Uncertainty Analysis of Capacity Estimates and Leakage Potential for Geologic Storage of Carbon Dioxide in Saline Aquifers

by

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**S.B., Engineering Science,
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Submitted to the Engineering Systems Division
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Abstract

The need to address climate change has gained political momentum, and Carbon Capture and Storage (CCS) is a technology that is seen as being feasible for the mitigation of carbon dioxide emissions. However, there is considerable uncertainty that is present in our understanding of the behavior of CO_2 that is injected into the sub-surface.

In this work, uncertainty analysis is performed using Monte Carlo simulations for capacity estimates and leakage potential for a saline aquifer. Six geologic parameters are treated as uncertain: porosity, irreducible water saturation, the endpoint relative permeability of CO_2, residual gas saturation, viscosity of water, and viscosity of the brine.

The results of the simulations for capacity indicate that there is a large uncertainty in capacity estimates, and that evaluating the model at using the mean values of the individual parameters does not give the same result as the mean of the distribution of capacity estimates. Sensitivity analysis shows that the two parameters that contribute the most to the uncertainty in estimates are the residual gas saturation and the endpoint relative permeability of CO_2.

The results for the leakage simulation suggest that while there is a non-zero probability of leakage, the cumulative amount of CO_2 that leaks is on the order of fractions of a percent of the total injected volume, suggesting that essentially all the CO_2 is trapped. Additionally, the time when leakage begins is on the order of magnitude of thousands of years, indicating that CCS has the potential to be a safe carbon mitigation option.

Any development of regulation of geologic storage and relevant policies should take uncertainty into consideration. Better understanding of the uncertainty in the science of geologic storage can influence the areas of further research, and improve the accuracy of models that are being used. Incorporating uncertainty analysis into regulatory requirements for site characterization will provide better oversight and management of injection activities. With the proper management and monitoring of sites, the establishment of proper liability regimes, accounting rules and compensation mechanisms for leakage, geologic storage can be a safe and effective carbon mitigation tool to combat climate change.

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List of Acronyms and Symbols

AOR	Area of Review
CCS	Carbon Capture and Storage
CO_2	Carbon Dioxide
DOE	Department of Energy
EPA	Environmental Protection Agency
GHG	Greenhouse Gas
Gt CO_2	Gigatonnes of CO_2
IPCC	Intergovernmental Panel on Climate Change
K^*_{rg}	Endpoint relative permeability of CO_2
MMV	Monitoring, Measurement and Verification
PDF	Probability Density Function
S_{gr}	residual gas saturation
S_{wc}	connate water saturation
SDWA	Safe Drinking Water Act
UIC	Underground Injection Control

Chapter 1: Introduction and Background

1.1 The Climate Crisis and the need for quick action

In the last decade, there has been a large effort from the scientific community to stress the importance of reducing carbon dioxide emissions to counter climate change. In its most recent report, the Intergovernmental Panel on Climate Change (IPCC) provided extensive scientific research and results from models indicating that that there has been a rise in global mean temperatures and 'that the warming of the climate system is unequivocal'. Additionally, it asserts that much of the temperature rise since "the mid-20th Century is very likely due to the observed increase in anthropogenic GHG concentrations.' (Alley *et al*., 2007)

The recognition of climate change as an imminent global crisis that needs to be addressed quickly has, in recent years, moved away from discussions in the academic and scientific arena to the public sphere. Policy makers, businesses and industries have acknowledged that carbon mitigation technology is a necessity to prevent further damage caused by anthropogenic greenhouse gas emissions, and there has been significantly increased reporting in the news media about climate change.

The direct linkage of carbon dioxide emissions with energy use and economic activity has turned the debate into one where global economic development is directly in competition with efforts to curb emissions through policy. However, with the recent change in administration in the United States, the commitment to finding solutions to climate change have been placed high on the agenda, and it remains to be seen how seemingly competing objectives of reducing emissions and increasing economic activity will be resolved.

In the Fourth Assessment report of the IPCC, Carbon Capture and Storage (CCS) technologies are referred to as the only way the continued use of fossil fuels can be 'environmentally sustainable' (Alley *et al.*, 2007). While renewable energy sources are touted as being the long-term solution to the emissions problem, issues such as cost, intermittency and energy storage provide challenges for wide scale deployment. CCS is often thought of as a transitional technology, which allows for the continued use of fossil fuels, but without the increase in GHG emissions. However, CCS technology itself has its own issues of scale and deployment that are yet to be addressed. While there are a number of CCS projects that are operational worldwide, no CCS projects have been completed in the United States that demonstrate the technology in a power plant setting.

Additionally, apart from the technological needs to make CCS viable, clear regulations are required particularly for the underground storage of carbon dioxide, the component of the process with which there is the least experience. Storage raises the most concern amongst critics of CCS because of the potential impacts to health and environment that could arise. The lack of experience, as well as the characteristics of geologic storage raises multiple issues where there is considerable uncertainty, which is the focus of this work.

The uncertainties related to geologic storage have many different dimensions, most importantly not knowing how a large quantity of CO_2 injected underground will travel and behave over time. The actual amount of CO_2 that can be stored underground is also uncertain, because of how little is known about the subsurface and the properties of the rocks into which the CO_2 may be injected.

The implications of these uncertainties are important from both a technical and a policy perspective. From a technical point of view, it is important to understand how much a certain reservoir can safely contain before the additional injection of material may damage the storage site. It is also important to characterize how far underground the CO_2 may travel so that it can be monitored and verified accurately. This is important from a regulatory standpoint, where requirements for siting a geologic storage site would require such analysis.

From a policy point of view, the uncertainties around both capacity and leakage are important to consider. Having a realistic estimate of capacity would allow for setting an attainable target for the level of carbon mitigation to be achieved through CCS. Additionally, with storage, the issues of permanence and leakage rates are also important, as they are indicators of the efficacy of CCS as a long-term solution to the climate problem. By being able to quantify leakage rates and the time frame of any leakage that may occur, the relevant policy can be designed, since a possibility of leakage within 50 years would require a much different set of regulations than leakage in 1000 years after injection.

1.2 Geologic Storage of Carbon Dioxide

Geologic storage of carbon dioxide refers to the injection of carbon dioxide into selected storage sites either in the subsurface or in the ocean. In the subsurface, the CO_2 can be stored in different underground formations that have porous rock. These include saline aquifers, depleted oil and gas reservoirs and unmineable coal seams. Of the three, saline aquifers are regarded as having the largest capacity for storage. The U.S. Department of Energy's Carbon Sequestration Atlas for the United States and Canada estimates that between 3,297 and 12,618 billion metric tons of CO_2 can be stored in saline aquifers on the continent alone (DOE, 2008). A study by the EPA on the Cost Analysis of Geologic Storage indicates that up to '88.6 percent of the capacity for CO_2 injection for geologic storage is in deep saline formations' (EPA, 2008). This thesis therefore restricts its analysis and discussion to storage in saline aquifers, and the model, described in section 2.1, is only applicable to saline aquifers.

When CO_2 is injected into the porous rock of a formation, there are multiple physical phenomena that allow it to remain trapped in the rock. Suitable formations are regarded as those 800m below the surface, so that the increased pressure due to the depth means that the CO_2 is in a supercritical phase. Apart from the rock that it is injected into being porous and able to store the CO_2, there must also be a layer of impermeable rock, the cap rock, on top of the formation to ensure that the CO_2 does not rise through the rock layers and leak through to the surface.

There are four trapping mechanisms that contribute to the storage of CO_2 in a site (fig 1):

1. Physical: structural and stratigraphic trapping
2. Physical: residual CO_2 trapping
3. Geochemical: solubility trapping
4. Geochemical: mineral trapping

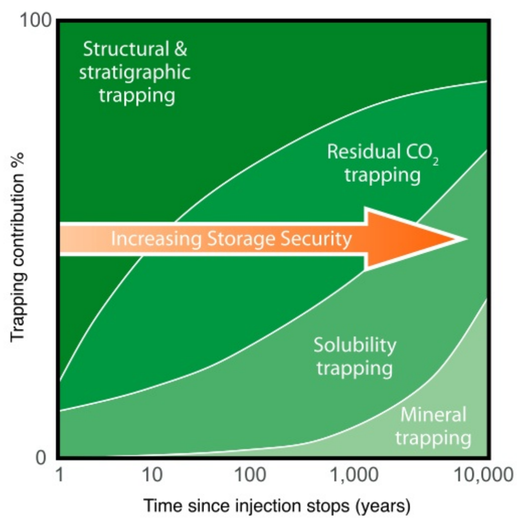

Figure 1.1 The timeframes for the different trapping mechanisms for geologic storage vary considerably. From (Metz *et al.*, 2005)

The time scales associated with geochemical trapping mechanisms is much larger than those of physical trapping mechanisms, and while they become important when talking about very long term (>1000 years) storage security, they are not as relevant as the physical trapping mechanism in the near to medium term, and therefore will not be discussed in this thesis.

Structural and stratigraphic trapping is the mechanism that relies on the geometry of the formation to store the CO_2. These are under a low permeability seal or caprock, or in areas where there are structural traps created by folds in the rock of the formation, or impermeable fractures that do not allow the flow of fluid out of the site once it has been injected there. These are the initial primary mechanisms through which CO_2 is stored underground.

Hydrodynamic, or residual gas trapping occurs in saline formations, where there is a fluid, usually brine, flowing through the formation, that causes the injected CO_2 to migrate slowly in the direction of the flow. The injected fluid displaces the brine, and because of differences in buoyancy, the CO_2 migrates upwards. During this movement of the plume, CO_2 becomes trapped in the pore spaces of the rocks of which it pushes the brine out of. The trapping is on the pore scale, but can trap significant amounts of CO_2, depending on the properties of the rock (IPCC, 2005). The model used for the analysis in this thesis is a residual trapping model that is used on the basin scale to estimate capacity and model leakage.

1.3 Capacity Estimation methods for Saline Aquifers

Attempts at quantifying the storage capacity for saline aquifers have lead to a large variation in the estimates of how much CO_2 can be stored. The Department of Energy's Carbon Atlas has recently attempted to quantify the storage capacity of various formations in the US (DOE, 2008). The large variation in the estimates comes from a number of sources, but is mainly from different approaches for how one can measure the capacity of the subsurface. Almost all the methods are based on approaches that are from reservoir modeling and estimation techniques from the oil and gas industry. However, even with sophisticated modeling, there are large uncertainties associated with those techniques. Additionally, saline aquifers are relatively unexplored in comparison to oil and gas fields, and so whether these techniques are directly applicable is not clear.

Almost all attempts at quantifying storage capacity in saline aquifers look at the structural and stratigraphic trapping mechanisms, as these are considered the most relevant and most likely to be used to determine potential injection sites. The most commonly used method is to use a volumetric estimate of the formation, and to then multiply it with an ‘efficiency’ factor that is site specific, determined using a combination of geologic and physical parameters, and use parameters representing high and low probabilities to determine the best and worse case estimates for capacity. This efficiency factor scales the total pore volume of the reservoir to volume of CO_2 that can be trapped (Frailey, 2008).

Additionally, a classification scheme for CO_2 storage space, based on the probability of its use, is proposed in the Carbon Atlas. In this scheme, a distinction is made between CO_2 storage ‘resource’ and ‘capacity’. Resource is used to describe the technical and scientifically useable pore space in which CO_2 can be stored, with the constraints applied being technical and scientific in nature. Capacity, on the other hand, refers to the pore space that is accessible and useable after economic and regulatory constraints have been applied. This classification scheme is similar to that used in the oil and gas industry, where a distinction is made between proved and probable reserves, based on the economic factors that affect extraction. For the purposes of this study, we will be referring to the scientific measurement of pore space as capacity, which parallels the terminology used in the models which will be used for uncertainty analysis.

To date, there have been no analyses that model carbon dioxide leakage on a basin scale. The work done on leakage focuses mainly on leakage mechanisms through abandoned wells or on the integrity of the cap rock, but no study has been conducted which estimates leakage rates and the time frame of leakage with models that include the migration of the CO_2 plume.

1.4 Regulation of Geologic Storage in the United States

In July 2008, the Environmental Protection Agency, (EPA) released a proposed rule for Geologic Storage under the Underground Injection Control (UIC) program of the Safe Drinking Water Act (SDWA). This rule regulates the injection of any 'fluid' into the subsurface, where a fluid is defined as 'any material which flows or moves whether in a semisolid, liquid, sludge, gas or other form or state'. The regulation covers CO_2 that is injected for enhanced oil and gas recovery. Additionally, UIC regulates the injection of both pollutants and commodities, and so the debate of whether CO_2 is a pollutant is not an issue in determining the Authority of the EPA to regulate geologic storage.

The existing UIC rule regulates injections for the protection of underground sources of drinking water (USDW) through five different classes of wells, for specific classes of materials that are injected. The injection of CO_2 for enhanced oil recovery is regulated under the class II wells, which are for hydrocarbon production. For the sole purpose of geologic storage, a sixth class of well is proposed, for which the regulations will take into account the specific nature of long-term storage of CO_2.

The UIC program is designed to prevent the flow of fluids into USDW, and in its components, it addresses pathways through which the injected fluids could potentially migrate into to USDWs. These components are:

1. Siting
2. Area of Review
3. Well construction
4. Operation
5. Mechanical Integrity Testing
6. Monitoring
7. Well Plugging and Post-injection site care

This thesis focuses on the first two components of the program- siting and area of review. Both of these come under site characterization, which needs to be conducted to ensure the safety and the efficacy of storage in a particular site, and to ensure that any effected regions do not have faults or fractures that may endanger USDWs. (EPA, 2008)

From the perspective of climate policy, the issue of storage permanence and the likelihood of leakage creates a challenge on many levels. Firstly, since the purpose of geologic storage is to prevent the addition of CO_2 into the atmosphere, any leakage compromises this objective. Secondly, in a foreseeable future where there is a monetary value attached to carbon dioxide or carbon credits allotted per unit of CO_2 stored, the presence of leakage can compromise the accounting in the system. The EPA regulations do not cover these aspects; the SDWA is designed to prevent contamination of ground water supply, not to prevent CO_2 being emitted into the atmosphere.

To issue a permit for a potential sequestration site, EPA would, according to the proposed rule, require the following information:

1. A geologic assessment that demonstrates the presence of geologic features that are suitable for CO_2 storage which will not endanger USDWs. Operators would have to submit maps of USDWs in the area near the injection site.
2. Geologic data about the rocks in the formation, including data about 'the lateral extent and thickness, strength, capacity, porosity and permeability' of the formation.
3. Results of seismic and geomechanical studies of the cap rock regarding its strength, rock stress, stability and ductility.
4. Geochemical data regarding the fluids in the aquifers and their mineral content.

Of these, the second requirement of geologic data is relevant to this thesis, as it requires not only estimates of the capacity of the formation, but also data about parameters that we are assuming to be uncertain in a given formation, such as porosity.

The regulation also requires a determination of the Area of Review (AOR), which the EPA defines as 'The region surrounding the geologic sequestration project that may be impacted by the injection activity'. Determining the AOR is important in site characterization and its suitability for GS because it requires any faults or penetrations that could endanger USDWs to be identified and evaluated.

Current UIC regulation for well classes I-III require that the AOR is either a fixed radius away from the injection site, or greater than the area above the pressure front of the injected fluid that has been determined through computational modeling. However, it is recognized that the CO_2 plume would cover a much larger range than those of other fluids that have been injected under the UIC program, and that neither the fixed radius nor computational methods are adequate to predict the movement of the plume. Therefore, the proposed rule suggests that 'computational multiphase fluid flow models' are used in determining the AOR. It specifies that the model should use site characterization data specific to a particular injection site, and takes 'into account any geologic heterogeneities, and potential migration through faults, fractures and artificial penetrations'.

In its discussions of models, the proposed rules suggest allowing the use of proprietary models that cannot be easily evaluated, as long as they are adequately documented. No one particular modeling approach is given preference, and uncertainty analysis is not mentioned.

The use of one particular model in this thesis that makes use of multi phase flow dynamics and its performance under uncertainty can provide insight onto how models and uncertainty analysis should be used as a part of site characterization.

In addition to the proposed rule, the EPA has also published a Vulnerability Evaluation Framework (VEF) in order to assist operators in determining the risks of geologic storage in a particular site (EPA, 2008). However, uncertainty regarding the behavior of the CO_2 plume is not discussed in the document, and there is a reliance on observed data from monitoring after injection to evaluate how the plume migrates.

1.5 Objective of this work

In this thesis, the research question I will address is, "How does variability in geologic parameters affect the storage capacity and the leakage potential for CO_2 injected into saline aquifers?". In order to answer this question, I will perform uncertainty analysis applied to a residual trapping model in a saline aquifer to evaluate:

1. The uncertainty in capacity estimates
2. The probability of leakage, and the uncertainty in both in quantity and in time to the start of leakage

The uncertainty analysis will look at the sensitivity of the estimates to individual parameters and variation of correlations between parameters and produce probability density functions (PDFs) to represent these. For the leakage, we will also look at the effects of uncertainty related to the spatial distribution of the leakage faults.

The characterization of these uncertainties is important, particularly because of the lack of data that is available about the properties of saline aquifers. The overall research goal of this work is to identify how the variability in certain geologic parameters can affect the performance of this particular model. By using this approach, we can also represent heterogeneity in the rock properties on a large basin better than by using a value from a small number of sites, which is a better representation of the physical characteristics of the subsurface.

The presence of uncertainty in geologic storage has implications for the further development of the science behind geologic storage, as well as policy implications. The proposed rules for the regulation of geologic storage as discussed in the previous section raise issues about how uncertainty is handled in the permitting process. Finally, by looking at uncertainty in potential leakage sites and how that affects the rate of leakage into the atmosphere, we can address the issues raised about permanence and storage efficacy. These issues are discussed in detail in chapter 4.

Chapter 2: Models and Methods

In order to perform uncertainty analysis, the following steps were performed:

1) Selecting the relevant models

2) Selecting the uncertainty analysis methods

3) Determining the input parameters

4) Characterizing the distributions of the input parameters

5) Performing the uncertainty analysis

Each of these steps is discussed in detail in the sections below.

2.1 Models used

The model that is used in this analysis is a dynamic, multiphase flow model for the trapping of CO_2 that can be used for capacity estimates on a basin scale (Szulczewski and Juanes, 2008). In comparison to the methods used by the Department of Energy, this is also a volumetric model adjusted using an efficiency factor to determine the storage volume. However, the underlying physical process that is modeled is different, and therefore, a straightforward comparison of results of the methods is difficult.

The model allows for capacity estimation for a simplified representation of a basin, as shown in fig 2.1 below. The basin is modeled as a rectangular volume of constant thickness at a constant depth below ground level, with the direction of natural groundwater flow taken as uniform. A maximum plume length is determined by demarking boundaries beyond which the geologic conditions such as the presence of faults or non-uniform groundwater flow make the model unsuitable for use.

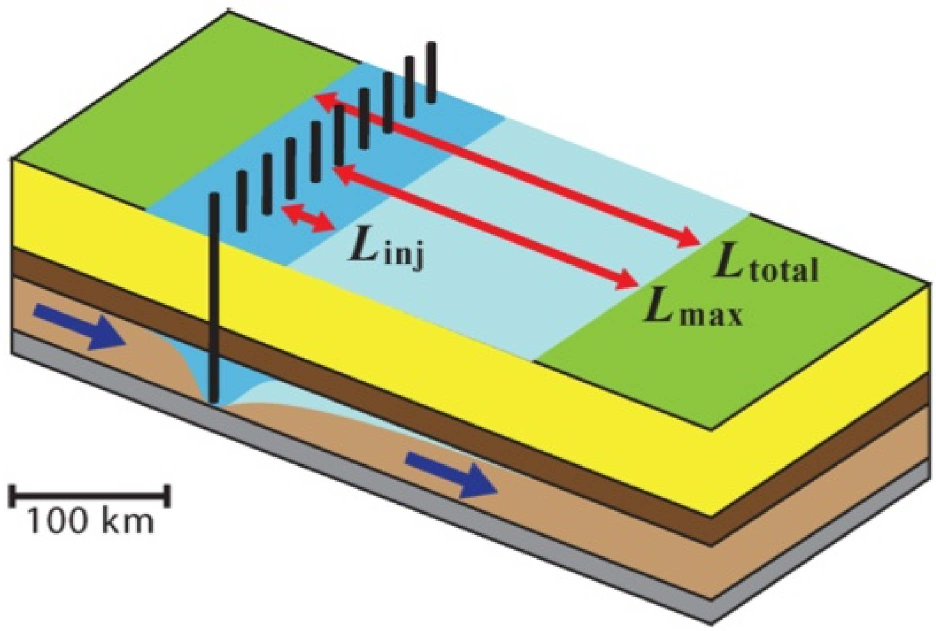

Figure 2.1: Schematic of basin, showing positioning of well array, and footprint of plume in the direction of the groundwater flow. From Szulczewski and Juanes (2008).

Using this information, the optimal positioning of the well array, perpendicular to the groundwater flow, can be determined. With the known location of the well array and a theoretical maximum boundary for the plume, we can calculate the capacity of the basin. This closed form solution for capacity as described by the multiphase flow model is shown below in equation 1:

$$C = \left[\frac{2M\Gamma^2(1-S_{wc})}{\Gamma^2 + (2-\Gamma)(1-M+M\Gamma)} \right] \rho_{co_2} \phi H W L_{total} \qquad (1)$$

Where C is the mass of the trapped CO_2, M is the mobility ratio, Γ is the trapping coefficient, S_{wc} is the connate water saturation, ρ_{CO2} is the density of the CO_2, ϕ is the porosity of the rock, H is the net sandstone thickness of the reservoir, W is the width of the well array, and L_{total} is the total extent of the plume.

In the above equation, M and Γ are defined as:

$$M = \frac{1/\mu_w}{k*_{rg}/\mu_g} \tag{2}$$

$$\Gamma = \frac{S_{rg}}{1 - S_{wc}} \tag{3}$$

Where μ_w is the viscosity of the brine,

μ_g is the viscosity of the CO_2,

$K^*_{rg.}$ is the endpoint relative permeability to CO_2,

S_{gr} is the residual saturation of CO_2

The same physical phenomenon is described separately in a complementary model that uses the same parameters to evaluate the footprint of the plume and its migration as a function of time (Juanes, MacMinn, and Szulczewski, 2009). The variation of the model characterizes the behavior of the plume in the subsurface as it interacts with the groundwater flow in the aquifer. Over time, the model shows the migration of the plume, breaking it down into two stages; during injection and post-injection. These are shown in the figure 2.2 below.

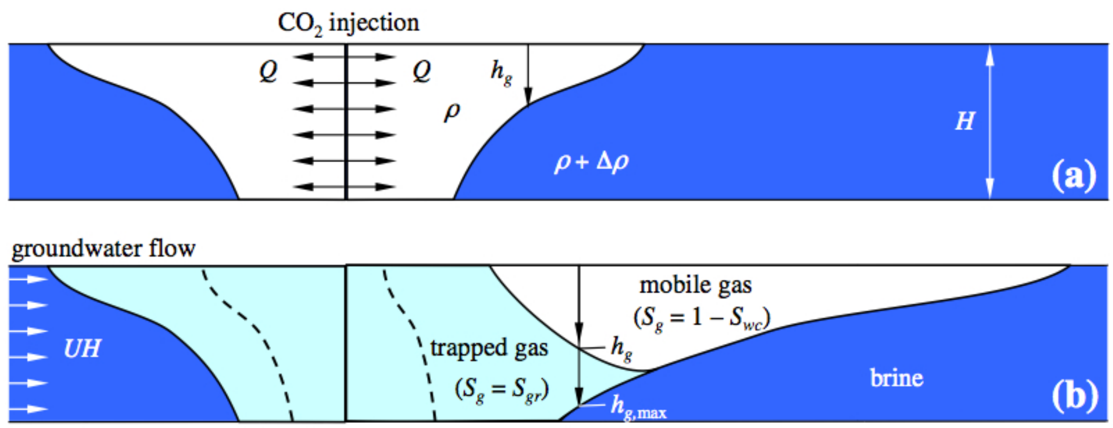

Fig 2.2 The two stages in the migration of the plume. White represents the mobile CO_2, light blue represents the trapped CO_2 and the dark blue is the brine into which the CO_2 is injected. From Juanes (2008).

During the injection stage, CO_2 is injected at a high flow rate, which displaces the water in the aquifer to its irreducible saturation. In the post injection stage, the groundwater flow and the buoyancy of the CO_2 allow it to migrate, with CO_2 being trapped in residual form at the trailing edge. The thickness of the mobile plume, h_g, decreases as the plume travels laterally.

The process can be broken down further into 3 phases in the post injection stage- the retreat, the chase and the sweep phases. The retreat and chase phases describe the behavior of the CO_2 that migrates in the opposite direction to the groundwater flow during injection, and for simplification of the model, we assume that these phases are of relatively short time periods and that there is no leakage, since we will model our faults to be a certain distance away from the injection wells in the direction of the water flow and plume migration. The sweep stage occurs when the mobile plume detaches from the bottom of the aquifer, below the injection well, and the entire mobile gas plume is moving away from the injection well in the direction of the groundwater flow. The leakage is therefore modeled during all stages of the plume migration.

This model incorporates the movement of the CO_2 plume in the reservoir because of initial excessive gravity override during injection, and the regional groundwater flow in the reservoir after the completion of the injection phase. The evolution of the plume, and the mass of CO_2 trapped in the pore spaces it travels along the reservoir can be modeled analytically in one dimension. By being able to evaluate the movement of the plume over time, we can then introduce a simple case of a fault in the migration path and develop a simplified scenario for leakage through this fault. By specifying a leakage length $L_{l,}$ we can calulate the time it takes for the mobile CO_2 to reach the location of the fault using the following equation:

$$\mathrm{T}_l^{begin} = \frac{L_l}{\mathrm{M}}\left(\frac{H\phi(1-S_{wc})}{Q_i T}\right) \tag{4}$$

Where Q_i is the injection rate, and T is the injection period. The time at which leakage ends is calculated using:

$$\mathrm{T}_l^{end} = \frac{1}{\mathrm{M}^2}\left\{\left[M(2-\Gamma)(M-(1-\Gamma))\right]^{1/2} + \left[L_l\left(\frac{H\phi(1-S_{wc})}{Q_i T}\right)M(1-\Gamma)^2\right]^{1/2}\right\}^2 \tag{5}$$

The set of equations used to evaluate leakage during injection and during the post injection period differ slightly because of the different conditions, but follow the same steps.

Once the times during which there is leakage are known, we can then evaluate the height, h_g of the plume at that location at a given time, using the following equations:

$$h_{l_{injection}} = \frac{H}{M-1}\left[\left(M\frac{Q_i T}{L_l H\phi(1-S_{wc})}\left[\left(\frac{t}{T}\right)\right]\right)^{1/2} - 1\right] \tag{6}$$

$$h_{l_{post-injection}} = \frac{H}{M-1}\left[\left(M\frac{Q_i T}{L_l H\phi(1-S_{wc})}\left[1+\frac{Q_n}{Q_i}\left(\frac{t-T}{T}\right)\right]\right)^{1/2} - 1\right] \tag{7}$$

where t is the time at which the expression is evaluated, and Q_n is the groundwater flow rate

The leakage flux can then be evaluated from h_g at each time period, using the following equations:

$$Q_{injection}(t) = Q_i\left(\frac{Mh_l}{(M-1)h_l + H}\right) \quad (8)$$

$$Q_{l,post-injection}(t) = Q_n\left(\frac{h_l}{h_l + \frac{1}{M}(H-h_l)}\right) \quad (9)$$

These set of equations describe the flux in a one-dimensional space. The total amount of CO_2 that leaks through a fault of a given width W_{leak} can be determined by multiplying the results of the leakage flux Q_l with the width. In order to evaluate the total injected CO_2 that leaks, a numerical integration between the time periods is performed.

2.2 Uncertainty Analysis

One of the most conceptually simple and widely used methods to perform uncertainty analysis is Monte Carlo Simulation. In its simplest form, the Monte Carlo simulation evaluates a given model using input values that are randomly selected from a defined probability distribution for each uncertain parameter, which gives a single estimate for the output of the model. This process is repeated a number of times where each set of input values are randomly drawn. The output of each set of input values is then a sample from the probability distribution of the output of the given model. With a large enough number of samples for a given distribution of inputs for a particular model, the frequency distribution of the output asymptotically approached the conditional PDF of the model.

As indicated above, the performance of the Monte Carlo simulation is only as effective as the selection of the input distribution functions for the model being evaluated. It is also important to understand the underlying model sufficiently to ensure that output values are realistic, and in this case where we are modeling a physical process, do not generate results that are impossible.

2.3 Parameters for uncertainty analysis

We can separate the parameters that are the inputs to this model into two groups; one group which describes the geometry of the basin: H, W, L_{total}, and a second group that characterizes the fluid flow properties of the rock and the injected fluids: ϕ, S_{wc}, S_{gr},, K^*_{rg}, μ_w, and μ_g. For the purposes of this analysis, the parameters in the second group will be treated as uncertain, with appropriate probability density functions determined from data that is available.

When performing uncertainty analysis, it is extremely important to ensure that any relationships between the parameters that are being varied are taken into consideration when sampling from the individual distributions. In order to do this, an understanding of the basic science between the parameters allows us to characterize these relationships better, and run simulations that are consistent with the physical processes. In the six parameters that we are treating as uncertain in this work, three of them- S_{wc} , the connate water saturation, S_{gr}, the residual gas saturation and K^*_{rg}, the endpoint relative permeability of CO_2, are related. Figure 2.3 shows a schematic of a relative permeability curve for CO_2, and these three values can be obtained from this graph.

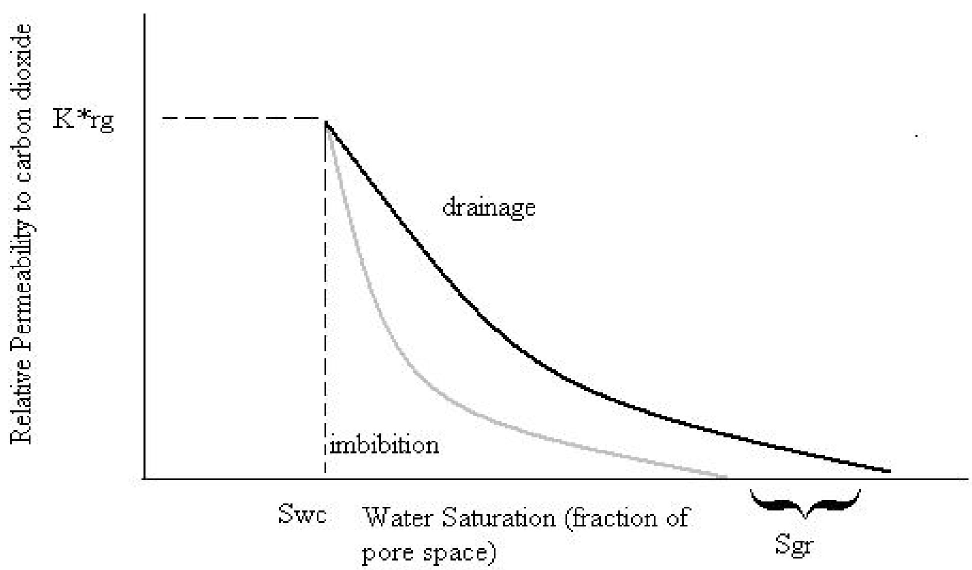

Fig 2.3 Schematic of relative permeability curves for water and CO_2 for drainage and imbibition cycles

This graph describes the relationship of the amount of CO_2 that a given rock sample is permeable to, given a certain saturation of water that is already present in the sample. This is the same scenario as injecting CO_2 into an aquifer that already has brine in it. S_{wc} and K^*_{rg} are the X and Y coordinates, respectively, of the same point on the line, which is the maximum point of the relative permeability curve in the drainage stage- where the CO_2 is passed through the wet rock and occupies the pore space that was previously occupied by the water, up to the point where it is no longer possible to reduce the saturation of water in the rock. This makes the relationship between S_{wc} and K^*_{rg} obvious- a lower S_{wc} leads to a higher K^*_{rg}, and vice versa.

S_{gr} measures the amount of CO_2 trapped in the pore spaces once the rock is flooded with water again- the imbibition stage, shown by the dotted line in the graph above. The two stages combine to form a hysteresis curve, with the difference on the water saturation of the sample once it is no longer permeable to CO_2 indicating the amount of CO_2 that is trapped. (Dullien, 1992)

The relationship between S_{gr} and S_{wc} is not as obvious. Both cases, a negative and a positive correlation between S_{gr} and S_{wc}, can be possible from a physical level. A lower S_{wc} would mean that a higher amount of CO_2 can pass through the rock, and that this higher quantity would lead to more trapping of CO_2, indicating a negative correlation between S_{gr} and S_{wc} . However, this does not completely eliminate the possibility of a positive correlation between the two parameters, as the amount trapped may not necessarily only depend on the amount that can pass through it, but can be a function of other properties, such as quality of rock. These relationships must be taken into consideration when simulating the model. Because the relationship between S_{wc} and K^*_{rg} is known, the relationship between S_{wc} and S_{gr} will then directly influence the relationship between K^*_{rg} and S_{gr}. (Juanes, personal communication).

2.4 Methods: Determining the Distributions of Uncertain Parameters

In order for the Monte Carlo simulation to effectively represent the uncertainties in a model that are a result of the variability in the input parameters, it is essential that the

PDFs that are selected for the input parameters characterize the likely values in a realistic manner.

For the parameters we have described above, there is very little data in the literature, particularly about the relative permeability characteristics of the sandstone/carbonate rock that is found in the saline aquifers with brine/CO_2 flowing through. This is because much of the previous literature has focused on the oil and gas industry, and geologic sequestration is a fairly new field. To determine the appropriate PDFs for ϕ, S_{wc} , S_{gr} and K^*_{rg}, we used data from Bennion and Bachu (2006), which were obtained from core samples for carbonate and Sandstone rock, taken from two regions in Alberta, Canada. We use this data as being a realistic scenario of the data that may be available about a particular sequestration site, with the heterogeneity that is present in the samples being representative of the fact that there can be differences within regions that are nearby. The data that is used is indicated in table 2.1 below.

Table 2.1: Data used to fit probability distribution functions for porosity, S_{wc} , K^*_{rg} and S_{gr}.

Sample	Rock Type	Porosity	S_{wc}	K^*_{rg}	S_{gr}
Cardium 1	Sandstone	0.1530	0.1970	0.5260	0.1020
Cardium 2	Sandstone	0.1610	0.4250	0.1290	0.2530
Viking 1	Sandstone	0.1250	0.5580	0.3319	
Viking 2	Sandstone	0.1950	0.4230	0.2638	0.2970
Ellerslie	Sandstone	0.1260	0.6590	0.1156	
Basal Cambrian	Sandstone	0.1170	0.2940	0.5446	
Wabamun 1	Carbonate	0.0790	0.5950	0.5289	
Wabamun 2	Carbonate	0.1480	0.5690	0.1883	
Nisku 1	Carbonate	0.0970	0.3300	0.1768	
Nisku 2	Carbonate	0.1140	0.4920	0.0999	0.2180
Cooking Lake	Carbonate	0.0990	0.4760	0.0685	

The values of S_{gr} are provided only for samples for which the imbibition cycle was part of the experimental process. The PDFs generated from the data in the table above for each of the parameters is shown in Figures 2.4 – 2.7.

As discussed in section 2.3, the correlations between S_{wc} , S_{gr} and K^*_{rg} must be defined in order to generate samples which are representative of the physical process. The negative correlation between K^*_{rg} and S_{wc} was fixed, with a correlation coefficient of -0.5. As part of the analysis, three cases for which the correlation coefficients between S_{gr} and S_{wc} were simulated: a base case, for which this correlation was set at 0, a positive correlation case, where the coefficient was set at 0.5, and a negative correlation case, where the coefficient was set at -0.5. These correlations do not effect the marginal distributions of the parameters, but are taken into consideration for each individual simulation performed during the Monte Carlo simulation.

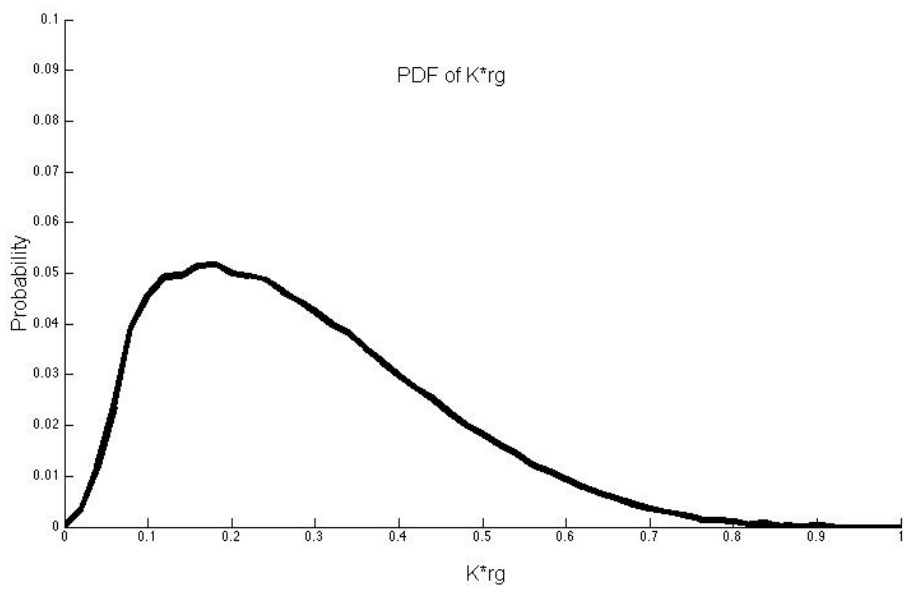

Fig 2.4 PDF of K^*_{rg}, samples from distribution fit to data from Bennion and Bachu (2006).

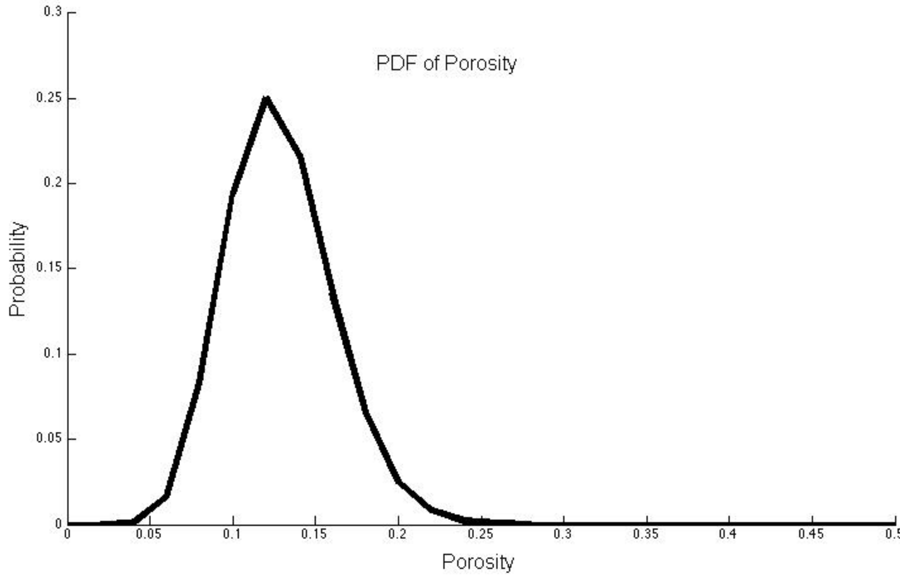

Fig 2.5 PDF of porosity, samples from distribution fit to data from Bennion and Bachu (2006).

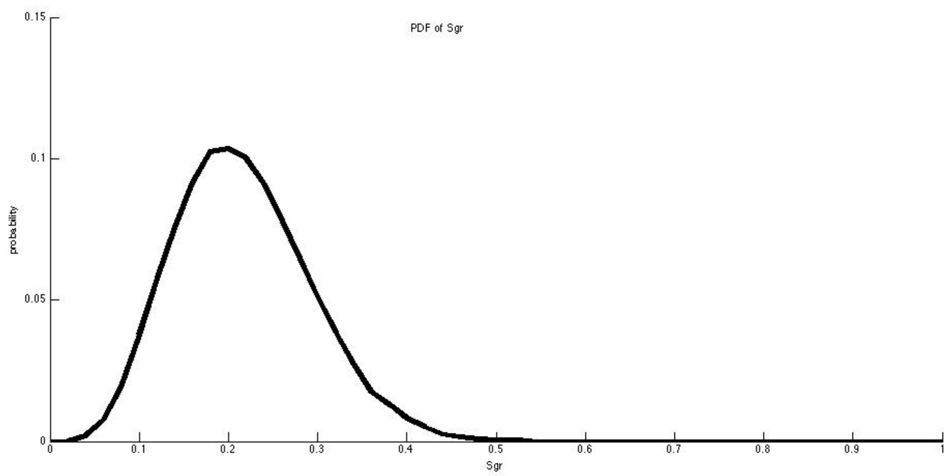

Fig 2.6 PDF of S_{gr}, samples from distribution fit to data from Bennion and Bachu (2006)

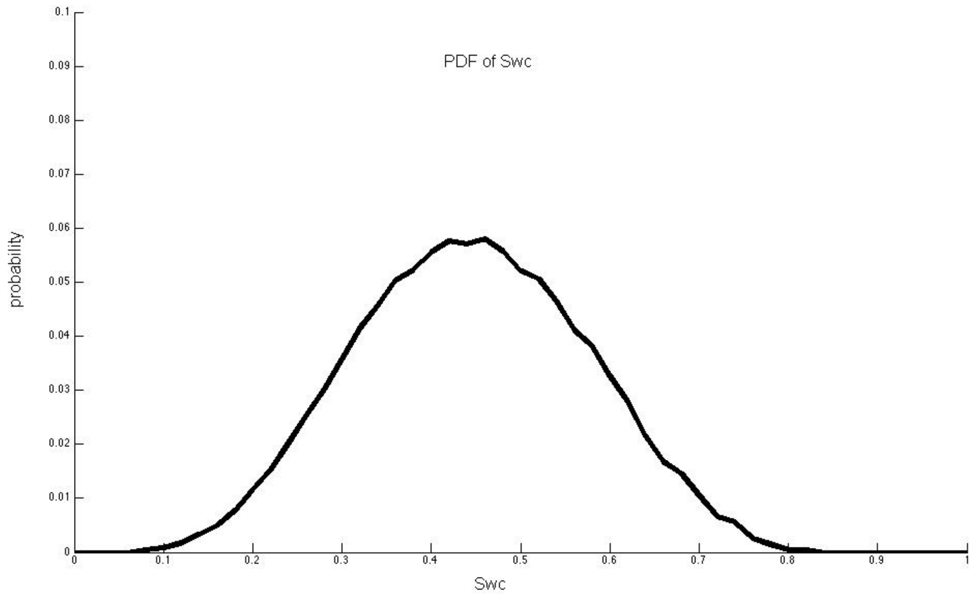

Fig 2.7 PDF of S_{wc} , samples from distribution fit to data from Bennion and Bachu (2006).

The descriptive statistics for the 5000 samples generated from these distributions during the simulation are shown in table 2.2. All the distributions are beta general distributions, which are continuous distributions defined on the interval [0,1].

Table 2.2: Descriptive Statistics for input distributions of uncertain parameters

	Porosity	S_{gr}	S_{wc}	K^*_{rg}
Distribution type	Beta General	Beta General	Beta General	Beta General
Mean	0.129	0.209	0.441	0.287
Median	0.126	0.204	0.441	0.262
5% Percentile	0.081	0.100	0.235	0.073
25% Percentile	0.106	0.157	0.352	0.161
50% Percentile	0.126	0.204	0.441	0.262
75% Percentile	0.149	0.256	0.531	0.389
95% Percentile	0.183	0.333	0.641	0.588

The viscosities of water and CO_2 are functions of the reservoir temperature and pressure, which in turn are functions of the depth of the reservoir. Therefore, in order to model the distribution for the viscosities, the distribution of the depths in the reservoir were modeled. Using a hypothetical reservoir of uniform thickness at a constant depth underneath the surface, the temperature and pressure for the reservoir were calculated using a geothermal gradient of 0.025^{o}C/m and a hydrostatic pressure gradient of 0.1 bar/m respectively. (Szulczewski, 2009)

The depth to the top of the reservoir was assumed to be 1000m. This is a realistic scenario, because for the purposes of storage and injection, depths of at least 800m are desirable. This is because at the temperature and pressure at that depth, CO_2 is in a supercritical fluid phase which is recommended for underground storage because it is at the appropriate density. The depth to the bottom of the reservoir is a constant, H, which is the net sandstone thickness. Consequently, the distribution of depths is between 1000m and 1000+H m. Within the reservoir, the CO_2 is not uniformly distributed, and as can be seen in fig 2.2, the CO_2 is more likely to be closer to the top of the reservoir than the bottom because of the differences in buoyancy. This affects the distribution of the depth measurements, and as an approximation, the distribution of the possible values of the depth of the stored CO_2 is assumed to be triangular, as shown in the Fig. 2.8 below.

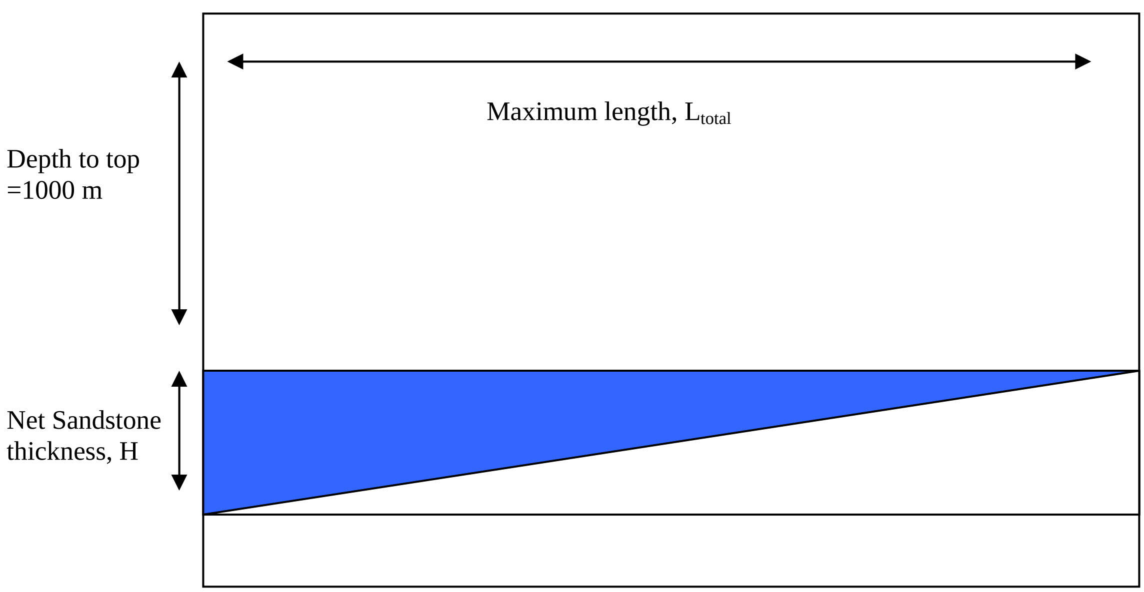

Fig 2.8 Schematic of reservoir depth, The blue shaded area indicates depths at which viscosities were calculated to create PDF for viscosity ratio.

Once a distribution for depth was obtained, the values for the viscosity of CO_2

at each depth was calculated using an online thermophysical properties calculator available publicly on the MIT Carbon Sequestration Initiative website (MIT,2009). The viscosity of water was calculated using a correlation function (Likhachev, 2003).
The ratio of the viscosities, for water/CO_2 ,was then calculated to provide the samples from which a PDF was generated. The ratio was used, as opposed to separate distributions for the viscosity of water and CO_2 to ensure that within each sample, the viscosities were consistent for both CO_2 and water.

2.5 Performing the Monte Carlo analysis

Once the input PDFs for the parameters were generated, the Monte Carlo analysis was performed using Palisade @Risk version 5.0 software, which is a plug-in into MS Excel that is used for uncertainty and risk analysis. Each Monte Carlo analysis performed ran 5000 samples of the model, using Latin Hypercube Sampling (Iman, Davenport and Ziegler, 1980).

The constant parameters H, L_{total}, and W were selected from the work by Szulzcewski and Juanes (2008) which describes the capacity model. However, because of the possible differences in the rock properties for the specific site that they modeled, this work will not attempt to compare results for capacity. Instead the same dimensions of the reservoir are used here to provide a realistic scale for a basin on which this analysis may be performed.

The values selected were:

- H=120m, L_{total}=299,300 m and W=42,000m. These were taken from the work in which the model is presented, and are used as being representative of the dimensions of a realistic injection site.
- The value for density of CO_2 was calculated using the average depth of the reservoir, and was 685 kg/m^3.

Using these values and the input PDFs, Monte Carlo simulations were performed for the following cases for the capacity model:

1. A base case, where the correlation between S_{gr} and S_{wc} was set to 0.
2. A Positive correlation case, where the correlation between S_{gr} and S_{wc} was set to 0.5.
3. A negative correlation case, where the correlation between S_{gr} and S_{wc} was set to -0.5.
4. 5 cases, where 1 parameter was varied at a time while the remaining four were held constant
5. 5 cases, where 1 parameter was held constant at a time, while the remaining four varied.

To evaluate the leakage, we defined a scenario where the output of the capacity model was used to determine how much CO_2 should be injected into a particular site. However, we assume that the existence of a fault some distance away from the injection site was unknown before the injection, and was not taken into consideration when boundaries were evaluated. The model then calculates the amount of CO_2 that escapes at that location. The location of the fault, or the leakage length, then becomes a variable in the model.

In order to model leakage, we construct a PDF of the distance of the fracture from the injection site. The distance was assumed to be exponentially distributed between the injection site and the maximum boundary at L_{total}, and that the probability of a fracture going undetected further away from the injection site is more likely than one that is closer. This distribution was selected to represent the intuition that as a site is selected for injection, the nearby area will be assessed more carefully than the areas further off for possible leaks and fractures.

After running the simulations, the samples were filtered to remove any that represented physically impossible scenarios. These were results from the model that were computed from combinations of the individual variables that combine to represent phenomena that are not possible, such as a trapping efficiency greater than 100% or negative leakage. These are:

1) Negative storage capacity rates

2) Negative lengths for plume length, as this would imply the CO_2 migrating against the groundwater flow

3) Values of the trapping coefficient greater than 0.7

4) Values for mobility ratio greater than 1.

5) Negative leakage rates for the leakage model

The results of the simulations are presented in chapter 3.

Chapter 3: Results

In this section, the results of the uncertainty analysis for the scenarios described in section 2.4 for storage capacity are presented.

3.1 Results of Capacity Simulations

Fig 3.1 shows the PDF of storage capacity, in Gt of CO_2 . From this figure, we can see that in the presence of uncertainty in the geology of the site, the estimate of storage capacity can vary greatly. The expected value of the distribution, as well as the median storage capacity is indicated on the graph.

In order to compare the performance of the model under uncertainty with a deterministic calculation, the capacity for the basin described in Section 2.5 was calculated using the mean values for each of the parameters, shown in table 2.2. The capacity for this aquifer was calculated as 2.62 Gt CO_2.

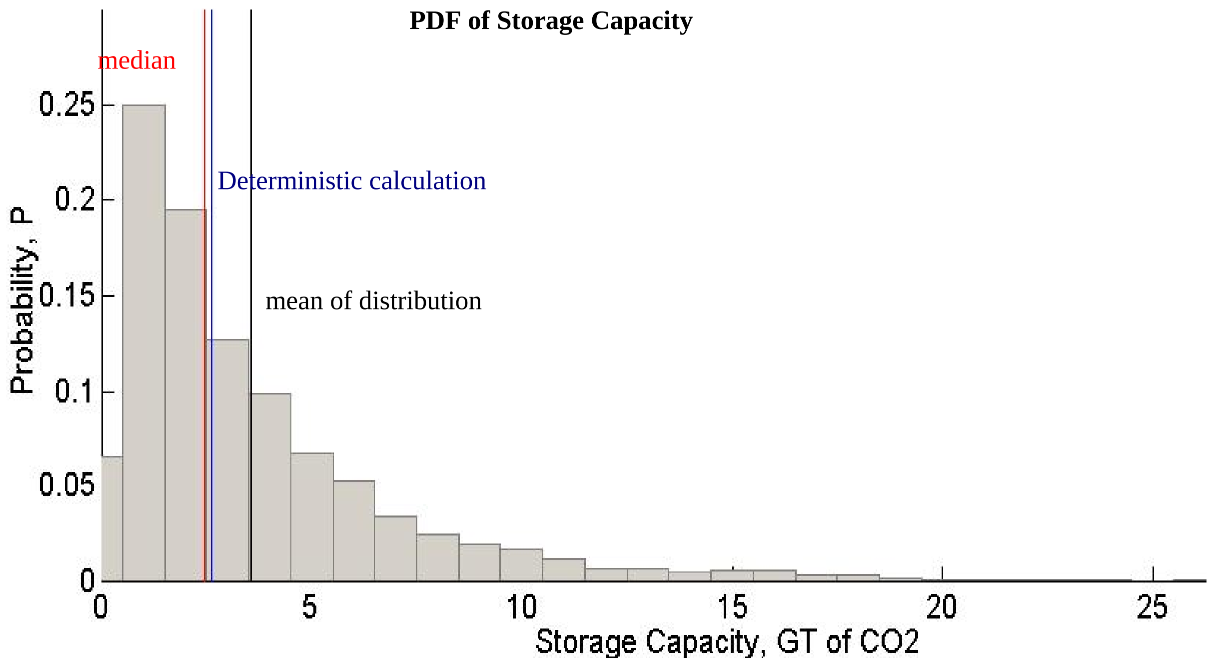

Figure 3.1 shows the PDF of capacity, in Gt of CO_2. The black line is the mean value of the distribution, the red line indicates the median, and the blue line is the capacity estimate from the deterministic calculation.

From the resulting distribution, it is evident that the deterministic calculation of storage capacity using the mean values of the model parameters is different from the expected value calculated from the Monte Carlo simulation with multiple parameters varying at the same time. The distribution has a negative skew, with the mean of the distribution being higher than that of the capacity determined using the mean of the input parameters. This is a significant result, as it illustrates the importance of having better information about the values of geologic parameters that characterize a site, and that the average value of important parameters may not be sufficient to provide an accurate estimate of storage capacity. In this case, the negative skew of the distribution implies that given the distributions of the inputs, it is much more likely that there are more combinations of them which result in smaller values of capacity than larger ones. The larger capacity estimates represent physical values that are physically extremely unlikely, although there is still a non-zero probability of these large values occurring.

The wide range of the capacity estimates which is evident in figure 3.1 is also significant. While there is a large mass of the distribution within a narrow range, between 1 Gt and 5 Gt of CO_2, there is still a non-zero possibility that the capacity of the given site can, for a particular set of geologic conditions, be more than three times as large the expected value. The DOE's Carbon Atlas, in its estimate of storage capacity in saline aquifers also presents a range where the upper estimate is four times as large as the lower estimate. However, unlike this analysis, it does not evaluate the relative likelihood of each of these scenarios. Our results show that while there is a possibility of extremely large storage capacities, there is a much lower chance of this occurring in comparison to the smaller values.

As discussed in Section 2.3, an important relationship between geologic parameters, for which there is very little data available, needs to be understood better. Its effect on capacity estimates can be seen in Fig 3.2, which shows the PDFs of capacity for three different assumptions about the correlations between S_{gr} and S_{wc} are varied. The base case, zero correlation between S_{gr} and S_{wc}, is the same case shown in fig 3.1

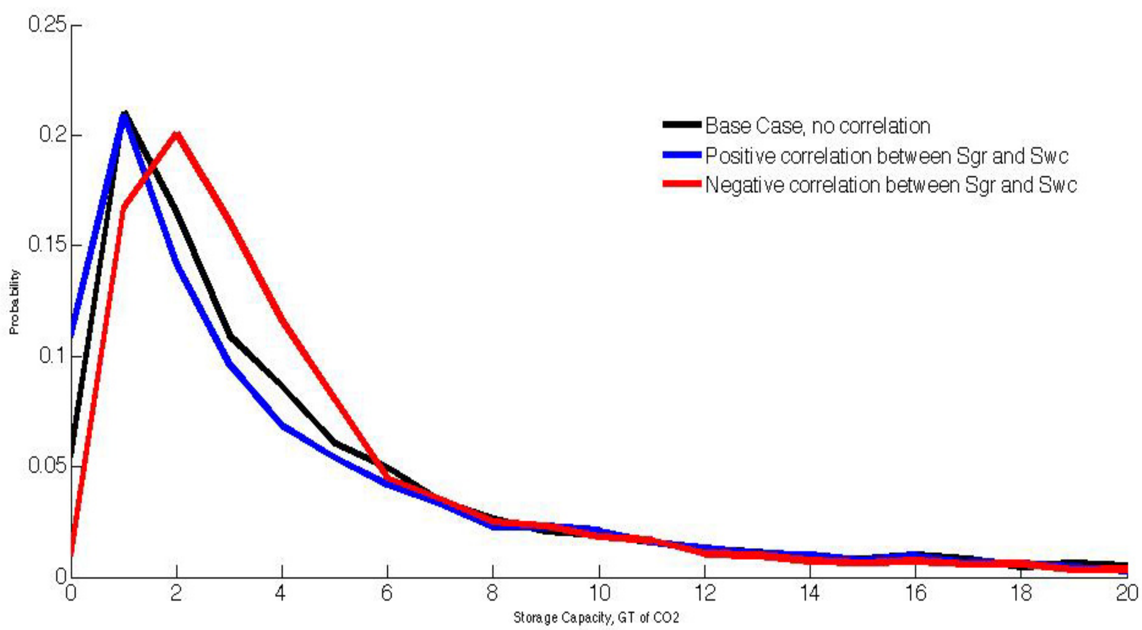

Fig 3.2 PDF of storage capacity for the cases with varying correlations between S_{gr} and S_{wc}.

Table 3.1 shows the mean, median, standard deviations and the fifth, twenty-firth, seventy-fifth and ninety-fifth percentiles for these three distributions.

Table 3.1 Statistics for the distribution of the capacity estimate simulations with varying correlations

	Mean	Median	Std dev.	5%	25%	75%	95%
Base Case	3.56	2.44	3.44	0.42	1.23	4.68	10.59
Positive correlation	3.46	2.21	3.67	0.23	0.93	4.68	11.09
Negative correlation	3.81	2.89	3.15	0.81	1.72	4.77	10.28

From figure 3.2, we can see that capacity estimates are sensitive to the correlations assumed. In the case of negative correlation between S_{gr} and S_{wc} , shown by the red line, we see that there is a larger variance, and higher probabilities of larger capacities. We would expect this because a lower S_{wc} , which is the irreducible saturation of the water, would mean that a higher amount of CO_2 can pass through the rock since there is more available pore space, and that this higher quantity would lead to more trapping of CO_2, which is represented by the higher S_{gr}.

Assuming positive correlation results in a narrower distribution of storage capacity, which demonstrates a physical behavior that is opposite to that of the negative correlation case. Physically, this would mean that even though there is less available pore space for the CO_2 to occupy in the first place, a large portion of it is still trapped. This analysis demonstrates the need to understand the properties of the rock into which CO_2 is being injected much better on a pore scale level.

It is useful to understand the relative contribution of parameters to uncertainty in the capacity estimates. As a first test, one parameter at a time was varied while holding the others constant (fig 3.3).

A second test held one parameter constant and varied the others (fig 3.4). For both analyses, the 5% to 95% percent range for the capacity estimates is shown.

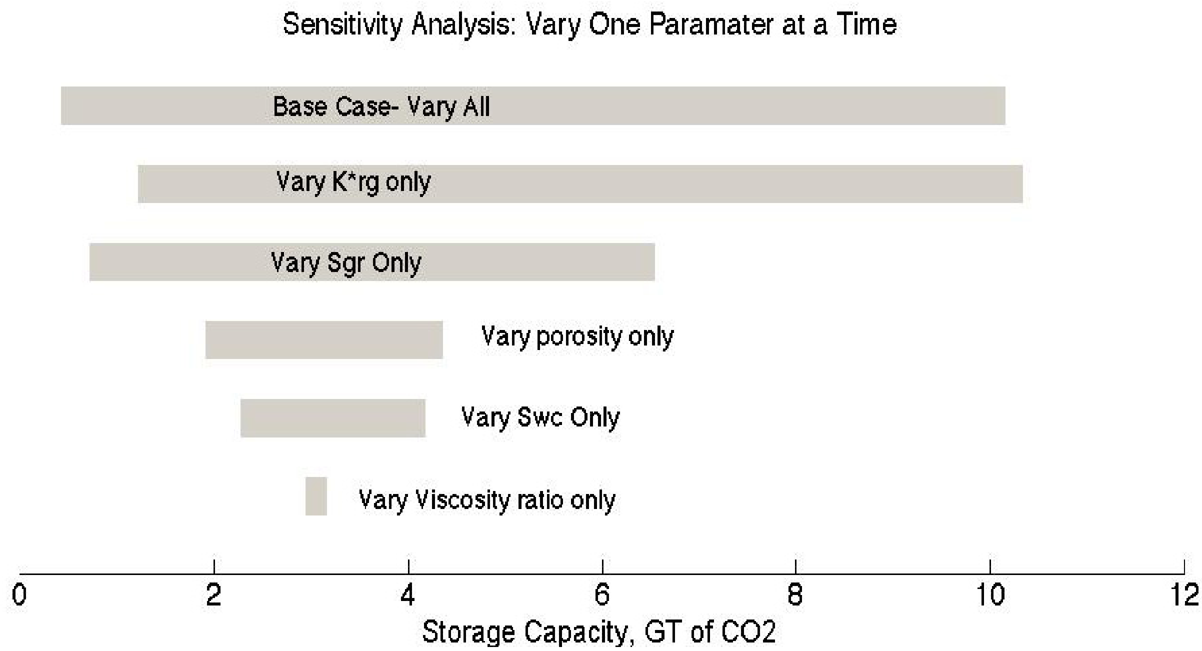

Fig 3.3 Sensitivity Analysis for one parameter variable at a time.

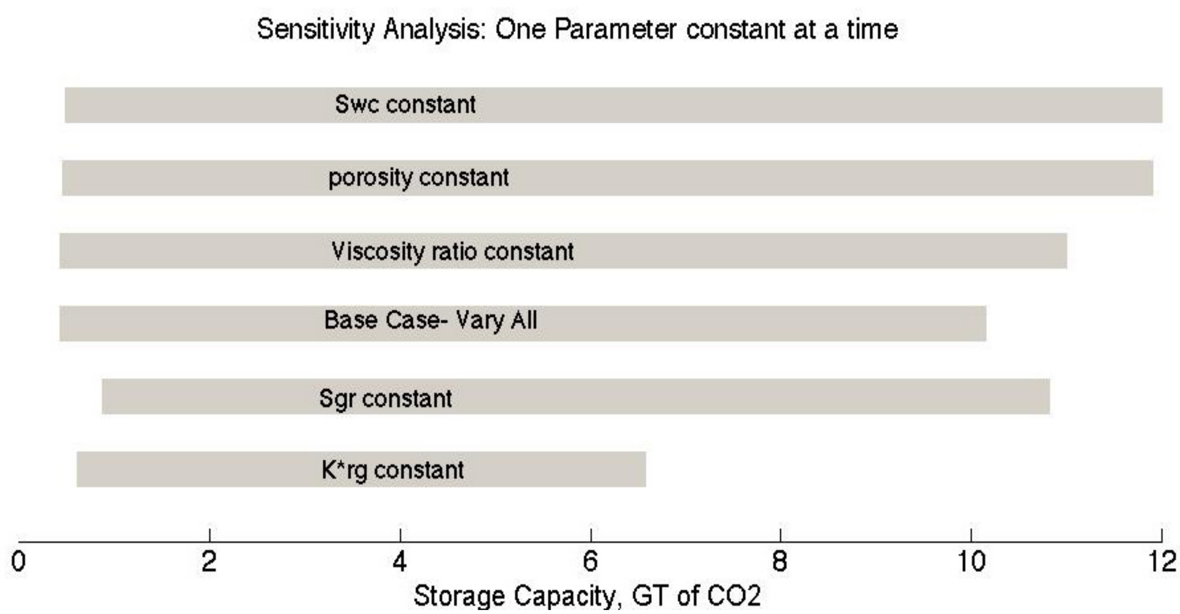

Fig 3.4, Sensitivity analysis for one parameter constant at a time.

The figures indicate that K^*_{rg} and S_{gr} are the greatest contributors to uncertainty in the capacity model. When they are the only variables in the Monte Carlo simulation, the ranges of the estimates are smaller in magnitude than only the base case. Holding them constant also leads the smallest ranges when all the other parameters in the simulation are variable.. The large variability introduced by the variation of K^*_{rg}, which is used to calculate the mobility ratio, is expected, because the solution to the model is highly sensitive to the value of M. (Juanes, 2008). S_{gr} determines the trapping ratio, which measures the amount of CO_2 that is trapped in the rock, and its contribution to the variability in the capacity estimates reflects that the measure of the residual gas that is trapped in the pores of the rock has a direct influence on the total capacity of the entire basin.This is extremely significant, as it implies that we can reduce uncertainty in estimates of geologic storage capacity by reducing the uncertainty in these parameters. Since these are quantities that are measurable from core samples in experimental lab settings, multiple measurements over a potential sequestration area are a straightforward way of reducing the uncertainty in estimates for a given site

In figure 3.3, we see much narrower ranges for the capacity estimates, as holding 4 of the parameters constant removes the variability that is introduced by the interactions between the parameters. This is reinforced by the fact that the case in which all the parameters are varied has the largest range of values. The small range for capacity in the case where viscosity ratio is the only variable is also a result of the fact that the range of values for the viscosity ratios is very small, and therefore, even at its extreme values, there is little variation to the model overall. While K^*_{rg} and S_{gr} have the greatest influence on variability, the other parameters do contribute significantly. Variability is not significantly reduced by holding porosity constant, because unlike the other parameters we are treating as variable, porosity varies directly with the capacity estimate. S_{wc}, which is used to calculate the trapping coefficient also contributes to the uncertainty, but not to the extent as S_{gr}.

3.2 Results of Leakage Simulations

As discussed in chapter 2, we modeled leakage by introducing fractures in the basin at various distances away from the injection well. The distances are presented as normalized to the maximum length, ranging from 0 to 1. The width of the fault for these cases is assumed to be 500m. The volume injected into the aquifer is the same in all the cases, which is 3.5 Gt of CO_2, injected at a constant rate over 30 years. This was selected from the capacity results above as being a 'best guess' value of the capacity of a given site, and this part of the analysis looks at the results of an unknown leak being present.

There are three main questions that we are looking to answer with the leakage model: what is the probability of leakage, what is the order of magnitude of the leakage in the cases where leakage occurs, and what is the timeframe for the start of any possible leakage. This section will present the results to each of these questions sequentially.

To demonstrate the behavior of the leakage model, we first present a test case in which only the distance of the fracture from the injection well, is varied, with all other parameters held constant at their mean values (i.e., no uncertainty). Fig. 3.5 shows whether leakage occurs at different distances away from the injection well.

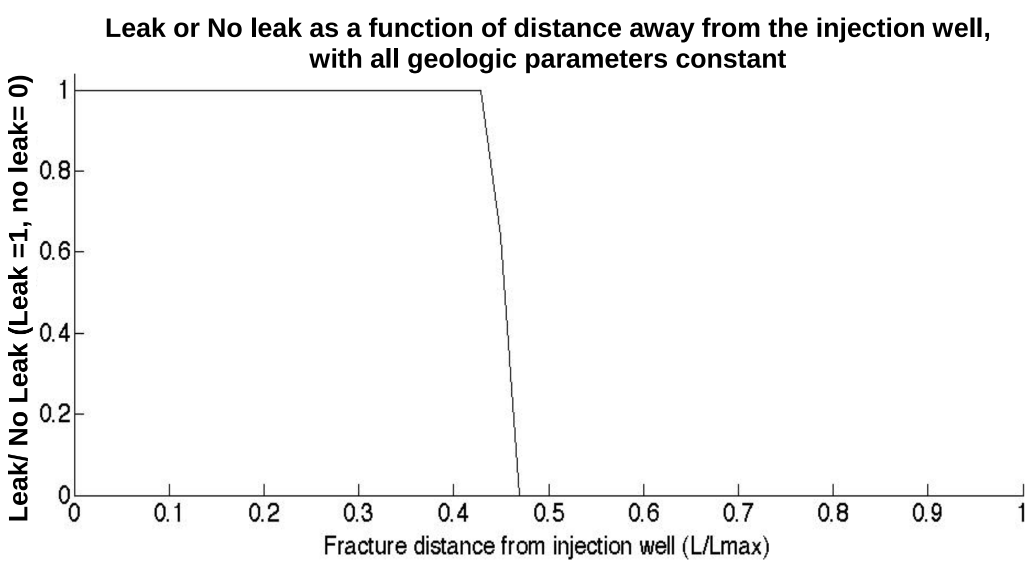

Fig 3.5. Leak/No leak at different distances away from the injection well.

From figure 3.5, we can see that if we have no uncertainty in the geologic parameters, we are able to define a boundary beyond which we know that the plume will not travel. This is because with no variability in the geologic parameters, we can calculate the plume length and the extent of its migration with its certainty. However, as already demonstrated above, there is significant uncertainty in the geology.

Figure 3.6 shows the results of the model for fixed distances away from the injection site, but with all the parameters varying. A Monte Carlo simulation was performed at each of the distances to determine the probability of leakage.

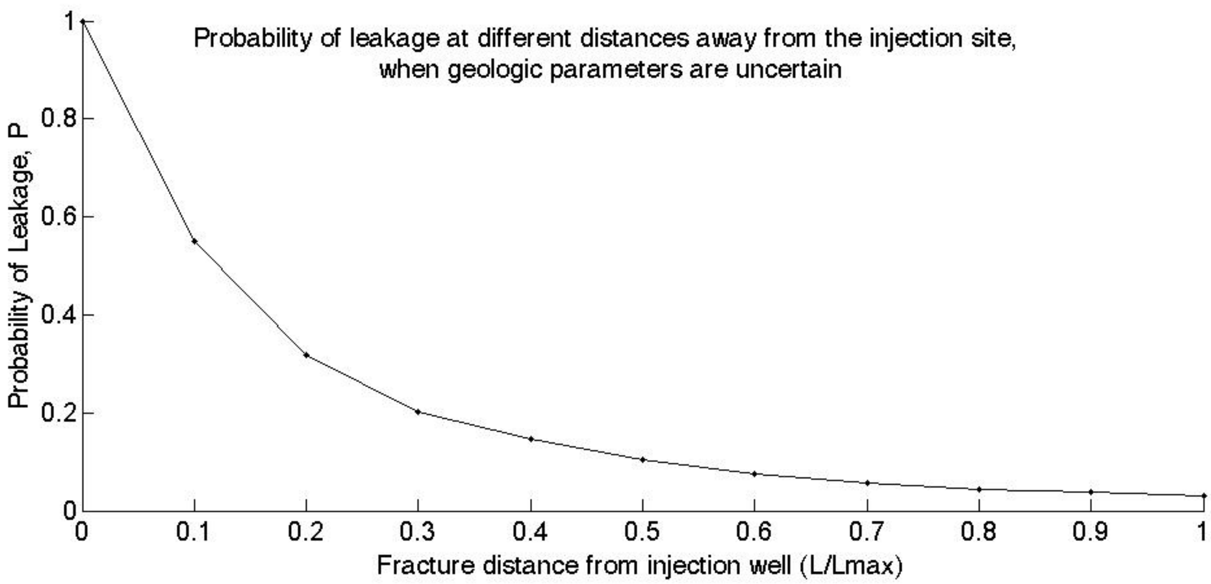

Figure 3.6 Fraction of samples for which there is leakage at different lengths, with all parameters varying.

We can see in figure 3.6 that in the presence of uncertainty in the geologic parameters, leakage can occur further away from the injection site. However the further away the leak is located, the less likely it is to leak. Unlike the deterministic case (fig 3.5), we cannot determine a cut off boundary beyond which we do not see any leakage.

A more realistic scenario to model leakage, as discussed in the previous chapter, is to use a distribution which represents the intuition that a leak that is close to the injection site is more likely be discovered and therefore taken into account in siting, while fractures further from the well are more likely to be missed. An exponential distribution of fracture location models this scenario. The input distribution is shown in fig. 3.7 below.

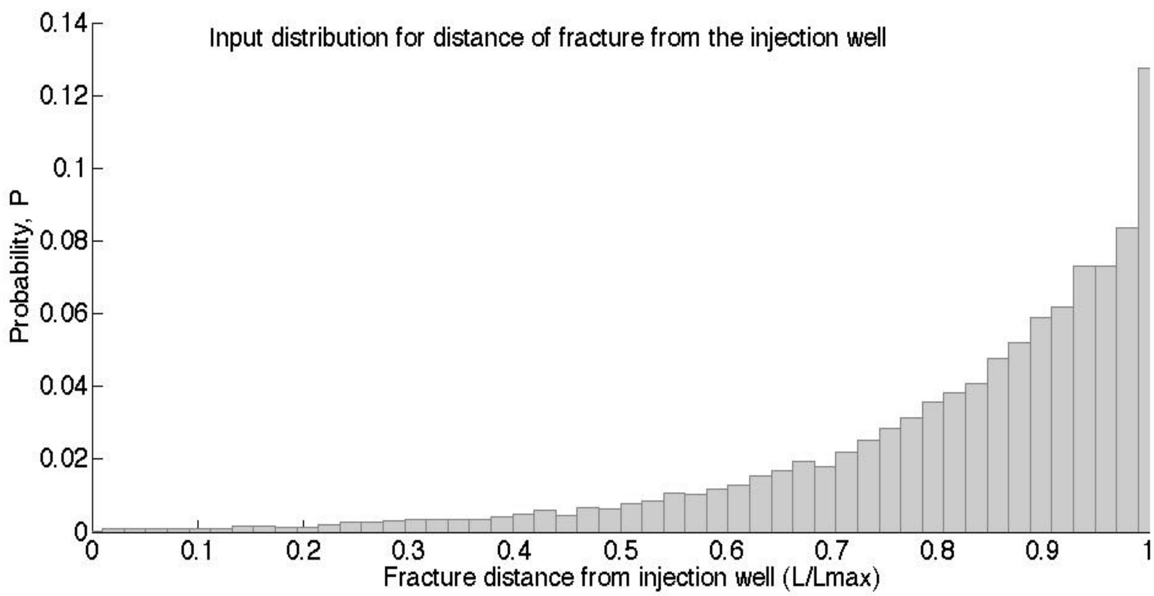

Figure 3.7 Input distribution for fracture distance from injection well.

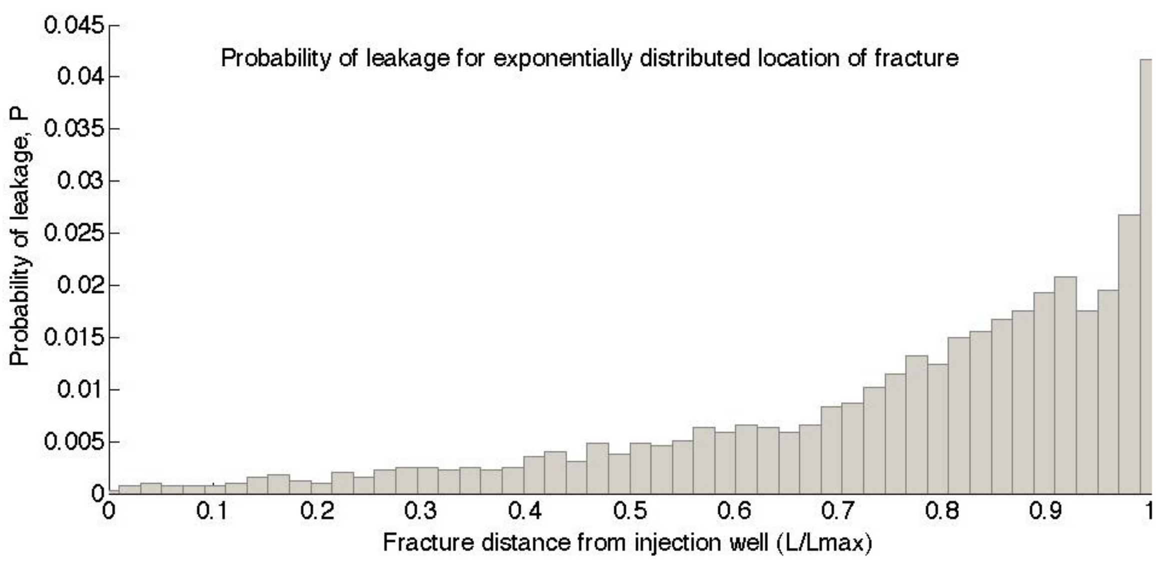

Fig. 3.8 Distribution of lengths at which leakage occurs.

Fig. 3.8 shows the probability of leakage at different distances from the injection site, which are exponentially distributed as shown above. Because of the larger number of samples toward the boundary of the site, the relative likelihood of leakage is higher further from the well. This does not reflect the amount of CO_2 that leaks, but rather only shows that there is more likely to be non-zero leakage. Overall, there was leakage in approximately 38% of the samples.

When leakage does occur, there are two model results that are of interest: the total amount of CO_2 that escapes over the duration of leakage, and the start time of the leakage. Probability distributions of both of these quantites are given in the figures below.

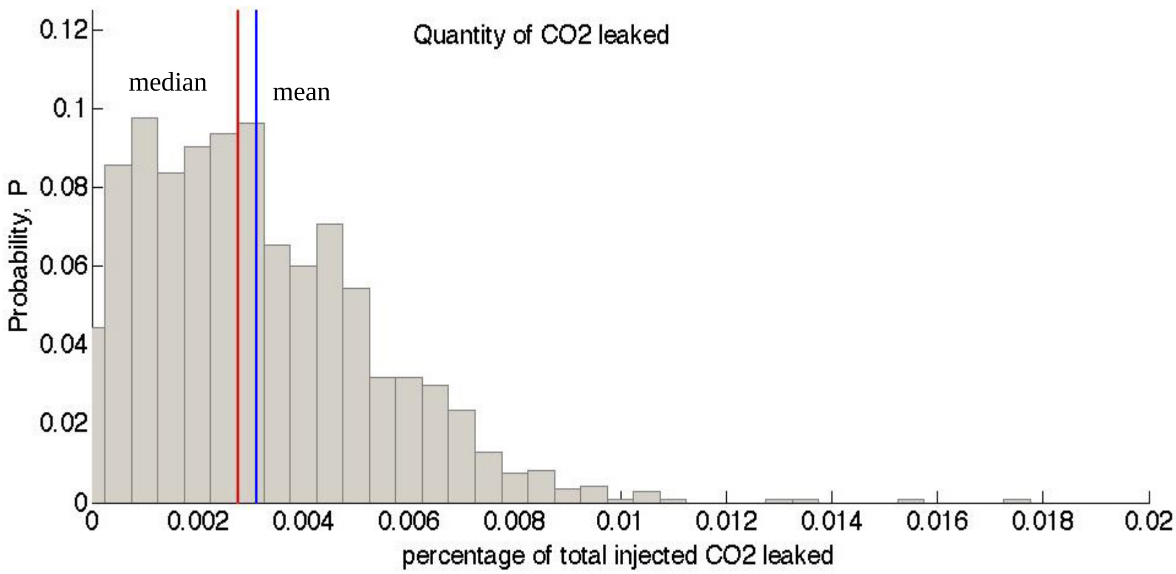

Figure 3.9 Distributions of total amount leaked, as a percentage of total injected volume of CO_2. The blue line indicates the mean of this distribution, and the red line is the median.

Figure 3.9 indicates that the total CO_2 injected that leaks is extremely small, for the majority of samples it is a fraction of a percentage. However, these amounts are directly proportional to the size of the fault, so if the fault was twice as big as the one modeled here (1 km vs 500m) the leakage amounts would be twice as large. Even with a 5 km fault, 10 times as large as assumed for Figure 3.9, almost all the likely leakage would be less than 0.1% of the total injected volume.

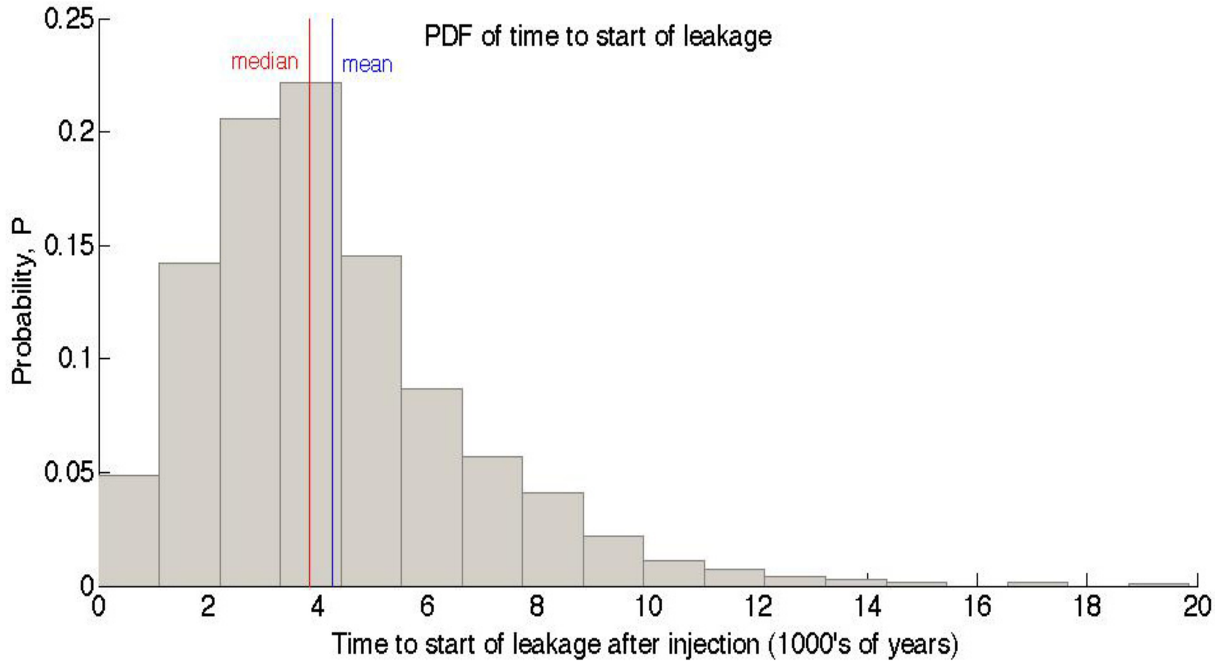

Figure 3.10 Distributions of start year of leakage.The blue line indicates the mean year, and the red line indicates the median

Table 3.2 Statistics for leakage simulation

	Mean	Median	Std. Dev.	5%	25%	75%	95%
For samples with leakage, start time for leakage (years)	4260	3830	2496	1139	2530	5370	8930
For samples with leakage, amount of leakage %	0.0031	0.0028	0.002	0.0002	0.0014	0.0045	0.0071
for all samples[1], leakage amount %	0.0012	0	0.002	0	0	0.0019	0.0056

The PDF of the year in which leakage begins is shown in figure 3.10. Table 3.2 below gives the descriptive statistics for the leakage simulation results. The conditional dataset excludes the simulations in which no leakage occurred. From these results we can see that according to this residual trapping model, there is a very low probability of large leakage amounts, and that the start of any leakage that occurs is on the order of thousands of years from the start of injection.

[1] For all samples in the simulation, 62% of the data demonstrated no leaks.

Chapter 4: Implications of Uncertainty in Geologic Storage

In chapter 3, the results of the Monte Carlo simulations performed on capacity estimates and leakage potential for storage in a single basin were presented. From these results, it is evident that in the presence of uncertainty in the geology of the site, it is difficult to accurately calculate the storage capacity of a site.

In the uncertainty analysis for leakage potential, we see that with the model used, we have a very low probability of large leakage amounts. In the cases in which there is leakage, the amounts that leak out are in fractions of a percentage of the total injected volume. Additionally, the timeframe of leakage occurring is on the order of thousands of years. These results indicate that if residual trapping is the primary trapping mechanism of CO_2, the injected gas is unlikely to leak in large amounts in the short and medium term. These results have important implications for the science and regulation of geologic storage, and its feasibility as a climate mitigation option.

4.1 Implications of uncertainty on the science of geologic storage

The uncertainty analysis performed on the residual trapping model for geologic storage presented in chapter 3 indicates that the variability in the rock properties can have a significant impact on the behavior of the CO_2 within the reservoir. Since this analysis was performed for a basin with realistic dimensions and a dataset of rock properties from a different geographical region, the exact numbers from the analysis are not comparable to other data; however the trends that are evident in the results provide important insights for research in the field of geologic storage.

Fig. 3.1 shows that when we perform the uncertainty analysis, the mean value of the distribution of potential capacity estimates is higher than the mean that would be calculated from the mean values of the input distributions in the given model. This is a demonstration of the fact that for a non-linear system, the expected value of the function is not equal to the function of the expected value, a fact that is often ignored in scientific research, particularly when there is no uncertainty analysis performed. It is also demonstrative of the fact that the storage capacity has a large possible range for a given basin, and the calculation of any one value as being representative of the capacity of the entire basin is problematic.

Considering the contribution of individual parameters to uncertainty, we see that the relationship between the relative permeability parameters — S_{wc} , S_{gr} and K^*_{rg} — and their individual effects on the model drive the majority of the uncertainty in the model results. This is not surprising, since these parameters are used to calculate the mobility ratio and the trapping coefficient, which describe the movement of the CO_2 plume and the amount that is trapped in the rock on a pore-scale, which is then used to describe the behavior of the CO_2 on a basin scale. This suggests the importance of further research into rock properties to understand these parameters better, and to narrow the distributions of the possible values that they may take. In this case, the uncertainty in the capacity of geologic storage could be significantly reduced by a straightforward set of experiments that can be conducted in a laboratory setting. Not only would this research improve the science of geologic storage, but it should also be a significant part of the site characterization process. The cost of performing the core-scale lab experiments that will lead to better data is likely justified by the reduction in the variability of the capacity. However, since a given reservoir will not be homogenous, a number of samples from any one area would need to be tested to ensure that the variability that is present in the rock can be characterized. The rise in the number of such experiments would also help bring down the cost and improve the experimental process, which in turn could bring down costs associated with site characterization.

The uncertainty in the location of leaks, leakage amounts and the start of leakage times indicates that when residual trapping is taken into account, the leakage potential is very small. The expected value of the amount of leakage is a small fraction of the total injected volume, and the expected value of the start of leakage is over a thousand years, indicating that geologic storage security exists over large a time frame for sites, even if they do not have structural traps preventing the migration of CO_2. It also confirms the assertion made in the IPCC's report (Metz *et al*., 2005) that over a long period of time, the contribution of residual trapping to the amount of CO_2 stored securely increases. This analysis also indicates that fractures that are further away from the injection site are less likely to be potential leaks, as the mobile CO_2 is less likely to reach that particular site.

While this analysis has provided us some insight into the uncertainty in one particular model, it is imperative that for a greater understanding of geologic storage, models of different processes of storage, plume migration and leakage are incorporated to ensure that the analysis is more complete. Other work in the area has demonstrated the variability in plume distribution depending on the geometry of the basins, including the thickness of the formation and structural traps, an element of geologic storage that was not taken into consideration by this model (Frailey, 2009). There are models which focus on dissolution, and not residual trapping as a large contributor to storage efficiency (Kumar, 2009), which leads to a different understanding of plume dynamics. A more complete model would combine both these processes to provide a better understanding of the evolution of the plume.

Additionally, core-scale experiments have also reinforced that the heterogeneity of the core can affect the multiphase brine displacement (Perrin, 2009), suggesting the need for more study in the area and for uncertainty and variability in geologic parameters to be taken into account. From an operational standpoint, relative permeability has also been shown to affect injectivity in the reservoir (Burton, 2009), and therefore uncertainty can affect the target rates of CO_2 injection into reservoirs.

The modeling of leakage processes can also have an impact on the leakage amounts and time frame associated with it, which can add more variability in the system. In this analysis, the mechanism behind leakage was not modeled in detail, creating a scenario that represented that all CO_2 that reaches a given location escapes into the atmosphere instantaneously. This is an unrealistic approach, and is representative of a worst case scenario. A number of different mechanisms to model leaks have been studied, and there are detailed models of leakage profiles through wells, fractures and faults, and diffusion through the cap rock driven by CO_2 buoyancy (Grimstad, 2009).

Additionally, the location of faults away from the injection site and the size of a fault can also be modeled, with work on the probabilistic estimates of fault and plume interaction looking at ways to characterize this process. (Oldenburg, 2009). With so many different physical processes occurring simultaneously, the variability in the entire system cannot be characterized as being limited to a subset of parameters. An important takeaway from this work is not just the importance of particular parameters in the light of uncertainty analysis, but of the process of modeling the associated uncertainty for the different models that may be used to gain a better understanding of the science.

4.2 Implications for the regulation of geologic storage

As discussed in section 1.4, the proposed rules for geologic storage require site characterization for geologic storage, which includes specifying storage capacity and an area of review (AOR) for which extensive geologic data must be submitted to the regulator.

Unlike the specifications for the area of review for other classes of injection wells, the proposed rule that creates a new category of wells for geologic sequestration of CO_2 does not state a fixed radius from the location of the injection well as the zone of influence, for which site characterization needs to be performed. This is in recognition of the fact that unlike other injected substances, the long-term natures of storage and the buoyancy of CO_2 will result in large but also uncertain behavior of the migration of the plume. However, since site characterization is an important part of the permitting process to ensure the safety of injection, there is a need to incorporate the uncertain nature of geologic sequestration and the evolution of the CO_2 plume over time into any future regulation.

There are two areas into which the issues surrounding the determination of the AOR can be broadly classified: 1) The models that are used in this process and the particular physical process that is modeled and taken into consideration 2) The economics of site characterization, which may prove to be significant hurdles for operators if the AOR is extremely large. Since there is no fixed boundary for the AOR, the rules propose that models are used to determine the lateral extent away from the injection site for which the geology needs to be characterized. The use of different models and the choice of parameter values for those models would likely lead to different results, and it is up to the operator to choose the model they wish to use. Additionally, the costs of site characterization could also influence the choice of model. These costs are typically per unit area, and so there is the possibility that in order to save on this costs, operators may avoid the use of models which result in larger areas of review.

As discussed in section 4.1, the various aspects of the science behind geologic storage- the different trapping and leakage mechanisms that are possible, as well as the variability introduced by heterogeneous geometry and geology- leads to a large number of sources of uncertainty in any attempt at modeling. From the results presented in chapter 3, it is evident that the presence of uncertainty, or heterogeneity in rock properties over a large geographic area, can lead to very different estimates of storage capacity and the migration of the plume. This model took only one trapping mechanism into account, and does not account for variability that may occur from variations in the geometry of the aquifer, or, from an operational point of view, variation in pressures that result from injection, which are only two examples of a number of other sources of variability.

The proposed rule indicates that the model used during the site characterization process, is a dynamic, multiphase flow model, but leaves the choice of model up to the operator that is applying for the permit. The trapping mechanism is not specified, nor is there a specification of the parameters that need to be included in any particular model. An issue that can arise here is one of quality control, and of the possible lack of consistency across the permits that are issued by different regions or states. While operators should be given the choice to use whatever computational models and simulations they deem appropriate, the regulators should ensure that these models take into consideration the different scientific processes that are at play in geologic storage.

Additionally, the proposed rule does not include a requirement for uncertainty analysis as part of the site characterization data. With more scientific data about a certain site, which could be obtained with a larger number of core samples and well tests in the area, one could reduce the uncertainty in the behavior of the plume. However, the area from which these samples are to be taken need to be delimited by some method since it is not practical to have a very large number of samples if they are not required.

The economics of site characterization create a trade-off between a complete site characterization that determines the AOR to be the maximum possible extent of the plume and one that limits the boundaries based on probabilistic estimates of leakage potential. The estimated costs of site characterization are high; these have been cited from industry to be \$38,610 per km^2 for 3-d seismic data collection, \$3,000,000 to drill and log a well, with one well required for every 65 km^2 of the area, and an additional 30% of costs for data processing and modeling (McCoy and Rubin, 2009). This means that the cost of an area covering 130 km^2, would be \$14.325 million; the lateral extent of a CO_2

plume is extremely variable depending on the rock properties and the formation structure of a given site.

Since the cost is per unit area, there is an incentive for the operator to limit the AOR. Consequently, there is a corresponding potential disincentive for the operator to present scenarios, through the exploration of model or parameter uncertainty, that show larger AOR since it would reduce their costs. One means of countering this disincentive is the design of liability rules regarding potential leakage. By making operators liable for any leakage during injection and for some pre-determined period after injection, regulators can ensure that operators are more diligent in their site characterization.

With the availability of probabilistic estimates of leakage potential as a function of the distance from the injection site as shown in chapter 3, one option is to determine a threshold for leakage amounts and start times, and use these thresholds to determine the extent to which the initial AOR is defined. This approach is feasible if combined with the requirement to remodel and reassess the site every 10 years, as is required in the proposed rule. With the availability of more data, the initial models could be verified or improved.

Previous studies of the assessment of sites at the Frio, Weyburn and Gorgon sequestration projects have used a number of different strategies to deal with uncertainty. The strategies for Frio and Weyburn include post-injection analysis, which confirms that the initial modeling of the CO_2 plumes were not accurate, as they did not account for geologic characteristics that influenced the plume migration. These strategies include i) sensitivity analysis for parameters included in models, ii) establishing a baseline for measurements can then be used to compare new data with, iii) iterative modeling using previously unavailable data and iv) monitoring of the sites (Bacanckas and Karimjee, 2009). While each of the sites used a subset of these, it is clear that all of these strategies can be incorporated in a single plan, which allows for continuous evaluation of the injected CO_2.

4.3 Implications of uncertainty on the feasibility of geologic storage as a carbon mitigation option

For climate policy, the long-term implications of geologic storage are extremely important. Even if the available storage capacity is a fraction of what the initial estimates are, it would still be enough to be an important component of the medium to long term solutions to prevent the addition of CO_2 into the atmosphere. The debates that make geologic storage controversial concern permanence of storage and leakage rates. This modeling exercise indicates that in the long run, the chances of large amounts of leakage are extremely small, and the amounts that may potentially escape into the atmosphere are fractions of a percentage of the total injected volume. Additionally, leakage would likely occur over a time frame of more than a thousand years, which is difficult to address in current policy discussions. The results here are consistent with the statement in the IPCC report (IPCC, 2005) that suggests that leakage is very likely to be less than 1% over 100 years, and likely to be less than 1% over 1000 years.

This implies that given the extent of storage security as represented in this model, issues around credits for leaked amounts are of a lesser impact, since the amount that will leak is so far out in the future and even then, such a small relative volume to that which is being stored, this should not be a hurdle in the development of climate policy. However, there is still a non-zero probability of leakage within a short time span, and in the context of a price on CO_2 that would result from a climate policy, this would need to be addressed in terms of carbon accounting and credits.

One aspect that is important to take into consideration is the applicability of the regulatory framework. Currently, the proposed rule is under the Safe Drinking Water Act, the mandate of which is to protect any potable groundwater from contamination. It does not take the effects of direct leakage into the atmosphere on carbon accounting and climate change. Since the entire purpose of geologic storage is for climate mitigation there is a need for an additional set of rules to ensure that the injected CO_2 is accounted for accurately.

Policy discussions regarding CCS suggest financial incentives for storage in the form of credits per ton of CO_2 sequestered. The volume of CO_2 injected into a site is easy to measure by measuring the flow rates in the injection wells, and this can be used for the initial assignment of credits. However, in the event of leakage, there is no clear way for the recipient of the initial credit to compensate for the amount lost. In a regulatory environment where this is a price on CO_2, a gap in the ability to account for CO_2 could leave CCS vulnerable to financial discrepancies and inefficiencies. Additionally, in the presence of national caps and targets for CO_2 mitigation, it is important to have a clear methodology to account for any amount that leaks back into the atmosphere, and a method to compensate for the initial credit that was given.

This poses a challenge, as there is no direct way to accurately measure the amount of CO_2 that escapes, or that remains trapped in the formation. With the uncertainty that is present in the migration of the plume, a measurement, monitoring and verification (MMV) plan needs to be in place. However, even MMV technology is limited in its accuracy, and is heavily reliant of the modeling of the subsurface that we have already demonstrated as being sensitive to variability in the geology. In the model we used, the presence of a leak would be easy to detect because of the assumption that the fracture is perfectly permeable and that all the CO_2 that reaches it escapes instantaneously. The plume could be tracked seismically and the fracture could be located, and the leakage rate could be monitored. In reality, both these assumptions are not physically realizable, and represent a worst case scenario in this analysis. The leakage amounts that are shown in the results of this exercise are extremely small; moreover, they are cumulative over the entire lifetime of the leakage, and so the annual rates are even smaller amounts. Based on this model, it would be extremely difficult to detect any leakage from the sites that may occur from a fault.

In order to be prepared for the case that there is leakage of large amounts of CO_2 in the short-term, as low as the probability may be, a system that can account for leakage must be designed. One option is to use bonds, or similar financial instruments that can be traded on a market, that lose their value as CO_2 leaks from storage. Additionally, in order to compensate for the leakage, the owner of the bond would have to compensate the regulatory body with a CO_2 emission certificate. The bond would be a guarantee of the security of the stored CO_2, and any loss in value would be a devaluation in the asset. Since an operator would not want to lose value on their assets, they would have an incentive to ensure the storage permanence of the injected CO_2.

Another option that is discussed is of temporary and partial credits for the stored CO_2, that only become permanent and complete once a certain pre-determined period of time for which there is an increased risk of leakage has passed (Held, Edenhofer, Bauer, 2009). All these accounting methods, however, are dependent on accurate MMV of the injected CO_2, which is an active area of research in CCS.

Any policy that is designed for geologic storage should take uncertainty into consideration, and include risk management strategies for events that while highly unlikely, still have a non-zero chance of occurrence. With the proper management and monitoring of sites, the establishment of proper liability regimes, accounting rules and compensation mechanisms for leakage, geologic storage can be a safe and effective carbon mitigation tool to combat climate change.

Chapter 5: Conclusions and Future work

Uncertainty analysis was conducted on a residual trapping model for geologic storage in saline aquifers. The conclusions that are drawn from this work are based on the uncertainty for this particular model. The use of other models that incorporate different scientific processes would further improve our understanding of uncertainty in geologic storage.

5.1 Conclusions

Uncertainty in geologic parameters has a significant effect on capacity estimates. Capacity estimates can vary by a factor of four in the presence of uncertainty in geologic parameters. By performing a probabilistic analysis, it is possible to narrow the range of values that are more likely than the extreme values. The Monte Carlo simulation also demonstrates that the expected value of the distribution of the capacity is not the same as the expected value that can be calculated deterministically from the expected values of the input parameters. This indicates the importance of performing uncertainty analysis.

Residual gas saturation and relative permeability of CO_2 have the maximum contribution to uncertainty in geologic storage in saline aquifers.

The sensitivity analyses performed on the capacity model indicate that residual gas saturation, , and the endpoint relative permeability of CO_2, k^*_{rg}, are the largest contributors to the uncertainty of the capacity estimates. Both of these values are easily measurable in a lab setting from core samples, and more extensive research can provide more extensive data from which the distributions of these parameters can be determined. Additionally, this points to the importance of multiple core samples in the process of site characterization

Correlation between geologic parameters that characterize the properties of the rock can vary the capacity estimates.

Assuming different correlations between the residual gas saturation and the connate water saturation S_{wc} varies the distribution of capacity estimates, indicating the need for further research into understanding the properties of the rock.

The likelihood of leakage decreases as the distance of a fracture away from the injection well increases.

As the plume migrates after injection, the amount of mobile CO_2 decreases and the amount that is trapped increases as the further away it travels from the injection well. This indicates that when fractures are further away, there is greater likelihood that the entire plume is trapped and therefore no mobile CO_2 reaches the fault, resulting in a lower likelihood of leakage. This suggests that when characterizing a site for injection, it is more important to assess areas closer to the injection well as opposed to areas much further away.

The quantity of CO_2 that leaks after injection, as a percentage of total injected volume of CO_2 is extremely small.

The quantity of CO_2 leaked in the simulations is on the order of fractions of a percentage of the total injected volume. This suggests that residual trapping is an effective trapping mechanism on its own, and can store large volumes, making geologic storage effective for carbon mitigation.

The time to the start of potential leakage of CO_2 after injection is extremely long. The expected time to the start of leakage is on the order of magnitude of thousands of years. This indicates that geologic storage has the potential to be a safe short to medium term carbon mitigation technology. While there is a very low non-zero probability of leakage in the short term, risk management strategies should be established using the appropriate policy and regulatory tools to ensure safety and proper accounting of CO_2 in the event there is leakage.

5.2 Future Work

Further work in this analysis would extend the uncertainty analysis to better understand the behavior of the injected CO_2. The analysis can be extended by including:

- More leakage scenarios, with different injection rates to reflect the different constraints- whether scientific, technical, or regulatory, that may restrict injection.
- Different assumptions about the distribution of fractures. Uncertainty analysis on the size of the fractures can be included as well.
- Uncertainty in the geometry of the basin, which we have assumed as being constant. This can also be treated as variable in order to better reflect the uncertainty in the entire basin.

References

Alley, R., Berntsen, T., Bindoff, N. L., Chen, Z., Chidthaisong, A., et al. (2007), "Climate Change 2007: The Physical Science Basis: Summary for Policymakers." Working Group 1, Intergovernmental Panel on Climate Change

Bacanskas,L., Karimjee,A., Ritter, K., (2009) "Toward practical application of the vulnerability evaluation framework for geological sequestration of carbon dioxide" *Energy Procedia*, Volume 1, Issue 1, GHGT9 Procedia Pages 2565-2572

Burton,M., Kumar,N., Bryant, S.L., (2009) "CO2 injectivity into brine aquifers: Why relative permeability matters as much as absolute permeability", *Energy Procedia*, Volume 1, Issue 1, GHGT9 Procedia, Pages 3091-3098,

Bennion DB, Bachu S (2006) Supercritical CO2 and H2 S–brine drainage and imbibition relative permeability relationships for intergranular sandstone and carbonate formations. In: *SPE Europec/EAGE Annual Conference and Exhibition*, Vienna, Austria, (SPE 99326)

Carbon Capture and Sequestration Technologies at MIT, CO2 thermophysical property calculator, http://sequestration.mit.edu/tools/index.html.

Department of Energy, National Energy Technology Laboratory, (2009) Carbon Sequestration Atlas of the United States and Canada, Second Edition, http://www.netl.doe.gov/technologies/carbon_seq/refshelf/atlas/

Dullien, F.A.L., (1992), Porous Media: Fluid Transport and Pore Structure. San Diego: Academic Press Inc.

Environmental Protection Agency, (2008) "Federal Requirements Under the Underground Injection Control (UIC) Program for Carbon Dioxide (CO2) Geologic Sequestration (GS) Wells Proposed Rule", http://www.epa.gov/fedrgstr/EPA-WATER/2008/July/Day-25/w16626.htm

Environmental Protection Agency, (2008) "Geologic CO2 Sequestration Technology and Cost Analysis", http://www.epa.gov/ogwdw/uic/pdfs/support_uic_CO2_technologyandcostanalysis.pdf

Environmental Protection Agency, (2008), "Vulnerability Evaluation Framework for Geologic Sequestration of Carbon Dioxide", http://www.epa.gov/climatechange/emissions/downloads/VEFTechnical_Document_072408.pdf

Frailey,S. M., Finley, R. J., (2009) "Classification of CO2 Geologic Storage: Resource and Capacity", *Energy Procedia*, Volume 1, Issue 1, GHGT9 Procedia, Pages 2623-2630

Frailey, S.M., Leetaru, H., (2009) "Geological factors affecting CO2 plume distribution", *Energy Procedia*, Volume 1, Issue 1, GHGT9 Procedia, Pages 3107-3112

Held,H., Edenhofer, O., (2009) "CCS-Bonds as a superior instrument to incentivize secure carbon sequestration" *Energy Procedia*, Volume 1, Issue 1, GHGT9 Procedia, Pages 4559-4566

Iman. R.L., Davenport, J.M., and Zeigler, D.K.,(1980), "Latin Hypercube Sampling (Program User's Guide), Sandia Labs, US Dept. of Energy.

Grimstad, A., Georgescu,S., Lindeberg, E., Vuillaume, J. (2009) "Modelling and Simulation of Mechanisms for Leakage of CO2 from Geological Storage", *Energy Procedia*, Volume 1, Issue 1, GHGT9 Procedia, Pages 2511-2518

Juanes, R., MacMinn, C. W., and Szulczewski, M. L., (2009) “The footprint of the CO_2 plume during carbon dioxide storage in saline aquifers: storage efficiency for capillary trapping at the basin scale.” , *Transport in Porous Media*, Accepted, in press.

Kumar, N.,Bryant, S., Nicot, J., (2009) “Simplified CO_2 plume dynamics for a Certification Framework for geologic sequestration projects”, *Energy Procedia*, Volume 1, Issue 1, GHGT9 Procedia, February 2009, Pages 2549-2556

Likhachev, E. R. (2003) Dependence of water viscosity on temperature and pressure, *Tech. Phy*. vol.48 no. 4, Pages 514-515

McCoy, S.T., Rubin, E.S., (2009) “Variability and uncertainty in the cost of saline formation storage”, *Energy Procedia*, Volume 1, Issue 1, GHGT9 Procedia, Pages 4151-4158

Metz, B., Davidson, O., De Coninck, H., Loos, M. & Meyer, L. (2005), "IPCC Special Report on Carbon Dioxide Capture and Storage." Intergovernmental Panel on Climate Change; Geneva (Switzerland); Working Group Iii, Cambridge University Press

Oldenburg, C.M, Nicot, J., Bryant, S. L., (2009) “Case studies of the application of the Certification Framework to two geologic carbon sequestration sites”,*Energy Procedia*, Volume 1, Issue 1, GHGT9 Procedia, Pages 63-70

Perrin, J., Krause, M., Kuo, C., Miljkovic. L, Charoba, E., Benson, S.M, “Core-scale experimental study of relative permeability properties of CO_2 and brine in reservoir rocks”, *Energy Procedia*, Volume 1, Issue 1, GHGT9 Procedia, February 2009 , Pages 3515-3522

Szulczewski, Michael., Juanes, R., (2009) “A simple but rigorous model for calculating CO_2 storage capacity in deep saline aquifers at the basin scale”, *Energy Procedia*, Volume 1, Issue 1, GHGT9 Procedia, Pages 3307-3314