability (\( k_{rg} \) at residual water saturation)
- \( S_g \) = Gas saturation
- \( S_{gcr} \) = Critical gas saturation
- \( S_{gcon} \) = Connate gas saturation
- \( k_{rw}^0 \) = Water end point relative permeability (\( k_{rw} \) at connate gas saturation)
- \( S_w \) = Water saturation
- \( S_{wr} \) = Residual water saturation
- \( S_{wr} \) = Irreducible water saturation
- \( N_g \) = Gas relative permeability exponent
- \( N_w \) = Water relative permeability exponent
Table 3-5 shows the parameters of relative permeability curves used in this study. Definition of end point saturations is illustrated in Figure 3-5 which shows the drainage relative permeability curves for both phases. Drainage relative permeability curves are defined by table entries in GEM using one of the following keywords:

*SLT

*SGT

This keyword must come after the *RPT keyword.

Table 3-5: Parameters of water and gas relative permeability curves

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Gas end point relative permeability, $k_g^0$</td>
<td>0.86</td>
</tr>
<tr>
<td>Connate gas saturation, $S_{gcon}$</td>
<td>0.10</td>
</tr>
<tr>
<td>Critical gas saturation, $S_{gcr}$</td>
<td>0.15</td>
</tr>
<tr>
<td>Gas relative permeability exponent, $N_g$</td>
<td>2.75</td>
</tr>
<tr>
<td>Water end point relative permeability, $k_w^0$</td>
<td>1.00</td>
</tr>
<tr>
<td>Irreducible water saturation, $S_{wir}$</td>
<td>0.15</td>
</tr>
<tr>
<td>Residual water saturation, $S_{wr}$</td>
<td>0.20</td>
</tr>
<tr>
<td>Water relative permeability exponent, $N_w$</td>
<td>2.00</td>
</tr>
</tbody>
</table>
3.5.2 Hysteresis in relative permeability

Our simulations show that gas saturation will increase, then decrease in some upper grid blocks of aquifer, which were initially saturated with water. This requires accounting for the hysteresis effect in relative permeability. It is also necessary to include relative permeability hysteresis to make a precise study of trapped gas saturation.

In GEM, $k_{rg}$ is always assumed to lie on the drainage curve initially. Drainage relative permeability curves are defined by table entries. The hysteresis effect on $k_{rg}$ is calculated as follows:

$$1 - S_{gcon} = 1 - S_{gcr}$$
\[
k_{rg}(S_g) = \begin{cases} \frac{k_{rg}^{\text{Drainage}}(S_g)}{S_g} & \text{during drainage} \\ \frac{k_{rg}^{\text{Imbibition}}(S_g)}{S_g} & \text{during imbibition} \end{cases}
\]

where:

\[
S_g^{\text{Shifted}} = S_{gr} + \frac{(S_{gh} - S_{gr})}{(S_{gh} - S_{grh})}(S_g - S_{grh})
\]

\(S_{gh} = \) the value of \(S_g\) when the shift to imbibition occurs.

\(S_{grh} = \) the value of \(S_{gr}\) corresponding to \(S_{gh}\) via Land’s equation as follows:

\[
\frac{1}{S_{grh} - S_{gr}} - \frac{1}{S_{gh} - S_{gr}} = \frac{1}{S_{gr}^{\text{max}} - S_{gr}} - \frac{1}{S_{g}^{\text{max}} - S_{gr}}
\]

where:

\(S_g^{\text{max}} = 1 - S_{wr}\).

\(S_{gr}^{\text{max}} = \) maximum residual gas saturation.

In summary, this \(S_{gr}^{\text{max}}\) is the adjustable parameter entered by user which determines the imbibition \(k_{rg}\) curve as a function of the given drainage curve. \(S_{gr}^{\text{max}}\) must lie between zero and \(1 - S_{wr}\).

In this study we use the following correlation developed by Holtz (2002) to calculate the maximum residual gas saturation:

\[
S_{gr}^{\text{max}} = 0.5473 - 0.9696\phi
\]

This correlation returns \(S_{gr}^{\text{max}}=0.286\) for average porosity \((\phi=0.269)\) which is used in our simulations.
3.5.3 Capillary pressure

To simplify reservoir simulations it is common to fit analytical models to capillary pressure curves. A popular empirical model for capillary pressure in petroleum engineering is Brooks-Corey model (Brooks and Corey, 1966). They proposed the drainage capillary pressure model of the form:

\[ p_c = p_e \left( S_w^* \right)^{\frac{1}{\lambda}} \]  

(3-14)

where:

- \( p_e \) = value of \( p_c \) at \( S_w = 1 \)
- \( \lambda \) = pore size distribution index
- \( S_w^* \) = reduced wetting phase saturation defined as:

\[ S_w^* = \frac{S_w - S_{wir}}{1 - S_{wir}} \]  

(3-15)

The parameter \( \lambda \) controls the slope of the plot. A large value of \( \lambda \) gives a small slope, which corresponds to the capillary pressure curve with a narrow pore size distribution whereas a small value of \( \lambda \) gives a large slope, which corresponds to the capillary pressure curve for a wide pore size distribution. A porous medium with a uniform pore size corresponds to \( \lambda = \infty \). \( \lambda \) is called the pore size distribution index in view of these observations.

The Brooks-Corey model cannot adequately fit an S-shaped capillary pressure curve with an inflection. It gives a good fit when the capillary pressure curve has a hyperbolic shape.

Table 3-6 shows the parameters of Brooks-Corey model for capillary pressure curve used in this study. Figure 3-6 below shows the calculated capillary pressure curve with those parameters. The curve is typical of sedimentary rocks with an entry capillary
pressure of 1.2 psi and a maximum capillary pressure of 2.3 psi at irreducible water saturation.

Table 3-6: Parameters of Brooks-Corey model for capillary pressure curve

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$p_e$</td>
<td>1.20</td>
</tr>
<tr>
<td>$\lambda$</td>
<td>8.49</td>
</tr>
<tr>
<td>Irreducible water saturation, $S_{wir}$</td>
<td>0.15</td>
</tr>
</tbody>
</table>

Figure 3-6: Reference capillary pressure curve

3.6 CAPILLARY PRESSURE SCALING

The capillary entry pressure is inversely proportional to the radius of a typical pore throat, while absolute permeability varies with the square of the pore throat radius. Thus heterogeneity of permeability, Figure 3-3, implies heterogeneity of capillary entry
pressure. In the other words, the capillary pressure curves for rock samples from the same reservoir having different permeabilities will be different. The heterogeneity of capillary pressure can be taken into account using the Leverett $J$-function, which is a dimensionless capillary pressure function (Leverett, 1941):

$$J(S_w) = \frac{p_c}{\sigma \cos \theta} \sqrt[3]{\frac{k}{\phi}}$$

(3-16)

where:

- $S_w$ = Water saturation,
- $p_c$ = Capillary pressure,
- $k$ = Permeability,
- $\phi$ = Porosity,
- $\sigma$ = Surface tension,
- $\theta$ = Contact angle.

It suggests that porous media that have the same pore structure but different permeability and porosity will have the same Leverett $J$-function. Therefore, if the different capillary pressure curves of the porous media are rescaled as a Leverett $J$-function, they should plot as one curve. This curve provides the means to average capillary pressure data. Figure 3-7 shows the Leverett $J$-function for several unconsolidated sands with widely different permeabilities. All the data are plotted as one single curve.
The Leverett $J$-function is an attempt to extrapolate capillary pressure data for a given rock to rocks that are similar but with differing permeability, porosity and wetting properties.
To scale the capillary pressure curve for each grid block in the aquifer, we assume that the wetting properties (interfacial tension and contact angle) do not vary spatially. Thus for any arbitrary grid blocks 1 and 2 we have:

\[
J(S_w) = \frac{P_{c1}(S_w)}{\sigma \cos \theta} \sqrt{\frac{k_1}{\phi_1}} = \frac{P_{c2}(S_w)}{\sigma \cos \theta} \sqrt{\frac{k_2}{\phi_2}}
\]

(3-17)

Hence,

\[
P_{c2}(S_w) = P_{c1}(S_w) \sqrt{\frac{k_1}{k_2}} \sqrt{\frac{\phi_2}{\phi_1}}
\]

(3-18)

Subscript 1 denotes the properties of the rock for which we know the capillary pressure curve. This is called reference rock and \(k_1\) and \(\phi_1\) are called reference permeability and porosity, respectively.

For example, if we assign a curve (\(p_{c1}\)) to capillary pressure of a rock (grid block) with permeability of 283.349 md and porosity of 0.30, then for another grid block which has \(k=127.904\) and \(\phi=0.15\), the capillary pressure curve would be:

\[
P_{c2}(S_w) = P_{c1}(S_w) \sqrt{\frac{283.349}{127.904}} \sqrt{\frac{0.15}{0.30}} = 1.0715 \times P_{c1}(S_w)
\]

Hence, if we have already introduced the reference capillary pressure curve (\(p_{c1}\)) to simulator, then we just need to give the scale coefficient of 1.0715 to it so that it would be able to find capillary pressure function for second grid block with \(k=127.904\) and \(\phi=0.15\).

In GEM, the keyword *PCGMAX is used to scale the gas-liquid capillary pressure table to a different end point value for each grid block. Therefore we use it to introduce the scaling coefficient for each grid block to simulator.
In summary, to implement a particular scaling we must choose a reference value of permeability and associate this value with the reference capillary pressure curve. Based on the chosen reference permeability and porosity, for each grid block in the domain we calculate the new gas-liquid capillary pressure value at the connate liquid saturation. We provide these values in the input deck to the simulator. The result is that the vertical scale in reference curve is stretched or contracted by a factor of PCGMAX.

In practice, measurements of the petrophysical properties on a single core sample would be the natural way to set the reference values. In this study, we assign the reference capillary pressure developed in previous section to several values of permeability for a single realization of permeability field. This better illustrates the influence of capillary heterogeneity.

Figure 3-8 shows the reference capillary pressure curve with two scaled curves for two other grid blocks, one with higher, another one with lower permeability than reference permeability, assuming equal porosities. The grid block with higher permeability than reference value has smaller entry pressure than reference and vice versa.
3.7 **LEAK MODEL**

At the end of buoyancy driven flow, CO$_2$ accumulates above residual saturations within some flow paths. To be able to assess the risk of CO$_2$ leakage and evaluate the stored CO$_2$ which is potentially mobile we need to model a leak at the top seal of the aquifer. We simulate an opportunity for all the stored CO$_2$ to move: the sudden development of a conductive leak in the aquifer seal.

As shown in Figure 3-9, our model of the leak is a high permeability (1 Darcy) channel of 4 ft width at the top seal. We assume that the formation above the leak has large permeability (1 Darcy) and porosity (30%). This facilitates the escape of CO$_2$ from
the storage formation, so that any hindrance to escape should be the result of behavior within the storage formation.

We study three different cases, depending on location of the upper aquifer with respect to storage formation:

- The first one has the high permeability formation immediately above the top seal.
- The second has the high permeability formation located above 50 feet impermeable shale layer at the top of the aquifer.
- The third case is similar to the second one, but the formation open to the leak is an active, open aquifer. This upper aquifer has a very low pressure gradient across it, so that water has a small horizontal velocity component through it.

The keyword *NULL can be used to model the shale barrier. The grid blocks which are supposed to act as very low permeability shale are set as null grid blocks using this keyword.

It is convenient to treat the leakage simulation as a “new” run of the simulator. The initial conditions within the storage formation in the new run correspond to the final conditions of the buoyant flow simulation in the storage formation without any leak at the top seal (Figure 3-2). Thus the global mole fraction of gas and water and also reservoir pressure after 25 years of buoyant flow in the lower aquifer without a leak are set as the initial conditions of the leak simulation.
Figure 3-9: Model of the leak is a high permeability channel of 4 ft width in the top seal. The formation open to the leak flow is assumed to have a large permeability and porosity which lets the gas to easily escape the aquifer. The schematic shows the second studied case, where the high permeability formation is located above 50 feet impermeable shale layer at the top of the aquifer. The global mole fraction of gas and water after 25 years of sequestration are set as the initial conditions of the leak simulation.

3.8 NUMERICAL METHODS

GEM can be run in explicit, fully implicit and adaptive implicit modes. In many cases, only a small number of grid blocks need to be solved fully implicitly; most blocks can be solved explicitly. The adaptive implicit option selects a block’s implicitness dynamically during the computation and is useful for coning problems where high flow rates occur near the wellbore, or in stratified reservoirs with very thin layers. Several options are provided for selecting implicit treatment.

The keyword *AIM controls the adaptive-implicit switching options. The default numerical method in GEM is adaptive implicit method with stability switching criterion.
Chapter 4: Simulation of CO2 Sequestration in Scaled Capillary Pressure Field

Determining the integrity of a sealing formation over a deep saline aquifer prior to CO2 injection, and then assuring its integrity after injection ends is feasible. Nevertheless, expediting the transition of injected CO2 into secure forms of storage is of great interest, either to reduce costs associated with seal integrity or to increase public acceptance of geologic storage.

Inducing residual trapping is an attractive means of immobilizing CO2 (Kumar et al., 2004; Ozah et al., 2005; Mo and Akervoll, 2005; Hesse et al., 2006). One way to do this is the “inject low and let rise” approach, in which CO2 is injected only into the bottom part of an aquifer. After injection ends, the CO2 moves upward due to buoyancy through previously uninvaded rock. Some CO2 remains in the displacement path as a residual phase because brine imbibes into the volume previously occupied by the mobile CO2. CO2 also dissolves in previously uncontacted brine on its way up. The dissolved CO2 then reacts with the other species present in the aqueous phase and also with the rock minerals. As a result, precipitation or dissolution of minerals occurs leading to storage of some part of the injected CO2 as minerals. Kumar et al. (2004), Xu et al. (2004) and Gunter et al. (1993, 2000) discuss the modeling of this complex process. Ozah et al. (2005) conclude that CO2 trapped in minerals even after thousands of years is small compared to the other forms of storage. Thus the extent of residual trapping is important for near-term and medium-term immobilization.

The nature of the rising CO2 front - smooth and compact vs. ramified and channeled - strongly affects the volume of rock in which a residual saturation is left.
Previous studies suggest that the intrinsic instability of a buoyancy-driven displacement has little effect on the front, and that the rising CO₂ instead follows channels of correlated larger-than-average permeability (Bryant et al., 2006). In these studies, capillarity was a second-order effect. It dampened the tendency toward channeling and increased the uniformity of the rising plume.

The previous studies use a single drainage capillary pressure curve or a few rock types, each with its own drainage curve, in a formation with a heterogeneous distribution of permeability, typically a geostatistical realization. Rocks with larger permeability tend to have larger pore throats and consequently smaller drainage entry pressures. This correlation means that the previous studies may not be physically representative, at least when capillary forces are comparable to the forces driving CO₂ movement. The reason is simple: even a highly permeable rock can form an effective (local) capillary barrier if placed above rock having a smaller entry pressure. This is shown schematically in Figure 4-1, where rock in region B has smaller permeability and therefore larger entry pressure than rock in region A.

To influence a buoyant displacement front, the barrier (region B) in Figure 4-1 need not have an entry pressure large enough to withstand the capillary pressure exerted by a long column of CO₂. That is, it need not be the petrophysical equivalent of a conventional seal, though such local barriers are commonly found within many aquifers. It need only prevent entry by a rising channel of CO₂ enough to redirect the CO₂ laterally, until the CO₂ encounters rock lying above it with sufficiently small entry pressure. At that point the CO₂ resumes its vertical migration. This corresponds to the path from region A to C to D in Figure 4-1(a). This redirection of the CO₂ can occur even if all the permeabilities, including $k_B$, are large; the only requirement is that the entry pressure in region B be sufficiently larger than in region A.
Figure 4-1: Schematic of path followed by bulk phase CO₂ rising under buoyancy in a heterogeneous domain. (a) Capillary entry pressures are scaled to permeabilities in each region using Leverett J-function. The CO₂ enters region A but has insufficient capillary pressure to enter region B. This can occur even if the permeability of region B is large. As a result, the CO₂ moves laterally into region C, then upward into region D. (b) Single capillary pressure curve is used for all regions. The CO₂ enters region A and can therefore enter region B. Since the driving force for movement is upward, the CO₂ will continue into region B, even if the permeability there is smaller than in the other regions.

If capillary heterogeneity is ignored, e.g. by applying the same drainage curve to all regions, the redirection effect is suppressed. In this case qualitatively different displacement patterns are possible. As indicated in Figure 4-1(b), capillary homogeneity would allow the CO₂ to continue rising into region B from region A, if all the permeabilities are large. This is because the driving force for buoyant displacement is vertical.
The sketch in Figure 4-1 contains no length scale. If region B extends $10^{+2}$ to $10^{+3}$ m, it corresponds to a conventional seal and region A is a structural trap, e.g. a conventional hydrocarbon reservoir. Several mechanisms can create arrangements like Figure 4-1 at the scale of $10^{-2}$ to $10^0$ m within an aquifer, such as grain size variation (e.g. a fining upwards sequence), changes in depositional environment over time, and nonuniform diagenetic alteration. It is at this local scale of heterogeneity that capillary trapping occurs.

These considerations indicate that the influence of heterogeneity of capillary entry pressure on buoyant displacement can overprint the influence of heterogeneity of permeability, even though these properties are strongly correlated. A different displacement front could also lead to different amounts of CO$_2$ being stored in two favorable modes, dissolution in brine and residual trapping. In this work, we study the consequences of this different behavior. In this chapter we show the results of simulations that account for capillary pressure in different ways, including no capillary pressure, single capillary pressure and scaled capillary pressure.

In section 4.1 the model used in our simulations is described and the base case is established. Results of different capillary schemes used with the base case are discussed in section 4.2 and completely changed qualitative behavior of buoyant movement is shown under the effect of heterogeneous capillary pressure field. In section 4.3, the results are given for a permeability field with different correlation length and the effect of correlation length in presence of heterogeneous capillary pressure is discussed. Section 4.4 discusses the effect of capillary pressure scaling on dissolution trapping. Section 4.5 summarizes the consequences of capillary pressure scaling.
4.1 **BASE CASE MODEL**

We idealize the distribution of CO$_2$ after injection phase as a large CO$_2$ saturation in the few bottom layers of a two dimensional aquifer, shown schematically in Figure 4-2. This is intended to approximate the result of high-rate injection into the bottom part of the aquifer.

The boundaries of the domain are closed, which leads to countercurrent flow inside the aquifer as brine falls to replace upward moving CO$_2$.

![Figure 4-2: Schematic of the initial condition for the buoyancy-driven flow simulations (base case). A large saturation of CO$_2$ is placed in the bottom 12 ft of the heterogeneous aquifer.](image)

Simulations are performed on a 100 ft high, 400 ft wide domain with grid blocks of 1 ft by 1 ft length. The aquifer is assumed to be located 5,300 ft below the surface, with initial pressure of 2,265 psi at constant temperature of 140°F which are typical of a deep saline aquifer.

Simulations are performed with GEM, Computer Modeling Group’s simulator. GEM is a general equation of state (EOS)-based compositional reservoir simulator for modeling the flow of three-phase, multicomponent fluids. Here it is used to model a two-phase (aqueous and gas), two-component (brine and CO$_2$) system.
4.2 EFFECT OF CAPILLARY PRESSURE SCALING

Here we present the results of 3 main approaches used to include capillary pressure in simulations. All the cases have the same permeability field with 5 ft correlation length (5 ft in horizontal direction, uncorrelated in vertical direction) which was discussed in previous chapter (Figure 3-3a). The 3 approaches are listed as follows:

1. **No capillary pressure**: to establish a reference case, we carry out a simulation that neglects the effect of capillary pressure entirely.

2. **Single capillary pressure curve**: we use the same capillary pressure curve for all of the grid blocks of the aquifer.

3. **Scaled capillary pressure curves**: we scale the typical capillary pressure curve of Figure 3-6 for each grid block of aquifer according to their different permeability using the Leverett $J$-function, as discussed in previous chapter.

Case 1: Figure 4-3 shows CO$_2$ saturation profile after 25 years, assuming no capillary pressure. The CO$_2$ plume is quite rough with several long, narrow preferential flow paths apparent. The rising CO$_2$ prefers the paths of less resistance, and these paths are determined by spatial correlation of permeability in the aquifer. Although these flow paths appear similar to viscous fingers, the governing factor here is heterogeneity in permeability field, not instability of the displacement. The entire CO$_2$ plume becomes trapped by dissolution and by residual saturation.

Case 2: Figure 4-4 shows CO$_2$ saturation profile when we use a single capillary pressure curve (Figure 3-6) for the entire aquifer. The introduction of capillary pressure dampens the instability of the movement and increases the uniformity of the front. The reason is that the capillary pressure at the leading edge of the CO$_2$ front must exceed the capillary entry pressure (1.2 psi in this simulation).
Figure 4-3: CO₂ saturation profile at 25 years, assuming no capillary pressure. CO₂ rises along preferential flow paths that correspond to regions of correlated, relatively large permeability.

Figure 4-4: CO₂ saturation profile at 25 years, using the single capillary pressure curve of Figure 3-6 for the aquifer. The CO₂ plume follows the preferential flow paths as in Figure 4-3, but is smoother and thus does not travel as far in the vertical direction.
Case 3: The capillary pressure required for a nonwetting phase to enter a pore is inversely proportional to pore throat size. Throat size in turn is correlated with the square root of permeability. In this set of simulations we assign the capillary pressure curve of Figure 3-6 to a particular value of permeability, and use the Leverett $J$-function to scale the curve for all other grid blocks with different permeability. Figure 4-5 through Figure 4-11 show the gas saturation profile at 25 years while assigning the reference capillary pressure curve to 0.57 md, 10 md, 100 md, 194 md, 400 md, 800 md and 2000 md, respectively and scaling the curve for other grid blocks according to their permeability and porosity via Equation (3-16).

If we assign the reference capillary pressure curve to grid blocks having the minimum value of permeability in the field (i.e. 0.57 md), then all other grid blocks would have higher permeability, thus lower entry capillary pressure. Since the distribution of permeability field is lognormal, Figure 3-4, most of the grid blocks have much larger values of permeability, thus nearly zero capillary entry pressure which leads to a behavior similar to that of no capillary pressure case. This can be seen by comparing Figure 4-3 and Figure 4-5. Figure 4-5 shows the CO$_2$ saturation profile at 25 years when the reference capillary pressure curve is assigned to the minimum permeability of the field. The general behavior is clearly the same for both cases. Close examination shows that some capillary barriers (just above the yellow and red pixels) have prevented CO$_2$ from sweeping the whole path it had traversed in no capillary pressure case.

As we increase the permeability associated with reference capillary pressure curve, the behavior dramatically changes. The front loses its uniformity and starts to branch (Figure 4-6). The behavior is intensified as reference permeability increases. In Figure 4-11, where the reference permeability is 2000 md, the gas upward movement is practically restricted to 3 main paths.
Figure 4-5: CO$_2$ saturation profile at 25 years. Capillary pressure scaling is used while reference curve is assigned to minimum permeability of the field (0.57md).

Figure 4-6: CO$_2$ saturation profile at 25 years. Capillary pressure scaling is used while reference curve is assigned to 10md.
Figure 4-7: CO₂ saturation profile at 25 years. Capillary pressure scaling is used while reference curve is assigned to 100md.

Figure 4-8: CO₂ saturation profile at 25 years. Capillary pressure scaling is used while reference curve is assigned to average (mean) permeability of the field (194md). The scaling causes many grid blocks to have large values of entry pressure and thus act as complete barriers to CO₂. Large saturations of CO₂ build up under these local barriers but do not migrate.
Figure 4-9: CO₂ saturation profile at 25 years. Capillary pressure scaling is used while reference curve is assigned to 400md.

Figure 4-10: CO₂ saturation profile at 25 years. Capillary pressure scaling is used while reference curve is assigned to 800md.
Figure 4-11 shows the case where the reference capillary pressure is assigned to the average (mean) permeability of the field and scaled for other grid blocks. This can be more representative of real physical situation in the aquifer. The CO$_2$ rises through some specific channels, which are surrounded by capillary barriers. Although the plume is much ramified, the structure is not the result of the hydrodynamic instabilities which lead to viscous fingering. Instead, some severe and extensive capillary barriers are present in the heterogeneous domain, and these govern the flow paths open to CO$_2$ brine. Moreover, because of countercurrent flow, the two phases compete for preferential flow paths (correlated regions of larger permeability) in a buoyancy-driven immiscible displacement. This makes it even harder for CO$_2$ to invade adjacent pores.

As the CO$_2$ rises, the capillary pressure at the leading edge of the displacement is in the range of 0.8 to 0.9 psi. The variance in the permeability distribution is such that
more than 70% of the grid blocks have capillary entry pressures exceeding 0.9 psi. Thus we expect significant redirection of the rising CO$_2$, as sketched in Figure 4-8. The presence of local capillary barriers within the aquifer traps high saturations of CO$_2$ within the flow paths. After 25 years of buoyant movement, this potentially mobile saturation has reached a relatively stable situation, giving it more time to go into solution in brine surrounding it. As discussed below, this leads to a significant amount of dissolution trapping. Indeed, the salient feature of the CO$_2$ saturation profile at the end of buoyant flow is that CO$_2$ rises through specific channels. As discussed later in this chapter in context of CO$_2$ accumulation as a bulk phase, this differs qualitatively from behavior in the same domain when a single capillary pressure curve is used.

The preferential flow paths in Figure 4-8 are capillarity dominated and it is the spatial correlation of entry pressure field that determines the path of CO$_2$ flow, as can be seen in Figure 4-13. The figure superimposes the saturation silhouette from Figure 4-8 on entry capillary pressure map of the aquifer, Figure 4-12. The plume is highly ramified but not because of the hydrodynamic instabilities (high mobility, less dense phase underlying low mobility, more dense phase) which lead to viscous fingering. Instead, extensive capillary barriers are present in the heterogeneous domain, and these govern the flow paths open to CO$_2$ and brine.
Figure 4-12: Entry capillary pressure (psia) of the aquifer corresponding to Figure 4-8.

Figure 4-13: Superimposing the saturation silhouette (black) from Figure 4-8 on entry capillary pressure map of the aquifer. Color scaling is that of Figure 4-12. The correlated regions of small entry pressure determine the paths followed by the buoyant plume.
4.3 EFFECT OF CORRELATION LENGTH

All the cases in previous section are also simulated with another permeability field with correlation length of 50 ft in x direction and uncorrelated in vertical direction (Figure 3-3b). Figure 4-14 and Figure 4-15 show the results for cases of no capillary pressure and single capillary pressure curve. Figure 4-16 through Figure 4-22 show the results for cases of scaled capillary pressure curves with reference curve assigned to minimum permeability (1.46 md), 10, 100, 190, 400, 800 and 2000 md, respectively.

As in the cases with shorter correlation length, accounting for capillary pressure as a single curve for the whole aquifer smooths the buoyant flow paths, cf. Figure 4-14 and Figure 4-15. But when the reference capillary pressure curve is assigned to minimum permeability of the field, the correlation length begins to affect the nature of the displacement, cf. Figure 4-14 and Figure 4-16. The reason is that in the correlated field with a larger range, capillary pressure barriers are more laterally extensive. Thus they impose a substantial horizontal flow component, even though only a small fraction of the grid blocks have significant entry pressures. Hence the capillary barriers take a more important role in buoyancy driven flow and change the qualitative behavior. Also the field has a vertical strip near the top right edge of the domain with a larger than average permeability which has created a low resistance channel for CO$_2$ to flow through, reaching the top seal of the aquifer in a potentially mobile saturation. This is very important in risk assessment of the project. The same region is present in the simulation with zero capillary pressure, Figure 4-14, but because more CO$_2$ rises throughout the width of the aquifer, there is less CO$_2$ to be focused in that region. In Figure 4-16, the capillary barriers significantly reduce the amount of CO$_2$ that rises from the initial location between x = 0 and x = 300 ft. Thus the mobile CO$_2$ is focused into the path on the far right side of the domain.
Figure 4-14: CO₂ saturation profile at 25 years, assuming no capillary pressure.

Figure 4-15: CO₂ saturation profile at 25 years, using the single capillary pressure curve of Figure 3-6 for the aquifer. Again, the CO₂ plume follows the preferential flow paths as in Figure 4-14, but is smoother and thus does not travel as far in the vertical direction.
Figure 4-16: CO₂ saturation profile at 25 years. Capillary pressure scaling is used while reference curve is assigned to minimum permeability of the field (1.46md).

Figure 4-17: CO₂ saturation profile at 25 years. Capillary pressure scaling is used while reference curve is assigned to 10md.
Figure 4-18: CO$_2$ saturation profile at 25 years. Capillary pressure scaling is used while reference curve is assigned to 100md.

Figure 4-19: CO$_2$ saturation profile at 25 years. Capillary pressure scaling is used while reference curve is assigned to average (mean) permeability of the field (190md).
Figure 4-20: CO₂ saturation profile at 25 years. Capillary pressure scaling is used while reference curve is assigned to 400md.

Figure 4-21: CO₂ saturation profile at 25 years. Capillary pressure scaling is used while reference curve is assigned to 800md.
Assigning the reference capillary pressure curve to average (mean) permeability again shows that CO$_2$ goes through some channels dominated by capillary barriers rather than producing a rough-edged plume, Figure 4-19. The number of channels is smaller than for the case of shorter correlation length, Figure 4-8, and they tend to spread horizontally rather than vertically. Hence the plume contains horizontal thin packs of high saturation CO$_2$ in channels or inside the initial accumulation. These thin packs are potentially mobile, but are trapped by local capillary barriers. In effect, the capillary heterogeneity distributes the CO$_2$ into many smaller stratigraphic traps. The risk of leakage from this arrangement is presumably smaller since the mass stored in each “mini-trap” is smaller. We will discuss it more later in this chapter.
4.4 DISSOLUTION OF CO₂ IN BRINE

The heterogeneity in capillary pressure dramatically changes the behavior of the rising plume and decreases the number of the invaded grid blocks. Remarkably, the amount of CO₂ dissolved in the aqueous phase changes relatively little compared to the cases with no capillary pressure or a single capillary pressure curve. Figure 4-23 and Figure 4-24 show the calculated values for dissolved CO₂ (as mass fraction of total CO₂ initially present in the domain) for permeability fields with 5 ft and 50 ft correlation length, respectively. The calculation uses six output variables of GEM in order to find the dissolved CO₂ in brine. Those six variables are:

- Pore volume,
- Gas saturation,
- Liquid phase mole density (mole/ft³),
- Gas phase mole density (mole/ft³),
- Liquid mole fraction of CO₂,
- Gas mole fraction of CO₂.

The following equations are used:

\[ m_{\text{dissolved CO}_2} = PV \cdot S_w \cdot \rho_{\text{l,molar}} \cdot X_{\text{CO}_2} \cdot MW_{\text{CO}_2} \]  \hspace{1cm} (4-1)

\[ m_{\text{gas CO}_2} = PV \cdot S_g \cdot \rho_{\text{g,molar}} \cdot Y_{\text{CO}_2} \cdot MW_{\text{CO}_2} \]  \hspace{1cm} (4-2)

where:

- \( PV \) = Pore volume, ft³
- \( S_w \) = Water saturation,
- \( S_g \) = Gas saturation,
\( \rho_{l,molar} \) = Liquid phase mole density, mole/ft\(^3\)
\( \rho_{g,molar} \) = Gas phase mole density, mole/ft\(^3\)
\( X_{CO2} \) = Liquid mole fraction of CO\(_2\)
\( Y_{CO2} \) = Gas mole fraction of CO\(_2\)
\( MW_{CO2} \) = CO\(_2\) molecular weight, 44 g/mole

For correlation length of 5 ft, Figure 4-23, where the no capillary pressure case and case of minimum permeability associated with reference capillary curve show similar CO\(_2\) displacement fronts, the latter has slightly larger amount of dissolved CO\(_2\). This is because despite similar front, the scaled \( p_c \) case has several tiny branches which increase the contact surface of gas and water and causes more CO\(_2\) to dissolve in brine. In two other scaled capillary pressure cases, the reduced number of invaded grid blocks due to capillary barriers has caused a significant drop in dissolved CO\(_2\). Although the amount of dissolved CO\(_2\) is less than the no capillary pressure case, it has not dropped proportional to the big drop in number of invaded grid blocks. Quantitatively speaking, we have calculated that more than 30\% of total grid blocks of storage formation are invaded by CO\(_2\) in single \( p_c \) case, while this number is less than 10\% in scaled \( p_c \) case \( (k_{avg}) \), i.e. a drop to one third of invaded grid blocks. At the same time, Figure 4-24 shows that at the time limit of 100 years or more (using extrapolation for scaled \( p_c \) case), 22\% of initial CO\(_2\) is dissolved in single \( p_c \) case, while this number is about 15\% for scaled \( p_c \) case, i.e. a drop to more than two third of the dissolved CO\(_2\) in single \( p_c \) case. In this sense, the scaled capillary pressure increases the dissolution trapping efficiency. That is, more CO\(_2\) is dissolved per unit volume of rock invaded by rising CO\(_2\).

The same behavior can be seen when permeability field with 50 ft correlation length is used for simulations.
Figure 4-23: Dissolved CO$_2$ as mass fraction of total CO$_2$ injected at the bottom of the aquifer for different cases with permeability field of 5 ft correlation length.

Figure 4-24: Dissolved CO$_2$ as mass fraction of total CO$_2$ injected at the bottom of the aquifer for different cases with permeability field of 50 ft correlation length.
Figure 4-26 to Figure 4-27 show the mole fraction of CO$_2$ in aqueous phase after 6 months for permeability field with 5 ft correlation length while reference $p_c$ curve is neglected, assigned to minimum permeability and assigned to average permeability of the field, respectively. In fact, since the dissolution process displaces the CO$_2$ slower than buoyancy-driven vertical displacement then the dissolved CO$_2$ profile looks smoother as scaling intensity increases, i.e. from Figure 4-25 toward Figure 4-27. However, the long term result is a uniform distribution of CO$_2$ in all cases which is achieved after CO$_2$ has enough time to go into solution in brine. This distribution accounts for more effective dissolution trapping in scaled cases after adequate amount of time (Figure 4-28 through Figure 4-30).

Figure 4-25: CO$_2$ mole fraction in aqueous phase after 6 months. Permeability field has 5 ft correlation length while capillary pressure is neglected.
Figure 4-26: CO$_2$ mole fraction in aqueous phase after 6 months. Permeability field has 5 ft correlation length while single capillary pressure curve is used.

Figure 4-27: CO$_2$ mole fraction in aqueous phase after 6 months. Permeability field has 5 ft correlation length. Capillary pressure scaling is used while reference curve is assigned to average (mean) permeability of the field.
Figure 4-28: CO₂ mole fraction in aqueous phase at 25 years. Permeability field has 5 ft correlation length while capillary pressure is neglected.

Figure 4-29: CO₂ mole fraction in aqueous phase at 25 years. Permeability field has 5 ft correlation length while single capillary pressure curve is used.
Figure 4-30: CO₂ mole fraction in aqueous phase at 25 years. Permeability field has 5 ft correlation length. Capillary pressure scaling is used while reference curve is assigned to average (mean) permeability of the field.

Figure 4-31 through Figure 4-33 show the mole fraction of CO₂ in aqueous phase after 1 year for permeability field with 50 ft correlation length while reference $p_c$ curve is neglected, assigned to minimum permeability and assigned to average permeability of the field, respectively. Similar to case of 5 ft correlation length, the dissolved CO₂ profile looks smoother as scaling intensity increases, i.e. from Figure 4-31 toward Figure 4-33.

After CO₂ has enough time to go into solution the result is a uniform distribution of CO₂ in all cases. Figure 4-34 through Figure 4-36 show the long term result for dissolution trapping in above cases after 25 years of buoyant flow.
Figure 4-31: CO$_2$ mole fraction in aqueous phase at 1 year. Permeability field has 50 ft correlation length while capillary pressure is neglected.

Figure 4-32: CO$_2$ mole fraction in aqueous phase at 1 year. Permeability field has 50 ft correlation length while single capillary pressure curve is used.
Figure 4-33: CO$_2$ mole fraction in aqueous phase at 1 year. Permeability field has 50 ft correlation length. Capillary pressure scaling is used while reference curve is assigned to average (mean) permeability of the field.

Figure 4-34: CO$_2$ mole fraction in aqueous phase at 25 years. Permeability field has 50 ft correlation length while capillary pressure is neglected.
Figure 4-35: CO₂ mole fraction in aqueous phase at 25 years. Permeability field has 50 ft correlation length while single capillary pressure curve is used.

Figure 4-36: CO₂ mole fraction in aqueous phase at 25 years. Permeability field has 50 ft correlation length. Capillary pressure scaling is used while reference curve is assigned to average (mean) permeability of the field.
4.5 SUMMARY AND IMPLICATIONS

Considering heterogeneity in capillary pressure has two main consequences for buoyancy-driven flow:

- First, it leads to the highly ramified displacement fronts just described.
- Second, local capillary barriers within the aquifer trap large saturations of CO₂ within the flow paths.

These consequences have competing effects on the extent of CO₂ immobilization. On one hand, less rock volume is invaded by rising CO₂ than when capillarity is homogeneous. On the other hand, large saturations of CO₂ occur within that rock volume. Thus the channeling caused by capillary heterogeneity need not lead to greater vertical extent of migration. A heterogeneous formation can store a volume of CO₂ comparable to that in an otherwise equivalent homogeneous formation. The difference is that the heterogeneous formation stores much of the CO₂ in many small regions of large saturations. These large saturations are potentially mobile, just as structurally trapped CO₂ is potentially mobile. But the accumulations in Figure 4-8 and Figure 4-19 cannot migrate unless all the local barriers lose their integrity. We examine this behavior in more detail in the next chapter.
Chapter 5: Risk Analysis: Simulation of Leak in Scaled Capillary Pressure Field

Three modes of secure (or permanent) storage are widely known for sequestration of CO$_2$ in geological formations: dissolution in brine as aqueous species, formation of disconnected blobs of CO$_2$ phase held by capillary forces (residual trapping), and precipitation of dissolved carbonate anions and metal cations as solids (mineral trapping). Each of these modes carries negligible risk of leakage over the long term. In contrast, accumulation of above-residual saturations of CO$_2$ as a bulk phase (within a structural trap or by any other means) introduces some uncertainty about long-term security, particularly for storage in deep saline aquifers. This is firstly because large saturations of CO$_2$ remain (potentially) mobile, and secondly because the Earth’s crust is inherently leaky. On one hand, many examples of seals enduring over geologic time are known, viz., all conventional oil and gas reservoirs. On the other hand, many examples of leakage of buoyant fluids from the subsurface are also known. Structurally held CO$_2$ can and will migrate should the permeability or capillary seal that forms the structure be breached.

In all of the cases studied in previous chapter, the volume of injected CO$_2$ (which is initial CO$_2$ at the bottom of the aquifer in our model) was chosen less than the threshold value such that the CO$_2$ will not reach the upper seal of the aquifer. A large fraction of CO$_2$ is stored in 2 favorable modes of trapping, i.e. residual and dissolution trapping. But still there is some above-residual saturation of CO$_2$ trapped below capillary barriers. We want to examine this group to see if this is just a temporary trapping below a barrier, like if there was a small flat vein of shale in some part of the aquifer, or if another mode of trapping exists which provides some secure storage for CO$_2$ in a heterogeneous aquifer.
In section 5.1 we increase the volume of injected CO₂ (which is initially present in the bottom of the domain in our model, Figure 3-1) to study the accumulation of CO₂ as a bulk phase held structurally in the storage formation. In section 5.2 we introduce the leakage scenario used in our simulations. In section 5.3 results of leak simulation are discussed and the new trapping mechanism is introduced. Section 5.4 quantifies different modes of trapping in cases studied in this chapter and makes conclusions.

5.1 EXCESSIVE CO₂

We increase the volume of CO₂ initially present in the domain several-fold to study the accumulation of CO₂ as a bulk phase in the upper part of the storage formation, driven by buoyancy. The heterogeneous part of the domain remains unchanged. We add $h_2$ feet of CO₂-saturated layers to the bottom of the simulation model, representing the result of injection into a greater fraction of a thicker aquifer. New layers are added to the bottom of the domain to hold additional CO₂, as indicated in Figure 3-2 and regenerated here in Figure 5-1. The new layers are homogeneous, with permeability and porosity equal respectively to the average permeability and porosity of the aquifer.

![Figure 5-1: Schematic of the initial condition used to study the accumulation of CO₂ beneath the top seal. The heterogeneous part of the domain ($H_1$) remains unchanged. New homogeneous layers are added to the bottom of the domain ($h_2$) to hold additional CO₂.](image)

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5.1.1 Permeability field with 5 ft correlation length

In this section results for the permeability field with 5 ft correlation length (Figure 3-3a) are discussed. Figure 5-2 through Figure 5-7 show the CO₂ saturation profile at 25 years for \( h_2 \) equal to 0, 10, 20, 30, 50 and 100 ft, respectively when capillary pressure scaling is used. In these figures, we can see that CO₂ follows capillary dominated flow paths to reach the top seal if adequate amount of CO₂ is provided. In case with \( h_2=10 \) ft, Figure 5-3, the CO₂ has just found a connecting path to the top seal and hence, the initial volume of CO₂ is the threshold value of injection that does not lead to accumulation of gas as bulk phase in the storage formation. When the injected volume of CO₂ is more than threshold value, Figure 5-4 to Figure 5-7, the excess CO₂ accumulates below the top seal but not uniformly.

Regardless of reaching the top or not, large saturations of CO₂ (70% and more) remain in its flow path. At the end of simulation, all the CO₂ is connected but through a wide spectrum of saturations. Above-residual saturations in the area below the seal are connected along the paths from the initial accumulation. However, still there exist some residual saturation and even un-invaded grid blocks in this upper “gas cap” section. The latter are the consequence of capillary barriers that resisted vertical migration from below and then from above as the accumulating CO₂ pushes downward. In other words, the barriers have been so severe that even pushing the gas downward by more CO₂ (which traveled upward due to buoyancy force) has not led the gas to invade those grid blocks. We want to know how much of this above-residual CO₂, within the “gas cap” and within the preferential flow paths below the gas cap, would escape if a leak develops in the seal. We address this question in the next section.
Figure 5-2: CO₂ saturation profile at 25 years for the aquifer of Figure 5-1 with $h_2=0$, assigning the reference capillary pressure curve to average (mean) permeability of the field. The permeability field of storage formation corresponds to that of Figure 3-3a.

Figure 5-3: CO₂ saturation profile at 25 years for the aquifer of Figure 5-1 with $h_2=10$ ft, assigning the reference capillary pressure curve to average (mean) permeability of the field. The permeability field of storage formation corresponds to that of Figure 3-3a.
Figure 5-4: CO₂ saturation profile at 25 years for the aquifer of Figure 5-1 with $h_2=20$ ft, assigning the reference capillary pressure curve to average (mean) permeability of the field. The permeability field of storage formation corresponds to that of Figure 3-3a.

Figure 5-5: CO₂ saturation profile at 25 years for the aquifer of Figure 5-1 with $h_2=30$ ft, assigning the reference capillary pressure curve to average (mean) permeability of the field. The permeability field of storage formation corresponds to that of Figure 3-3a.
Figure 5-6: CO₂ saturation profile at 25 years for the aquifer of Figure 5-1 with $h_2=50$ ft, assigning the reference capillary pressure curve to average (mean) permeability of the field. The permeability field of storage formation corresponds to that of Figure 3-3a.

Figure 5-7 shows the gas saturation profile at 25 years when $h_2=100$ ft, i.e. the volume of injected CO₂ is more than pore volume of the storage formation. This causes the CO₂ to almost spread over the whole area of storage formation. In fact, CO₂ first rises through capillary dominated flow paths due to buoyancy and then sweeps the aquifer downward due to rise of more CO₂ in those channels. In this case, the aquifer is divided into two parts, with no distinguishable transition zone in between: an upper section (the gas cap) in which CO₂ accumulates in high saturations within the flow channels, and a lower section with residual CO₂ saturation where CO₂ was initially injected. A similar final pattern will be seen in no capillary pressure and single capillary pressure cases, but different in nature and development.
Figure 5-7: CO₂ saturation profile at 25 years for the aquifer of Figure 5-1 with $h_2=100$ ft, assigning the reference capillary pressure curve to average (mean) permeability of the field. The permeability field of storage formation corresponds to that of Figure 3-3a.

Figure 5-8 and Figure 5-9 show the CO₂ saturation profile again at 25 years using no capillary pressure and single capillary pressure curve, respectively. In both cases $h_2=50$ ft. The CO₂ has risen through essentially vertical channels and swept almost the whole aquifer, then filled the upper section of the storage formation like a gas cap. In the cap, the bulk CO₂ phase has accumulated below the top seal uniformly, unlike the scaled $p_c$ case (Figure 5-6). The storage aquifer is thus divided into two sections, an upper section (the gas cap) in which CO₂ has displaced water to residual saturation, and a lower section with residual CO₂ saturation within the flow channels. These flow channels are the consequence of correlation in the permeability field.
Figure 5-8: CO₂ saturation profile at 25 years for the aquifer of Figure 5-1 with \( h_2 = 50 \) ft, while capillary pressure is neglected. The permeability field of storage formation corresponds to that of Figure 3-3a.

Figure 5-9: CO₂ saturation profile at 25 years for the aquifer of Figure 5-1 with \( h_2 = 50 \) ft, while single capillary pressure curve is used. The permeability field of storage formation corresponds to that of Figure 3-3a.
5.1.2 Permeability field with 50 ft correlation length

In this section we discuss the results when the permeability field of Figure 3-3b with 50 ft correlation length is used. Figure 5-10 and Figure 5-11 use no capillary pressure curve and a single capillary pressure curve, respectively. The results are shown for \( h_2 = 50 \) ft more initial volume of CO\(_2\). The CO\(_2\) first follows vertical channels resulting from correlation in the permeability field. These wide stripes expand gradually and join together after sufficient amount of CO\(_2\) leaves the injection zone and rises. The CO\(_2\) then accumulates in the upper section of the storage formation, again uniformly like a gas cap. Two zones are clearly distinguished in the storage aquifer: residual water in upper section (the gas cap), and residual gas in lower section.

In Figure 5-12 through Figure 5-14 capillary pressure scaling is used. Figure 5-12 shows the threshold value of injection volume in order for CO\(_2\) to be securely trapped without accumulating as a bulk phase. There is \( h_2 = 20 \) ft more CO\(_2\) injected initially at the bottom. There are two differences between this case which has 50 ft correlation length and the case of section 5.1.1 which has 5 ft correlation length. The longer correlation length can accommodate more amount of CO\(_2\) securely, and also it takes a longer time for the CO\(_2\) to get trapped as residual saturation or dissolved gas. In Figure 5-3 it takes less than 25 years for CO\(_2\) to get to a stable position, while this time is about 100 years for Figure 5-12. The reason is higher tendency of CO\(_2\) for horizontal rather than vertical movement in longer correlation length permeability field.

Figure 5-13 and Figure 5-14 show the CO\(_2\) saturation profile with \( h_2 = 50 \) ft at 25 and 100 years, respectively. Again, we can see that CO\(_2\) follows capillary dominated flow paths (which are horizontally aligned) to reach and non-uniformly accumulate below the top seal. Because of the slower displacement of CO\(_2\), it is still moving after 100 years.
Figure 5-10: CO₂ saturation profile at 25 years for the aquifer of Figure 5-1 with $h_2=50$ ft, while capillary pressure is neglected. The permeability field of storage formation corresponds to that of Figure 3-3b.

Figure 5-11: CO₂ saturation profile at 25 years for the aquifer of Figure 5-1 with $h_2=50$ ft, while single capillary pressure curve is used. The permeability field of storage formation corresponds to that of Figure 3-3b.
Figure 5-12: CO$_2$ saturation profile at 25 years for the aquifer of Figure 5-1 with $h_2$=20 ft, assigning the reference capillary pressure curve to average (mean) permeability of the field. The permeability field of storage formation corresponds to that of Figure 3-3b.
Figure 5-13: CO₂ saturation profile at 25 years for the aquifer of Figure 5-1 with $h_2=50$ ft, assigning the reference capillary pressure curve to average (mean) permeability of the field. The permeability field of storage formation corresponds to that of Figure 3-3b.

Figure 5-14: CO₂ saturation profile at 100 years for the aquifer of Figure 5-1 with $h_2=50$ ft, assigning the reference capillary pressure curve to average (mean) permeability of the field. The permeability field of storage formation corresponds to that of Figure 3-3b.
5.2 LEAKAGE SCENARIO

We simulate the sudden development of a leak in the top seal after 25 years of buoyant flow. The leak is a set of high permeability grid blocks extending through the impermeable layer at the top of the aquifer. This could represent a damage zone around a fault, defects in the cemented annulus of a well, or a fracture induced during injection. The storage formation containing the CO$_2$ remains closed, so any CO$_2$ that leaks out must be replaced by water sinking into the aquifer. This does not prevent the migration of any potentially mobile CO$_2$ although it does affect the rate at which CO$_2$ escapes.

As shown in Figure 3-9 and reproduced here in Figure 5-15, we model the leak as a high permeability (1 Darcy) channel of 4 ft width at the top seal. The leak has a width of four grid blocks in order to accommodate countercurrent flow within it. We assume that the formation above the leak has large permeability (1 Darcy) and porosity (30%). This facilitates the escape of CO$_2$ from the storage formation, so that any hindrance to escape should be the result of behavior within the storage formation. Details of modeling in GEM are explained in section 3.7.

Figure 5-15: Model of the leak is a high permeability channel of 4 ft width in the top seal. The schematic shows the second studied case, where the high permeability formation is located above 50 feet impermeable shale layer at the top of the aquifer.
We study three different cases, depending on location of the upper aquifer with respect to storage formation:

- The first one has the high permeability formation immediately above the top seal (Figure 3-9 with $h_{\text{shale}}=1$ ft).
- The second has the high permeability formation located above 50 feet impermeable shale layer at the top of the aquifer (Figure 3-9).
- The third case is similar to the second one, but the formation open to the leak is an active, open aquifer. This upper aquifer has a very low pressure gradient across it, so that water has a small horizontal velocity component through it.

5.3 SIMULATION OF LEAK: LOCAL CAPILLARY TRAPPING

5.3.1 Thin sealing layer ($h_{\text{shale}}=1$ ft)

The first case has the high permeability formation immediately above the top seal, i.e. the height $h_{\text{shale}}=1$ ft consist of a thin seal (one layer of grid blocks). Figure 5-16 shows the CO$_2$ saturation profile at the beginning of leak simulation. The resulting configuration after 25 years of buoyant flow in the lower aquifer without a leak (Figure 5-6) is set as the initial condition of the leak simulation.

The results 25 years after the leak opens are shown in Figure 5-17 through Figure 5-19. In order to analyze the risk involved in each case, we quantify the CO$_2$ escaped through the leak. In following discussion, the “gas cap” refers to top 30 ft of the storage formation in which excess CO$_2$ has accumulated. First, we calculate the initial mass of CO$_2$ in the gas cap that is potentially mobile, i.e. that part of CO$_2$ which is beyond maximum residual gas saturation in Figure 5-16. For this simulations, $S_{g}^{\text{max}}=0.286$. In fact, the following equation is used for every grid block with $S_{g}>0.286$ in the gas cap:
\[ m_{\text{potentially mob CO}_2} = \sum_{\text{gas cap, } S_g > 0.286} \left( PV \cdot (S_g - 0.286) \cdot \rho_{g,\text{molar}} \cdot Y_{\text{CO}_2} \cdot MW_{\text{CO}_2} \right) \] (5-1)

where:

- \( PV \) = Pore volume, ft\(^3\)
- \( S_g \) = Gas saturation,
- \( \rho_{g,\text{molar}} \) = Gas phase mole density, mole/ft\(^3\)
- \( Y_{\text{CO}_2} \) = Gas mole fraction of CO\(_2\)
- \( MW_{\text{CO}_2} \) = CO\(_2\) molecular weight, 44 g/mole

Then the mass of total CO\(_2\) in the upper aquifer after the leak (whether dissolved in water or residually trapped or accumulated in above-residual saturation) is calculated \( m_{\text{escaped CO}_2} \). A security index can be defined for every leak position using the ratio of these two variables as:

\[ S.I. = 1 - \frac{m_{\text{escaped CO}_2}}{m_{\text{potentially mob CO}_2}} \] (5-2)

which is a measure of how secure the configuration is if a leak develops in that specific location in the seal. The index varies between 0 and 1, with higher indexes showing higher security.

In Figure 5-17 the leak is placed 110 feet from the left boundary of the domain. About 54\% (mass percent) of the above-residual saturation of CO\(_2\) in the gas cap escaped 25 years after development of the leak, forming an accumulation of a few CO\(_2\)-saturated layers at the top of the upper aquifer. This gives a security index value of \( S.I. = 0.46 \). Most of the grid blocks at the upper layers of storage formation only contain the residual gas
saturation after the leak. Sinking brine dissolved the residual phase just below the leak. However, as discussed below, much of the CO$_2$ in the flow channels did not escape.

In Figure 5-18 the leak is placed 300 feet from the left boundary of the domain. In contrast to Figure 5-17, less than 4% of the above-residual saturation of CO$_2$ in the gas cap has leaked, mostly in form of dissolved gas in brine, and a large fraction of potentially mobile CO$_2$ has remained in place. The security index is then $S.I=0.96$ which shows a highly secure configuration of stored CO$_2$ if a leak develops at $x=300$ft.

So, we can conclude that the location of fracturing in the top seal is important in evacuation of CO$_2$ to adjacent formations when the storage formation is heterogeneous. In other words, not every leak in storage formation in which CO$_2$ has accumulated in local capillary traps leads to extensive contamination of neighboring waters.

Figure 5-16: CO$_2$ saturation profile just before leak evolves. The leak is assumed to emerge instantaneously after 25 years of buoyant flow of the CO$_2$ initially in the storage formation. In fact, CO$_2$ saturation profile of Figure 5-6 is set as the initial condition before the leak opens in the top seal of the aquifer.
Figure 5-17: CO$_2$ saturation profile at 25 years after a leak opens in the top seal of the aquifer. The high permeability formation is immediately above the top seal. The leak is located at 110 ft distance to the left boundary.

Figure 5-18: CO$_2$ saturation profile at 25 years after a leak opens in the top seal of the aquifer. The high permeability formation is immediately above the top seal. The leak is located at 300 ft distance to the left boundary.
In Figure 5-19 both leaks in the last two figures are assumed to develop simultaneously after 25 years of buoyant flow, i.e. there are two leaks at 110 ft and 300 ft from the left boundary of the domain. Calculation shows that about 57% of the above-residual CO$_2$ in gas cap has escaped through the leak which is equal to sum of the escaped gas in the last two cases. The resulting security index of $S.I._t=0.43$ shows a fairly insecure storage for this leak combination. However, simulation shows that the amount of gas that escaped through each single leak is different from the amount escaped when that was the only leak in the aquifer. This can be better understood by comparing Figure 5-20 and Figure 5-21. Both figures show the CO$_2$ saturation profile at 10 years after leaks open. Apparently much more CO$_2$ is escaping through right-hand side leak in Figure 5-21 than in Figure 5-20.

![Figure 5-19: CO$_2$ saturation profile at 25 years after two leaks open in the top seal of the aquifer. The high permeability formation is immediately above the top seal. The leaks are located at 110 ft and 300 ft distance to the left boundary.](image)
Figure 5-20: CO$_2$ saturation profile at 10 years after a leak opens in the top seal of the aquifer. The high permeability formation is immediately above the top seal. The leak is located at 300 ft distance to the left boundary.

Figure 5-21: CO$_2$ saturation profile at 10 years after two leaks open in the top seal of the aquifer. The high permeability formation is immediately above the top seal. The leaks are located at 110 ft and 300 ft distance to the left boundary.
Regardless of leak location, above-residual saturations of CO\textsubscript{2} remain trapped by local capillary barriers in several scattered regions throughout the domain. Some examples are indicated by pink arrows in Figure 5-17 and Figure 5-18. This mode of trapping is analogous to filling a hydrocarbon trap beyond the spill point. Once CO\textsubscript{2} fills the local trap, subsequent migration of CO\textsubscript{2} past the spill point has no effect on the trapped CO\textsubscript{2}. It does not matter if the migration is a continuation of buoyant flow from below, or induced by leakage above. This secure mode of CO\textsubscript{2} storage could not be seen when neglecting capillary pressure or using a single capillary pressure curve for the whole aquifer. We suggest that an appropriate term for this mode of storage is \textit{local capillary trapping}. 
5.3.2 Thick sealing layer ($h_{\text{shale}}=50$ ft)

To see whether countercurrent flow within the leakage path (a narrow column of grid blocks) has any effect on the behavior, a second case has been set to have the high permeability formation located above a 50 feet thick impermeable shale layer at the top of the storage formation (Figure 3-9). The leak is assumed to develop 110 feet from the left boundary. The gas saturation profile 25 years after the leak opens is shown in this section. In Figure 5-22 a single capillary pressure curve is used for the whole aquifer, while in Figure 5-23 capillary pressure scaling is used.

In Figure 5-22 gas cap has almost entirely discharged to upper aquifer, leaving the storage formation filled with residual gas saturation in gas cap zone. The CO$_2$ is still moving toward the leak in very few grid blocks at top right of the storage formation where it has more than residual saturation. When the top seal is breached there is no hindrance for CO$_2$ escaping to upper formations. Thus about 93% of the above-residual CO$_2$ in the gas cap, i.e. the portion of the CO$_2$ that was structurally “trapped”, escapes through the leak. A large amount of still potentially mobile CO$_2$ accumulates at the top of the upper aquifer. The security index of the storage formation for this leak is $S.I.=0.07$ which is a very low value.

In Figure 5-23 the mobile CO$_2$ phase accumulated at the top left of the aquifer is evacuated through the leak. This leads to an accumulation of a thin layer at the top of the upper aquifer. The amount of this still potentially mobile CO$_2$ is much smaller than in Figure 5-22. The CO$_2$ saturation in the storage formation falls to residual values in the vicinity of the leak, but elsewhere large saturations of CO$_2$ remain trapped below capillary barriers. This is true for barriers not only in the preferential flow paths, but also in the gas cap at the top of the storage formation. About 43% of the above-residual CO$_2$
in the gas cap has leaked 25 years after the leak opens. This is two thirds the amount that leaked in Figure 5-22. The security index is $S.I. = 0.57$ which shows that the storage formation is much more secure if we use capillary pressure scaling for analysis. The large saturations of CO$_2$ remaining at the top right of the storage aquifer are also mobile, but this CO$_2$ would escape only if another leakage path through the seal were to emerge. Local capillary trapping is visible also in the preferential flow paths below the gas cap (the red arrows, yellow and orange pixels at the bottom).

Comparison of Figure 5-22 and Figure 5-23, and continued simulation of leakage for 150 years suggest that the thickness of the seal affects the leakage rate but not the final distribution of CO$_2$ in the storage formation.

Local capillary trapping and residual phase trapping are both the result of capillary forces. But there is an essential difference in the way capillary forces act. In residual trapping, capillary forces lead to spontaneous disconnection of volumes of CO$_2$ phase at the pore scale. The volumes are then immobilized by capillary forces. In local capillary trapping, no pore-scale disconnection of the bulk phase occurs. Instead local accumulations of CO$_2$ are formed when capillary forces prevent the CO$_2$ from rising further.
Figure 5-22: CO₂ saturation profile at 25 years after a leak at x=110 ft opens in the 50 ft thick seal at top of the aquifer. Single reference capillary pressure curve of Figure 3-6 is used. Permeability field has 5 ft correlation length.

Figure 5-23: CO₂ saturation profile at 25 years after a leak at x=110 ft opens in the 50 ft thick seal at top of the aquifer. Capillary pressure scaling is used. The red arrows indicate regions where local capillary trapping has immobilized CO₂. Permeability field has 5 ft correlation length.
5.3.3 Thick sealing layer \((h_{\text{shale}}=50 \text{ ft})\) leaking to active aquifer

The third case presented in this section is similar to the second case, but the formation open to the leak is an active, open aquifer. This upper aquifer has a very low pressure gradient across it, so that water has a small horizontal velocity component through it.

Figure 5-24 through Figure 5-28 show the results of simulation at 6 months, 5, 10, 15 and 25 years, respectively. The pressure gradient across the upper aquifer is such that brine has a horizontal velocity component of about 0.03 ft/day (reservoir condition) from left to right. As can be seen in the figures, the effluent CO\(_2\) has vertical velocity component comparable to horizontal velocity of brine. Hence, CO\(_2\) first rises to the top of the upper aquifer and then moves horizontally toward right boundary. Gas continues to leave the aquifer up to about 10 years (Figure 5-26), which is less than the time it takes while the upper aquifer is also static (see Figure 5-23). But the amount of escaped gas is similar in both cases, i.e. 42% of the above-residual CO\(_2\) in the gas cap or \(S.I.=0.58\). Hence, an active aquifer seems to increase the rate of gas leakage from the storage formation, but does not change the volume of CO\(_2\) that leaks out of it.
Figure 5-24: CO₂ saturation profile at 6 months after a leak at x=110 ft opens toward an active aquifer. Capillary pressure scaling is used.

Figure 5-25: CO₂ saturation profile at 5 years after a leak at x=110 ft opens toward an active aquifer. Capillary pressure scaling is used.
Figure 5-26: CO₂ saturation profile at 10 years after a leak at x=110 ft opens toward an active aquifer. Capillary pressure scaling is used.

Figure 5-27: CO₂ saturation profile at 15 years after a leak at x=110 ft opens toward an active aquifer. Capillary pressure scaling is used.
Figure 5-28: CO₂ saturation profile at 25 years after a leak at x=110 ft opens toward an active aquifer. Capillary pressure scaling is used.

5.4 SUMMARY AND IMPLICATIONS

Table 5-1 summarizes the value of security index, as defined in section 5.3.1, for four of the cases studied in this chapter:

- leak at x=110 ft in thin shale layer, using capillary pressure scaling, Figure 5-17.
- leak at x=300 ft in thin shale layer, using capillary pressure scaling, Figure 5-18.
- leak at x=110 ft in thick shale layer, using capillary pressure scaling, Figure 5-23.
- leak at x=110 ft in thick shale layer, using single capillary pressure curve, Figure 5-22.

Low value of $S.I.$ in case with single capillary pressure field suggests that ignoring capillary pressure scaling can underestimate, in a significant extent, the ability of aquifer to securely store CO₂.
Table 5-1: Security index for different cases

<table>
<thead>
<tr>
<th>Case</th>
<th>Seal Thickness</th>
<th>Leak Position</th>
<th>Security Index (S.I.)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Scaled</td>
<td>Thin, h=1 ft</td>
<td>x=110 ft</td>
<td>0.46</td>
</tr>
<tr>
<td>Scaled</td>
<td>Thin, h=1 ft</td>
<td>x=300 ft</td>
<td>0.96</td>
</tr>
<tr>
<td>Scaled</td>
<td>Thick, h=50 ft</td>
<td>x=110 ft</td>
<td>0.57</td>
</tr>
<tr>
<td>Single</td>
<td>Thick, h=50 ft</td>
<td>x=110 ft</td>
<td>0.07</td>
</tr>
</tbody>
</table>

Figure 5-29 compares the escaped CO$_2$ as mass percent of total CO$_2$ initially injected in the aquifer for the above four cases. While all cases have equal amount of initial CO$_2$, using capillary pressure scaling reduces the estimation of escaped CO$_2$ to less than half than using single capillary pressure field.

Figure 5-29: Amount of trapping in aquifer for single and scaled capillary pressure fields, 25 years after leak development. x denotes the location of the leak from the left boundary of the aquifer.
Figure 5-30 shows the distribution of CO$_2$ in various storage mechanisms in simulations with single and with scaled capillary pressure fields. The figure compares mass percent of CO$_2$ for the above four cases, 25 years after leak development.

For the purpose of quantification, the CO$_2$ escaped from the leak to the upper aquifer is defined as “free gas”, while the above-residual saturations of CO$_2$ remaining in the storage formation are considered as local capillary trapped. No local capillary trapping can exist when using single capillary pressure. (The tiny percent seen in the chart is due to incompleteness of CO$_2$ escaping after 25 years. The limit value is zero.)

A remarkable consequence of capillary heterogeneity is greater immobilization of CO$_2$ even though less residual trapping occurs. This only becomes apparent when a leak is simulated, and the amount of CO$_2$ that escapes is found to depend on heterogeneity and on location of the leak. The maximum amount of “free gas” occurs when capillary heterogeneity is ignored. Thus Figure 5-30 suggests that CO$_2$ sequestration risk assessment based on simple assumptions for $p_c$, i.e. a homogeneous capillary pressure field or neglecting $p_c$, is pessimistic when significant buoyancy-driven displacement occurs. However, a wide range of CO$_2$ leakage amounts below this maximum can happen in a storage formation, depending on the position of the presumptive leak. On one end the total mass of above residual gas can be secured by local capillary trapping, while on the other end almost all of this mass can escape the storage formation when different leaks develop in different positions in the top seal. The cases studied here illustrate the intermediate situations between these limits.
Figure 5-30: Distribution of CO$_2$ in various modes of storage for single and scaled capillary pressure fields, 25 years after leak development. $x$ denotes the location of the leak from the left boundary of the aquifer.
Chapter 6: Conclusions and Recommendations

6.1 CONCLUSIONS

This research work was performed with the main objective of studying the dynamics of buoyancy-driven flow in CO₂ bulk phase storage. The following conclusions are made from this work:

- Considering heterogeneous capillary pressure introduces a new control parameter in buoyancy-driven flow of CO₂ in deep saline aquifers, which is capillary barriers.

- As the heterogeneity of the aquifer increases, capillarity begins to dominate the intrinsic instability of a buoyant displacement.

- In some regions, capillary barriers confine CO₂ to a particular flow path even when the value of absolute permeability would allow significant flow of a single phase. This can cause trapping of CO₂ below some barriers in above-residual saturations.

- Modeling and simulations of a leak in the top seal show that CO₂ in a large portion of these above-residual accumulations can remain trapped. Accordingly, a new mode of trapping is identified, termed “local capillary trapping” as it is associated with conterminous regions of larger-than-average capillary entry pressure. The regions are scattered throughout the domain according to the correlation structure of the permeability field and contain CO₂ accumulations at saturations much larger than residual.
In formations with sufficiently heterogeneous capillarity, the structure of the rising CO₂ plume reduces the volume of rock invaded. This necessarily implies a reduction in residual phase trapping. In the cases examined here, this reduction is more than balanced by local capillary trapping within the storage formation.

Consequently heterogeneity does not reduce the security of sequestration that relies on buoyancy-driven displacement. In fact, the amount of CO₂ that leaks through a channel in the caprock is smaller when capillary heterogeneity is accounted for.

However, the extent of local capillary trapping depends on the location of the leak.

6.2 RECOMMENDATIONS

As stated above, our study implies that the extent of local capillary trapping depends on the location of the leak in the top seal of the aquifer. This suggests that a probabilistic appraisal of the increase in security will be necessary.

Further research considering following issues could be conducted in order to improve the risk estimate of the sequestration projects:

- The hysteresis effect in capillary pressure is neglected in this work. Some preliminary simulations using two different curves for drainage and imbibition capillary pressure suggest that capillary hysteresis can change the behavior of the buoyancy driven flow. However, a model needs to be established and verified to be able to handle capillary hysteresis. This parameter not only adds to complexity of the simulation and makes it take longer to get solved, but also adds to stiffness of the mathematical problem.
The results presented in this work are based on two-dimensional simulations. Three-dimensional studies may reveal new behavior of the front or change the storage capacity of the aquifer. However, finding an upscaling method seems to be necessary before conducting a three-dimensional simulation. Fine grid blocks of 1 ft by 1 ft which were used in this work cannot be used for a three-dimensional simulation, since they lead to a very large number of grid blocks even for a small aquifer used for analyzing the behavior.
Appendix: Input Files

GEM INPUT FILE: BASE CASE

The simulation input file for the base case while capillary pressure scaling is used is presented here. The permeability, porosity and capillary pressure scaling ratio of grid blocks are in separate files included to the input file, namely 'Perm-5-5-1.txt', 'Por-5-5-1.txt' and 'PcScale-5-5-1-P.txt', respectively. The resulting CO₂ saturation profile is given in Figure 4-8.

RESULTS SIMULATOR GEM
RESULTS SECTION INOUT
 *******************************************************************
** Base Case
** Purpose: Effect of capillary pressure scaling
** All 40000 grid blocks have different Pc curves, scaled with J-function
 *******************************************************************
*INUNIT *FIELD
*INTERRUPT *INTERACTIVE
*RANGECHECK *ON
*XDR *ON
*MAXERROR 20
*DIARY *CHANGES

** Output Print File:
*WPRN *ITER *NONE
*WPRN *GRID *TIME
*OUTPRN *GRID *PRES DROP PCG SATP
*KRG KRO
*DEN O RHOG RHOO MWG MWO VISG VISO FRG
*SG SO
*Z 'CO2' Z 'H2O'
*Y 'CO2' Y 'H2O'
*X 'CO2' X 'H2O'
*K 'CO2' K 'H2O'
*SIG
*VELOCRC
** Simulation Results File:  
*WSRF *GRID *TIME  
*OUTSRF *GRID *PRES DROP  
*PCG SATP  
*KRG KRO  
*DENG DENO RHOG RHOO MWG MWO VISG VISO FRG  
*SG SO  
*Z 'CO2' Z 'H2O'  
*Y 'CO2' Y 'H2O'  
*X 'CO2' X 'H2O'  
*K 'CO2' K 'H2O'  
*SIG  
*VELOCRC  
*OUTSRF *RES *VELOCRC  

** Restart File (To restart at the last time step in RST file):  
*WRST 100000  
*REWIND 2

*********************************************************************  
Aquifer details  
*GRID *CART 400 1 100  
*KDIR *DOWN  
*DI *CON 1  
*DJ *CON 1  
*DK *CON 1  
*DEPTH *TOP 200 1 1 5300.  
=NULL *CON 1  

** No Anisotropy:  
*PERMI *ALL *INCLUDE 'Perm-5-5-1.txt'  
*PERMJ *EQUALSI  
*PERMK *EQUALSI  
*POR *MATRIX *ALL *INCLUDE 'Por-5-5-1.txt'  
*CPOR *MATRIX 3.0E-6  
*PRPOR *MATRIX 14.7

*********************************************************************  
Component properties for EOS model  
*MODEL *PR  
*NC 2 2  
*COMPNAME 'CO2' 'H2O'  
*HCP 0 0  
*VISCO *PEDERSEN  
*VISCOEFF 0.291  
1.4  
0.0005747  
4.265  
1.0579
** Relative permeability

*ROCKFLUID
*RPT *SCALING-NEW

** Water-Oil relative perm table: NOT USED in simulation
*SWT
0.000000 0.000000 1.000000 0.000000
0.0524375 0.0008203 0.8400835 0.000000
0.104875 0.0032813 0.6973033 0.000000
0.1573125 0.0073828 0.5708514 0.000000
0.209750 0.013125 0.4599021 0.000000
0.2621875 0.0205078 0.3636104 0.000000
0.314625 0.0295313 0.2811098 0.000000
0.3670625 0.0401953 0.211510 0.000000
0.419500 0.052500 0.1538931 0.000000
0.4719375 0.0664453 0.1073101 0.000000
0.524375 0.0820313 0.0707757 0.000000
0.5768125 0.0992578 0.0432609 0.000000
0.629250 0.118125 0.0236831 0.000000
0.6816875 0.1386328 0.0108919 0.000000
0.734125 0.1607813 0.0036447 0.000000
0.7865625 0.1845703 0.0005609 0.000000
0.839000 0.210000 0.000000 0.000000

** Oil-Gas relative perm table: USED in simulation
*SLT
**SL Krg Krog Pco
0.15 0.860969388 0 2.291009 ** SLCON: Connote Liq. Sat.
0.2 0.7 0 1.698
0.25 0.560459184 0.005102041 1.556611 ** SLRG: Residual Liq. Sat.
0.3 0.440816327 0.020408163 1.479537
0.35 0.339540816 0.045918367 1.427207
** Initial condition**

*INITIAL
*USER_INPUT
*NREGIONS 1

*SW  *CON 0
*PRES  *CON 2265.5
*ZGLOBALC 'CO2' KVAR 88*0 12*0.8
*ZGLOBALC 'H2O' KVAR 88*1 12*0.2

** Numerical control**

*NUMERICAL
*DTMAX  1.0
*DMIN  1.0E-05
*NORM  *PRESS 1000.
*MAXCHANGE *GMOLAR 0.5
*MAXCHANGE *SATUR 0.5
*CONVERGE *PRESS 0.514884

** Well and run details**

*RUN
*DATE 2000 01 01
*DATE 2000 01 10
*DATE 2000 01 20
*DATE 2000 01 30
*DATE 2000 02 30
*DATE 2000 03 30

*DTMAX 2.

*DATE 2000 06 30
*DATE 2000 09 30
*WRST *TNEXT
*DATE 2001 01 01

*DTMAX 10.

*DATE 2002 01 01
*DATE 2003 01 01
*DATE 2004 01 01
*WRST *TNEXT
*DATE 2005 01 01

*DATE 2006 01 01
*DATE 2007 01 01
*DATE 2008 01 01
*DATE 2009 01 01
*WRST *TNEXT
*DATE 2010 01 01

*DATE 2015 01 01
*DATE 2020 01 01
*WRST *TNEXT
*DATE 2025 01 01

*STOP

******************************************************************************** TERMINATE SIMULATION ********************************************************************************
RESULTS SECTION WELLDATA
RESULTS SECTION PERFS
GEM INPUT FILE: LEAK

The input file for leak simulation is presented here. The case has an upper aquifer located above a 50 ft thick sealing layer. The initial pressure and initial global mole fraction of gas and water in grid blocks are in separate files included to the input file, namely 'Pressure-25yrs.txt', 'ZGlobal-CO2-25yrs.txt' and 'ZGlobal-H2O-25yrs.txt', respectively. The resulting CO2 saturation profile is given in Figure 5-23.

RESULTS SIMULATOR GEM
RESULTS SECTION INOUT
*******************************************************************
** Leak simulation
** Purpose: Effect of countercurrent flow within the leakage path
** Thick sealing layer (h_shale=50 ft)
*******************************************************************

*INUNIT *FIELD
*INTERRUPT *INTERACTIVE
*RANGECHECK *ON
*XDR *ON
*MAXERROR 20
*DIARY *CHANGES

** Output Print File:
*WPRN *ITER *NONE
*WPRN *GRID *TIME
*OUTPRN *GRID *PRES DROP PCG SATP
*KRG KRO
*DENG DENO RHOG RHOO MWG MWO VISG VISO FRG
*SG SO
*Z 'CO2' Z 'H2O'
*Y 'CO2' Y 'H2O'
*X 'CO2' X 'H2O'
*K 'CO2' K 'H2O'
*SIG
*VELOCRC

** Simulation Results File:
*WSRF *GRID *TIME
*OUTSRF *GRID *PRES DROP
*PCG SATP
*KRG KRO
*DENG DENO RHOG RHOO MWG MWO VISG VISO FRG

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**Restart File (To restart at the last time step in RST file):**
*WRST 100000
*REWIND 1

*********************************************************************
Aquifer details

**GRID *CART 400 1 250
*DI *CON 1
*DJ *CON 1
*DK *CON 1
*DEPT *TOP 200 1 1 5300.
** No Anisotropy:
*PERMI *ALL 40000*1000
**INCLUDE 'Perm-5-5-1.txt'
20000*194
*PERMJ *EQUALSI
*PERMK *EQUALSI
*POR *MATRIX *ALL 40000*0.3
**INCLUDE 'Por-5-5-1.txt'
20000*0.246
*CPOR *MATRIX 3.0E-6
*PRPOR *MATRIX 14.7

*********************************************************************
Component properties for EOS model

**MODEL *PR
**NC 2 2
**COMPNAME 'CO2' 'H2O'
**HCFLAG 0 0
**VISCOR *PEDERSEN
**VISCOEFF 0.291
1.4
0.0005747
4.265
1.0579
*MIXVC  1
*TRES  140.
*PCRIT  72.809000  217.754600
*TCRIT  304.12780  647.09440
*AC  0.223940  0.344000
*VCRIT  0.094000  0.056000
*MW  44.01000  18.01500
*PCHOR  78.00000  52.00000
*SG  0.818000  1.000000
*TB  -109.21000  212.00000
*ZCRIT  0.274139  0.229409
*VISVC  0.094000  0.056000
*VSHIFT  0.024668  0.234867
*OMEGA .457235530 .457235530
*OMEGB .077796074 .077796074
*BIN  -0.0576003
*PHASEID  *DEN

*******************************************************************
** Relative permeability

*ROCKFLUID
*RPT *SCALING-NEW

** Water-Oil relative perm table: NOT USED in simulation
*SWT
0.000000  0.000000  1.000000  0.000000
0.0524375  0.0008203  0.8400835  0.000000
0.104875  0.0032813  0.6973033  0.000000
0.1573125  0.0073828  0.5708514  0.000000
0.209750  0.013125  0.4599021  0.000000
0.2621875  0.0205078  0.3636104  0.000000
0.314625  0.0295313  0.2811098  0.000000
0.3670625  0.0401953  0.211510  0.000000
0.419500  0.052500  0.1538931  0.000000
0.4719375  0.0664453  0.1073101  0.000000
0.524375  0.0820313  0.0707757  0.000000
0.5768125  0.0992578  0.0432609  0.000000
0.629250  0.118125  0.0236831  0.000000
0.6816875  0.1386328  0.0108919  0.000000
0.734125  0.1607813  0.0036447  0.000000
0.7865625  0.1845703  0.0005609  0.000000
0.839000  0.210000  0.000000  0.000000

** Oil-Gas relative perm table: USED in simulation
*SLT
**SL  Krg   Kgq   Pcog
0.15  0.860969388  0  2.291009  ** SLCON: Connate Liq. Sat.
0.2  0.7  0  1.698
0.25  0.560459184  0.005102041  1.556611  ** SLRG: Residual Liq. Sat.
0.3  0.440816327  0.020408163  1.479537
0.35  0.339540816  0.045918367  1.427207
0.4  0.255102041  0.081632653  1.387907
0.45  0.185969388  0.12755102  1.356607
0.5  0.130612245  0.183673469  1.330698
0.55  0.0875  0.25  1.308658
0.6  0.055102041  0.326530612  1.289521
0.65  0.031887755  0.413265306  1.272641
0.7  0.016326531  0.510204082  1.257562
0.75  0.006887755  0.617346939  1.243953
0.8  0.002040816  0.734693878  1.231564  ** 1-SGCRIT: Critical Gas Sat
0.85  0  0.862244898  1.220204
0.9  0  1  1.209723
0.95  0  1  1.205
1  0  1  1.2  ** 1-SGCON: Connate Gas Sat.

** Max residual gas saturation
*HYSKRG  0.286

** End-point value to scale the relative permeability tables of each grid block
*SWCON  *CON  0
*PCGMAX  *ALL  40000*0.44
  *INCLUDE  'PcScale-5-5-1-P.txt'
  20000*1
  *MOD  *  2.291009

******************************************************************************
** Initial condition
*INITIAL
*USER_INPUT
*NREGIONS  1

*SW  *CON  0
*PRES  *ALL  *INCLUDE  'Pressure-25yrs.txt'
*ZGLOBALC  'CO2'  *ALL  40000*0
  *INCLUDE  'ZGlobal-CO2-25yrs.txt'
*ZGLOBALC  'H2O'  *ALL  40000*1
  *INCLUDE  'ZGlobal-H2O-25yrs.txt'

******************************************************************************
** Numerical control
*NUMERICAL
*DTMAX  1.0
*DTMIN  1.0E-05
*NORM  *PRESS  1000.
*MAXCHANGE  *GMOLAR  0.5
*MAXCHANGE  *SATUR  0.5
*CONVERGE  *PRESS  0.514884

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*** Well and run details

*RUN
*DATE 2025 01 01
*DATE 2025 01 10
*DATE 2025 01 20
*DATE 2025 01 30
*DATE 2025 02 30
*DATE 2025 03 30

*DTMAX 2.

*DATE 2025 06 30
*DATE 2025 09 30
*WRST *TNEXT
*DATE 2026 01 01

*DTMAX 10.

*DATE 2027 01 01
*DATE 2028 01 01
*DATE 2029 01 01
*WRST *TNEXT
*DATE 2030 01 01

*DATE 2035 01 01
*DATE 2040 01 01
*DATE 2045 01 01
*WRST *TNEXT
*DATE 2050 01 01

*STOP

**************************************** TERMINATE SIMULATION ****************************************
RESULTS SECTION WELLDATA
RESULTS SECTION PERFS
MATLAB INPUT FILE: CALCULATION OF MASS OF CO₂

The MATLAB m-file for calculation of mass of CO₂ in different parts of aquifer is presented here. The code reads the data from six output files of “CMG Results” in SRF format (section 4.4). The calculations are for the case in Figure 5-23.

%% Read Data and Calculate Mass of CO₂ in Different Parts of Aquifer
% The input files should be in SRF format
% Use "Export Property Values..." in CMG Results

%% Read input files
clear;
delimiter = '';
R1 = 2;
C1 = 0;

fname = 'Leak3-110-Scaled-5-k=Avg-150 Gas Saturation-50yrs.txt';
M  = dlmread(fname, delimiter, R1, C1);
Sg = M(:,1:6);

fname = 'Leak3-110-Scaled-5-k=Avg-150 Net Pore Volume-50yrs.txt';
M  = dlmread(fname, delimiter, R1, C1);
PV = M(:,1:6);

fname = 'Leak3-110-Scaled-5-k=Avg-150 Oil Mole Fraction(CO2)-50yrs.txt';
M = dlmread(fname, delimiter, R1, C1);
Xco2 = M(:,1:6);

fname = 'Leak3-110-Scaled-5-k=Avg-150 Gas Mole Fraction(CO2)-50yrs.txt';
M = dlmread(fname, delimiter, R1, C1);
Yco2 = M(:,1:6);

fname = 'Leak3-110-Scaled-5-k=Avg-150 Oil Phase Mole Den-50yrs.txt';
M = dlmread(fname, delimiter, R1, C1);
RHOoil = M(:,1:6);

fname = 'Leak3-110-Scaled-5-k=Avg-150 Gas Phase Mole Den-50yrs.txt';
M = dlmread(fname, delimiter, R1, C1);
RHOgas = M(:,1:6);
%% Calculate Mass of CO2 - ABOVE THE SEAL

Ni = 400;  % Number of grid blocks in the x-direction
TOP = 1;  % Top layer of the range
BOTTOM = 50;  % Bottom layer of the range

Lim_L = 1;  % If TOP = 1
%Lim_L = floor((TOP-1)*Ni/6);  % Otherwise
Lim_H = ceil( BOTTOM*Ni/6 );

Gdis1 = sum(sum(Xco2(Lim_L:Lim_H,:).*RHOoil(Lim_L:Lim_H,:).*PV(Lim_L:Lim_H,:).*
(1-Sg(Lim_L:Lim_H,:))*44));
Gfree1 = sum(sum(Yco2(Lim_L:Lim_H,:).*RHOgas(Lim_L:Lim_H,:).*PV(Lim_L:Lim_H,:).*
Sg(Lim_L:Lim_H,:)*44));
G1 = Gdis1 + Gfree1;

%% Calculate Mass of CO2 - IN THE GAS CAP

TOP = 101;  % Top layer of the range
BOTTOM = 129;  % Bottom layer of the range

Lim_L = floor((TOP-1)*Ni/6);  % Otherwise
Lim_H = ceil( BOTTOM*Ni/6 );

Gdis2 = sum(sum(Xco2(Lim_L:Lim_H,:).*RHOoil(Lim_L:Lim_H,:).*PV(Lim_L:Lim_H,:).*
(1-Sg(Lim_L:Lim_H,:))*44));
Gres2 = sum(sum(Yco2(Lim_L:Lim_H,:).*RHOgas(Lim_L:Lim_H,:).*PV(Lim_L:Lim_H,:).*
(Sg(Lim_L:Lim_H,:)<=0.286).*Sg(Lim_L:Lim_H,:)*44))...
+ sum(sum(Yco2(Lim_L:Lim_H,:).*RHOgas(Lim_L:Lim_H,:).*PV(Lim_L:Lim_H,:).*
(Sg(Lim_L:Lim_H,:)>0.286)*0.286*44));
Gcap2 = sum(sum(Yco2(Lim_L:Lim_H,:).*RHOgas(Lim_L:Lim_H,:).*PV(Lim_L:Lim_H,:).*
(Sg(Lim_L:Lim_H,:)>0.286).*(Sg(Lim_L:Lim_H,:)-0.286)*44));

%% Calculate Mass of CO2 - BELOW THE GAS CAP

TOP = 130;  % Top layer of the range
BOTTOM = 250;  % Bottom layer of the range

Lim_L = floor((TOP-1)*Ni/6);  % Otherwise
Lim_H = ceil( BOTTOM*Ni/6 );

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\[ G_{\text{dis}}^3 = \sum_{\text{Lim}_L: \text{Lim}_H} \sum_{:} (X_{\text{co}_2} \times \text{RHO}_{\text{oil}} \times \text{PV} \times (1 - S_{\text{g}}) \times 44) \]\[ G_{\text{res}}^3 = \sum_{\text{Lim}_L: \text{Lim}_H} \sum_{:} (Y_{\text{co}_2} \times \text{RHO}_{\text{gas}} \times \text{PV} \times (S_{\text{g}} \leq 0.286) \times S_{\text{g}} \times 44) + \sum_{\text{Lim}_L: \text{Lim}_H} \sum_{:} (Y_{\text{co}_2} \times \text{RHO}_{\text{gas}} \times \text{PV} \times (S_{\text{g}} > 0.286) \times 0.286 \times 44) \]\[ G_{\text{cap}}^3 = \sum_{\text{Lim}_L: \text{Lim}_H} \sum_{:} (Y_{\text{co}_2} \times \text{RHO}_{\text{gas}} \times \text{PV} \times (S_{\text{g}} > 0.286) \times (S_{\text{g}} - 0.286) \times 44) \]

%% Calculate Distribution of Mass of CO2
\[ G_{\text{dis}} = G_{\text{dis}}^2 + G_{\text{dis}}^3 \quad \text{\% Dissolution trapping} \]
\[ G_{\text{res}} = G_{\text{res}}^2 + G_{\text{res}}^3 \quad \text{\% Residual trapping} \]
\[ G_{\text{cap}} = G_{\text{cap}}^3 + G_{\text{cap}}^2 \quad \text{\% Local capillary trapping} \]
\[ G_{\text{free}} = G_1 \quad \text{\% Free gas} \]
Glossary

ROMAN SYMBOLS

\( D \quad \text{Aquifer thickness, m} \)

\( k \quad \text{Absolute permeability, md} \)

\( k_r \quad \text{Relative permeability} \)

\( k_r^0 \quad \text{End point relative permeability} \)

\( MW \quad \text{Molecular weight, lb/lb-mol} \)

\( MW_n \quad \text{Mole fraction averaged molecular weight, lb/lb-mol} \)

\( MW_w \quad \text{Weight fraction averaged molecular weight, lb/lb-mol} \)

\( N_g \quad \text{Gas relative permeability exponent} \)

\( N_w \quad \text{Water relative permeability exponent} \)

\( p_a \quad \text{Aquifer pressure, psi} \)

\( p_c \quad \text{Capillary pressure, psi} \)

\( P_c \quad \text{Critical pressure, psi} \)

\( p_e \quad \text{Capillary pressure at } S_w = 1, \text{ psi} \)

\( p_i \quad \text{Injection pressure, psi} \)

\( PV \quad \text{Pore volume, ft}^3 \)

\( Q \quad \text{Mass injection rate, ton/day} \)

\( r_e \quad \text{Radius of injection influence, ft} \)

\( r_w \quad \text{Radius of the injection well, ft} \)

\( S \quad \text{Salinity, ppm} \)

\( S_g \quad \text{Gas saturation} \)

\( S_{gcon} \quad \text{Connate gas saturation} \)
$S_{g_{cr}}$ Critical gas saturation

$S_{gr}$ Residual gas saturation

$S_{w}$ Water saturation

$S_{w_{ir}}$ Irreducible water saturation

$S_{wr}$ Residual water saturation

$T$ Temperature, °F

$T_c$ Critical temperature, °R

$X_{CO_2}$ Liquid mole fraction of CO$_2$

$Y_{CO_2}$ Gas mole fraction of CO$_2$

**GREEK SYMBOLS**

$\alpha$ Rotational coupling coefficient

$\phi$ Porosity

$\lambda$ Pore size distribution index

$\mu$ Dynamic viscosity, mPa.s

$\theta$ Contact angle, rad

$\rho$ Density, kg/m$^3$

$\rho_{molar}$ Mole density, mole/ft$^3$

$\rho_r$ Reduced density

$\sigma$ Surface tension, dyne/cm

**SUBSCRIPTS**

0 Reference substance

g Gas

l Liquid

mix Mixture
$w$  Water

**ACRONYMS**

- **BIC**  Binary Interaction Coefficient
- **VSP**  Volume Shift Parameter
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