Storing CO2 in geological reservoirs

Lagring av CO2 i geologiska reservoarer

Matilda Einemo

ABSTRACT

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Climate change has received considerable exposure in media during the last years. The general public is increasingly aware of the effects of greenhouse gas emissions and many governments and organizations have become involved in finding solutions. The most important contributor to the enhanced global warming is carbon dioxide (CO_2) produced by burning of fossil fuels. One of the considered possibilities to reduce emission of greenhouse gases is capturing CO_2 at the source and storing it in geological formations. Deep saline aquifers are the geological formations that are considered to have the largest storage potential. Another possible formation type that is usually not considered geologically optimal and has therefore not been subject to similar research as deep saline aquifers is a rock type common in Sweden, namely fractured crystalline rock.

In this Thesis simulations of CO_2-storage are carried out for two geological formation types relevant for Sweden. The first one is a deeply situated fracture zone in crystalline rock, with characteristic typical of such zones even though not based on data at any specific location. The second one is an actual saline aquifer situated in Skåne, Sweden. For this aquifer the properties are based on data from an observation well in Malmö, Skåne.

The simulations are carried out with TOUGH2 simulator. This is a numerical model that has been developed at Lawrence Berkeley Laboratory in USA for simulations of multi-component and multiphase flow in porous and fractured media. ECO2N is a fluid property module that has been developed to function together with TOUGH2 for simulating storage of CO_2 in saline aquifers.

The results of these preliminary simulations indicate that storage of CO_2 in fractured crystalline rock may be possible but the injection would probably have to be of small scale and the risk of seepage is considerable. Some CO_2 remain as immobile, residual saturation in the fracture zone when the injected plume leak, making it possible to store some CO_2 in a fracture zone. The saline aquifer appears to be a potential storage site, but again further investigations and simulations are required in order to carry out an injection project. The quantity of CO_2 that can be stored in a fracture zone is small compared to the potential storage in a saline aquifer.

Keyword: TOUGH2, ECO2N, Geological storage, CO_2, saline aquifer, fractured rock

REFERAT

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Utsläpp av växthusgaser och klimatförändringar har fått stor uppmärksamhet i media under de senaste åren. Både allmänhet och makthavare blir mer och mer medvetna om problematiken och vikten av att agera snabbt i frågan. Den viktigaste växthusgasen är koldioxid (CO_2) som bildas vid förbränning av fossila bränslen som kol och olja i till exempel kolkraftverk eller bilar. En metod att minska utsläppen av koldioxid är att fånga in den vid utsläppskällan och lagra den i geologiska formationer. Salina akviferer är den geologiska formation som anses ha störst potential för lagning av CO_2. Sprucket kristallint berg är en formation som inte har undersökts tidigare då det oftast är poröst material som är av intresse.

TOUGH2 är en numerisk modell utvecklad vid Lawrence Berkeley Laboratory i USA för simuleringar av multikomponent och flerfas-flöden i sprucket och poröst material. Flödesmodulen ECO2N är framtagen för att användas tillsammans med TOUGH2 vid simulering av geologisk lagring av CO_2 i salina akviferer.

Simuleringar har genomförts av lagring av CO_2 i en teoretisk sprickzon i kristallint berg samt i en salin akvifer belägen i Skåne, Sverige. Simuleringarna av akviferen har genomförts med hjälp av fältdata från en undersökningsbrunn i Malmö. Slutsatserna som kan dras från arbetet är att lagring av CO_2 i sprucket kristallint berg eventuellt är möjligt men att nyttan av lagringen möjligen kan vara begränsad då projekten blir småskaliga och risken för läckage är betydande. Vid läckage blir en del av den injicerade plymen kvar som immobil, residual mättnad vilket innebär att lagring av CO_2 ändå sker. Den salina akviferen förefaller vara en möjlig lagringplats, dock krävs ytterligare undersökningar och simuleringar för att kunna dra säkra slutsatser och för att ett lagringsprojekt skall kunna genomföras.

PREFACE

This master thesis is part of my MSc degree in Aquatic and Environmental Engineering program at Uppsala University. It covers 30 ECTS credits and Auli Niemi at the Department of Earth Sciences, Uppsala University has been the supervisor. I would like to thank her for all the help and feedback she has given me during my work with this thesis. I would also like to thank Christopher Juhlin for help with information about the fractured crystalline rock, and Mikael Erlström at SGU for all help with the Composit log for the saline aquifer. Tanks go also to Eon for providing the data from the Malmö aquifer.

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Matilda Einemo

POPULÄRVETENSKAPLIG SAMMANFATTNING

Utsläpp av växthusgaser och klimatförändringar har fått stor uppmärksamhet i media under de senaste åren. Både allmänhet och makthavare blir mer och mer medvetna om problematiken och vikten av att agera snabbt i frågan. Den viktigaste växthusgasen är koldioxid (CO_2) som bildas vid förbränning av fossila bränslen som kol och olja i till exempel kolkraftverk eller bilar. En metod att minska utsläppen av koldioxid är att fånga in den vid utsläppskällan och lagra den i geologiska formationer djupt ner i marken. Detta är en metod som bara fungerar för stora, stationära utsläppskällor och är inte något som kan appliceras på transportsektorn.

De geologiska formationer som brukar nämnas i samband med koldioxidlagring är uttjänta olje- och gasfält, obrytbara kollager och salina akviferer. Det mest använda alternativet är oljefält där denna typ av projekt har bedrivits länge på grund av att injektion av CO_2 kan öka uttaget av olja. Fokus har då legat på ökad oljeproduktion och inte lagring av koldioxid, men tekniken är densamma. Salina akviferer är det alternativ som anses ha störst potential. En salin akvifer utgörs ofta av sedimentära bergarter med hög porositet och hög permeabilitet, till exempel sandsten. I södra Sverige, Skåne med intilliggande vatten, finns det sedimentär bergart där förekomsten av akviferer gör området intressant för lagring av CO_2. Ett alternativ som också kan vara av intresse i Sverige men som inte tidigare undersökts är lagring av koldioxid i sprucket kristallint berg. För att en plats skall vara lämplig för injektion av CO_2 finns det några grundläggande krav. Till exempel bör injektionen ske på större djup än 800 m för att garantera att den injicerade koldioxiden är i flytande form, vilket ökar lagringsförmågan. Oavsett i vilken typ av geologisk formation man lagrar koldioxiden är det av yttersta vikt att det finns ett tätt lager ovanför som kan fungera som lock över formationen. Flytande CO_2 är lättare än vatten och kommer därför att stiga uppåt och om det inte finns något tätare lager som hindrar stigningen kommer koldioxiden så småningom att läcka ut. Vid injektion ökar trycket i formationen och det är även viktigt att bevaka detta så att inte en alltför stor tryckökning uppstår.

Detta arbete utgörs av simuleringar av CO_2-lagring dels i en teoretisk sprickzon med egenskaper som är typiska för svenska förhållanden, dels i en akvifer i Skåne. I sprickzonsimuleringen antas dels en helt horisontell zon och dels en zon med en lutning på 3°. Simuleringen av akviferen genomfördes med hjälp av mätdata från en undersökningsbrunn i Malmö hamn som borrats med syfte att undersöka möjligheterna för bergvärme. Alla simuleringar gjordes för 50 år med injektion av CO_2 under de första två åren.

Simuleringarna av sprucket kristallint berg genomfördes med en låg injektionshastighet för att inte CO_2-plymen skulle få för stor lateral spridning eller för stor tryckökning. Trots detta läckte CO_2, främst löst i vattenfasen men även som CO_2-fas, in i det täta lagret av intakt berg. Detta var förvånande då den erhållna tryckökningen inte var större än vad som borde vara acceptabelt. Eftersom sannolikheten att en sprickzon skall vara helt horisontell är väldigt liten genomfördes samma injektion även i en lutande sprickzon. Resultaten visar att den injicerade koldioxiden rör sig snabbt uppåt på grund

av densitetsskillnaderna och redan efter tio år har en stor del av plymen försvunnit ut ur systemet. Kvar blir den CO_2 som hunnit lösa sig i vattenfasen samt residualmättnad av CO_2-fasen. Residualmättnad är den lägsta mättnadsgrad som kan nås genom fri dränering och vid residualmättnad är CO_2-fasen immobil. Simuleringarna indikerar att det är osannolikt att geologisk lagring av koldioxid i sprucket kristallint berg är ett möjligt alternativ utan att läckage uppstår. Men trots läckage lagras dock en del av den injicerade koldioxiden eftersom residualmättnad av CO_2-fasen finns kvar i sprickzonen. Injektionen måste vara småskalig och en stor del av den injicerade koldioxiden förefaller kunna läcka ur reservoaren vilket gör det tveksamt om nyttan med ett dylikt projekt uppväger kostnaderna.

Malmö-akviferen har både högre permeabilitet och porositet än sprickzonen och därför kan en högre injektionshastighet användas här. Då akviferen är uppbyggd av flera sandstenslager separerade av lersten kördes simuleringen för det lager som har högst permeabilitet och omkringliggande lersten. Simuleringarna indikerar att CO_2 inte tränger igenom lerstenen inlagrad i akviferen vilket innebär att injektionsmängden blir något begränsad i jämförelse med om lerstenen inte skulle vara tät. Men akviferen förefaller kunna vara en bra plats för lagring av CO_2 och saken borde definitivt undersökas närmare. Simuleringarna bygger på information från enbart en brunn och det är troligt att injektion kan vara mer lämplig på annan plats i akviferen. Om ett svenskt projekt med geologisk lagring av CO_2 skall genomföras kan möjligen denna plats vara av intresse.

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1. INTRODUCTION

Climate change is a topic that has received a lot of exposure in media during the last years amongst other things as a consequence of IPCC receiving the 2007 Nobel Peace Prize. The general public is increasingly aware of the effects of greenhouse gas emissions and many governments and organizations have become involved in finding solutions. The most important contributor to the enhanced global warming is carbon dioxide (CO_2) produced by burning of fossil fuels. One of the possibilities considered in order to reduce emission of greenhouse gases enough is the capturing and geological storing of CO_2 (International Energy Agency, 2003). This is not a method that can be applied to the transport sector with its many small sources, but rather at large stationary sources of CO_2 such as fossil-fueled power plants. The CO_2 can there be separated and injected into deep geological formations such as saline aquifers, depleted oil and gas fields and coal seams (Cook, 2006).

Geological formations considered for storage of CO_2 commonly consist of sedimentary rocks. Crystalline rocks are usually not considered and thus the option of storing CO_2 in fractured bedrock has not been subject to any previous research. The option may however be of interest in Sweden due to the occurrence of useful fracture zones here. When it comes to porous media, sedimentary bedrock is especially interesting due to the occurrence of deep aquifers. In Sweden there are only two larger continuous areas with sedimentary bedrock that can be considered for CO_2 storage. One of those is located in south-west Skåne with adjoining sea and this area has already been the site of geological investigations due to search for gas and oil in the seventies (Lövgren, 2004). In the area around Malmö there are investigation wells that were drilled with the purpose to examine the possibility to use area in geothermal projects (Erlström, personal communication 2007).

The aim of this project is to simulate and assess the feasibility of storage of carbon dioxide in geological reservoirs using the model TOUGH2 with the fluid property module ECO2N. The simulations considered both the aquifer situated in Malmö and a theoretical fracture zone in a crystalline rock. The thesis starts with a literature study that will give a brief insight into the available options for geological storage of CO_2, the required reservoir properties and problems associated with storage. The study will also function as a base for determining if the results from the simulation runs are enough to decide whether or not the site is suitable for injection.

2. GEOLOGICAL STORAGE OF CO_2 - A REVIEW

2.1. GEOLOGICAL RESERVOIRS

2.1.1. Depleted oil and gas fields
The storage possibility that is the most well known and has been used in most cases is injections of CO_2 into depleted oil or gas fields. It has been ongoing as enhanced oil

recovery (EOR) and enhanced gas recovery (EGR) operations long before the recent interest for CO_2 storage. These injection projects have developed as an option to increase the mobility of the oil or repressurize the gas reservoir and thus enhance the production. Much of the injected CO_2 does however remain in the reservoir when the operation is completed even though the main focus of these operations often is not to maximize the CO_2 storage. The main advantage of these operations as a way of reducing CO_2 emissions is that the cost of the injection can be balanced by the profits from an increased oil or gas output. Both gas and oil fields also have another economic advantage in the fact that the reservoir properties often have been extensively characterized during the production of oil and gas. It is therefore often not necessary with further expensive geological investigations in order to decide whether or not the site is appropriate for storage of CO_2 (International Energy Agency, 2003). EGR has so far not been applied to the same extent as EOR (International Energy Agency, 2004).

2.1.2 Unmineable coal seams
Injection of CO_2 into unmineable coal seams is an alternative for geological storage that is under development but still a great deal of research is needed. Enhanced coal-bed methane recovery (ECBM) has been discussed for some time although it is still a speculative method and it can only be applied to unmineable coal seams with high enough permeability. The coal matrix tends to swell due to injection of CO_2, which reduces permeability and makes this method difficult. There are some demonstration projects in progress but it is still some way to go before a decision can be made on whether this is an acceptable option for geological storage (International Energy Agency, 2004). One of the interesting aspects of unmineable coal seams as storage sites for CO_2 is that the injected CO_2 is considered to be trapped in the coal by sorption to the coal surface and physical trapping within the coal. That implies that if the coal is never mined the CO_2 will remain in the coal deposit forever, at least in theory. In some regions this type of geological storage can be an important alternative. The coal seams do however not offer enough storage capacity to have any significant impact on a global scale (Gale, 2004).

2.1.3. Deep saline aquifers
The storage option that is considered to have the largest potential is deep saline aquifers and it is one of the most interesting options based solely on the large possible storage volume. There is ongoing research in order to determine how large the storage potential is in saline aquifers (Gale, 2004). The cost for storage of CO_2 in saline aquifers is higher than for storage in oil and gas fields since for saline aquifers as often thorough geological investigations prior to injection are needed (Cook, 2006). Storage in saline aquifers has not been in use as long as EOR operations, but there is much ongoing research and one important project is the Sleipner Demonstration Project. At the Sleipner gas field in the North Sea, CO_2 has been injected into a saline aquifer 1000 m below the sea bottom since 1996 and ten years into the project about 8 million ton CO_2 had been injected. The project was undertaken with the sole purpose to reduce the release of greenhouse gases and was the first industrial project of its kind (NGU, 2007). Another interesting pilot project is Vattenfall's Schwarze Pumpe in north-east German where Vattenfall is building a pilot-scale power plant that is expected to function by 2008. The main focus is to validate and further develop technology around capturing CO_2 and the captured gas will be injected into saline aquifers at depths of about 1500 m (NGU, 2007).

2.1.4. Fractured crystalline rock

The possibility of geological storage of CO_2 in fractured rock has not been investigated earlier and hence there is very little information available on the subject. The option is interesting and research on the subject is needed. In Sweden frequently occurring fracture zones are expected to have a thickness of 10-20 m and might provide an alternative for small scale operations (Juhlin, personal communication 2007).

2.2. STORAGE

The main storage mechanisms for CO_2 in reservoir rock are *structural/stratigraphical trapping*, *residual saturation trapping*, *dissolution trapping* and *geochemical trapping* (NGU, 2007). The *structural and stratigraphical trapping* occurs when the upwards migration of CO_2 is prevented by barriers with low permeability e.g. layers of mudstone. *Residual saturation trapping* is when some of the injected CO_2 remains trapped in the rock matrix due to capillary forces. *Dissolution trapping* occurs when the CO_2 dissolves into the formation water and becomes trapped. *Geochemical trapping* takes place when the injected CO_2 reacts with the minerals and the native fluid to form solid minerals or aqueous complexes dissolved in the water. This is a very slow process and it can be ignored as a significant trapping mechanism unless the time perspective is hundreds to thousands of years. Geochemical trapping is desirable since the injected CO_2 will be permanently trapped in the reservoir. To some extent mineral trapping can be expected, but it does not contribute significantly to the storage in sandstone or carbonate reservoirs (Gale, 2004).

Another important aspect of storage is the nature of the reservoir boundaries (NGU, 2007). These greatly affect the storage capacity of the reservoir and needs therefore to be considered. In an aquifer with perfectly sealed non-elastic boundaries only very little CO_2 can be stored since the only volume available for storage is the one created by compression of water and rock.

Beside the occurrence of a geological reservoir with suitable properties for CO_2 storage there is also a need for a geographical match between the storage site and emission source in order for the storage to be viable. It is not practical to transport the CO_2 large distances and research on the topic of correlating potential storage sites with areas of large emissions is therefore underway in North America, North Western Europe and Japan (Gale, 2004).

2.3. SITE CHARACTERIZATION

Site characterization is made by collecting and analysing surface and subsurface data with the aim to judge whether or not a site will store a certain quantity of CO_2 for a long period of time without compromising the health, safety and environmental standards (Cook, 2006). One of the fundamental geological requirements is the presence of a large enough formation with high permeability. The depth of the formation is commonly required to be greater than 800 m to ensure that the injected CO_2 remains in dense form (Friedmann, 2006). Compared to storage of CO_2 in a gaseous state, storage as supercritical CO_2 or as a liquid improves the storage efficiency considerably (NGU, 2007). To avoid vertical migration of CO_2 the reservoir needs to be capped by a formation with low permeability and ideally there is also a seal underlying the storage site (Friedmann, 2006).

When characterizing a site for storing CO_2 there are three important criteria of the system that must be fulfilled for an injection program to succeed. These criteria are

called the ICE framework and it includes the reservoirs injectivity, capacity and effectiveness (Friedmann, 2006).

2.3.1. Injectivity

The injectivity describes how high injection rate can be maintained over long intervals of time. Injectivity depends on properties like bulk connectivity and permeability. Other important aspects are down-hole pressure and effective thickness over the injection point (Friedmann, 2006). The most important property affecting injectivity is the absolute permeability of the rock. Irrespective of porosity the injected amount of CO_2 increases nearly linearly with the reservoir permeability (Law & Bachu, 1996).

2.3.2. Effectiveness

The effectiveness of a reservoir is the formation's ability to store CO_2 under long periods of time. To characterize the effectiveness of a reservoir approximations of seal integrity and geomechanical and hydrodynamic properties of the rock are required. Capillary entry pressure and fault reactivation potential are also aspects that need to be considered. Important issues will include mapping of potential fast-paths out of the reservoir, description of subsurface heterogeneity and geomechanical characterization (Friedmann, 2006).

Densities of pure CO_2 at the depths of interest for geological storage are in the range of 0.3-0.8 times the density of water. After injection into a water-filled reservoir the CO_2 will thus migrate upwards due to buoyancy forces. One important issue when ensuring a reservoir's effectiveness is therefore the properties of the reservoir seal. When the CO_2 is rising towards the surface due to buoyancy it places a pressure drop across the seal. Capillary entry pressure of the intact rock needs to be able to resist any expected pressure drop due to the injection or buoyancy driven accumulation of CO_2 to ensure the integrity of the seal (NGU, 2007). The capillary entry pressure is inversely proportional to the radius of the pore throat and if the CO_2 does not overcome that entry pressure, no flow will occur. A proper reservoir seal should thus have small pore throats (Christopher & Iliffe, 2006). The cap rock should not be rich in carbonates since dissolution of carbonate rich layers could cause reduction of the sealing capacity, creating pathways for the CO_2 past the cap rock. Analysis of mineralogy and capillary entry pressure is thus important in characterizing the properties of the seal (NGU, 2007).

2.3.3 Capacity

The storage capacity is the volume of CO_2 that potentially can be stored in the formation. This is a property that can be difficult to estimate since the effective volume depends on reservoir heterogeneity. Also the amounts of CO_2 stored in dissolved phase, trapped residual phase and trapped buoyant phase influence the volume of CO_2 that can be stored in a reservoir (Friedmann, 2006). Since the nature of the boundaries also affects the storage capacity it is important to take these into account as well. If the formation water cannot be displaced only very little CO_2 can be injected into the reservoir (NGU, 2007). To properly evaluate the storage capacity there is need for a considerable quantity of reservoir information and numerical simulations can be useful when it comes to estimate the achievable CO_2 saturation, dissolution and the residual saturation. Numerical simulations can also be an important method when reviewing pressure constraints (NGU, 2007).

There can be some undesirable effects that will limit the quantity of injected CO_2 before the theoretical maximum storage capacity is reached. Such effects include rise in

reservoir pressure towards the capillary entry pressure of the seal and migration of saline formation water or CO_2 into fresh-water supplies or other areas where it is not wanted (NGU, 2007). In cases where the boundary conditions allow rapid displacement of formation water the pressure build up will have less impact than on a closed reservoir (NGU, 2007). A rule of thumb is that the pressure should not rise to more than 1.6 times the original hydrostatic pressure. (Lund & Zoback, 1999)

The volume fraction of the reservoir pore space that can be filled with CO_2 is one of the greatest uncertainties in storage estimation. It depends not only on the heterogeneity and the structural geometry but also on the effort undertaken to achieve high saturations (NGU, 2007).

2.4. HEALTH, SAFETY AND ENVIRONMENTAL RISKS

When storing supercritical CO_2 for geological timescales, there is a possibility that it could migrate out of the reservoir. It is however not easy to assess the environmental consequences without knowing the CO_2 flux (Gale, 2004). A leakage of CO_2 as a sudden release from a geological storage site is a most unlikely event. This should be prevented by comprehensive geological investigations of the site before injection and if there is a risk of sudden release the site should not be used for storage (NGU, 2007).

It is more likely that CO_2 reaches the surface through small-scale leakage that could result in different impacts depending on where it takes place. On-shore there can be accumulations of CO_2 in depressions in the ground or in basements of buildings that are harmful to humans and animals. Naturally occurring accumulations of this kind can take place as a result of volcanic activity (Gale, 2004). CO_2 is a non-toxic gas but it can still be dangerous to humans and animals if it reaches concentrations above 10% by volume since it can cause suffocation. In the subsurface, even small fluxes of CO_2 will have a harmful effect on flora and fauna since the poor mixing of soil air quickly results in dangerous concentrations. If carbonated ground water leaks it can cause damage to foundations of buildings and destroy historical buildings or archeological sites (NGU, 2007).

When CO_2 leaks into the ocean it causes changes in pH on a local scale that can possibly affect the marine ecosystem (Gale, 2004). The CO_2 that does not dissolve into the ocean water will quickly escape to the atmosphere. This situation does not result in any great risks unless perhaps possibly if humans are located directly above the leakage (NGU, 2007).

There are also risks that are not directly related to an actual leakage of CO_2, there can be geomechanical effects by injections that can cause damage. Reactivation of existing faults in the cap rocks could cause shallow earthquakes. This has happened during production of natural gas in several countries and anthropogenic induced earthquakes due to production of natural gas in The Netherlands have reached magnitudes of 3.5 on the Richter scale. CO_2 storage can also cause non-seismic deformation that can damage buildings and an uplift of the earth's surface could shift streams in lowland areas. Mudflows, sinkholes at the surface and saline water intrusion in fresh water aquifers are also possible effects of CO_2 storage (Gale, 2004).

3. TOUGH2/ECO2N

3.1. TOUGH2

The TOUGH (Transport of Unsaturated Groundwater and Heat) (Pruess et al, 1999) family of models solves conservation of mass and conservation of energy equations. Fluid advection is expressed by an expansion of Darcy's law and both advection and diffusion are considered in the calculation of fluid fluxes. Transport of heat is assumed to occur through both conduction and convection. The governing equations for the fluid and heat flow can be found in appendix 1.

TOUGH2 (Pruess et al, 1999) is a numerical model that has been developed at Lawrence Berkeley Laboratory in USA. It is developed for simulations of multi component and multiphase flow simulations in porous and fractured media and it is capable of simulating one, two or three dimensions. It can be used for geothermal reservoir engineering, studies involving isolation of nuclear waste, environmental assessments and simulation of transport and flow in media at different levels of saturation. It is written in FORTRAN77 and was originally launched in 1991 but has been updated since then. The TOUGH2 program is composed of several functional units. Regardless of the components present and the nature and number of fluid phases, the governing equations for fluid and heat flow have the same form. This allows the flow and transport modules of TOUGH2 to be used together with different modules that express fluid properties. It is thus possible to choose the fluid property module that best suits the scenario to be simulated. This model architecture was in the eighties used in MULKOM, which laid the foundation for the TOUGH family of models.

The time and space variables have to be discretised in order to solve the equations numerically. In the TOUGH family of models the space discretisation is not made from partial differential equations but directly from the integral form of the conservation equation. This method has the advantage of being able to do regular or irregular discretisations in one, two or three dimensions. First-order backward finite difference is used to discretise the time. The result is a set of coupled nonlinear algebraic equations where the time dependent variables are unknown in every gridblock. The equations are all solved with Newton-Raphson iterations and in order to receive an efficient solution the time steps are automatically adjusted during a simulation. The change made at a time step is depending on the convergence rate of the iteration process. If the program does not succeed to calculate the thermo physical parameters, fail to solve the linear equations or does not converge within a given number of iterations the increase in time, Δt, will be reduced and the same time step will be repeated. The simulations will continue until one of the termination criteria is fulfilled. These can be user specified like maximum number of time steps or a particular simulation time. They can also be predestined in the model such as the criteria that if a simulation achieves convergence on the first iteration for ten consecutive steps, the program takes this as an indication of steady state and the execution will be terminated. The latter termination criteria can also be satisfied when the initial time step is chosen so small that the convergence tolerance are fulfilled without any updating of thermodynamic variables.

3.1.1. Relative permeability and capillary functions

There are several options in TOUGH2 for calculating relative permeability and capillary functions. In this thesis only the van Genuchten-Mualem model is used to describe the relative permeability function (van Genuchten, 1980; Mualem, 1976)

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$$k_{rl} = \sqrt{S^* \left\{ 1 - \left(1 - \left[S^* \right]^{1/\lambda} \right)^{\lambda} \right\}^2} \qquad \text{if } S_l < S_{ls} \qquad (1)$$

$$k_{rl} = 1 \qquad\qquad\qquad\qquad \text{if } S_l \geq S_{ls} \qquad (2)$$

and

$$k_{rg} = 1 - k_{rl} \qquad\qquad\qquad \text{if } S_{gr} = 0 \qquad (3)$$

$$k_{rg} = \left(1 - \hat{S} \right)^2 \left(1 - \hat{S}^2 \right) \qquad \text{if } S_{gr} > 0 \qquad (4)$$

Where

$$S^* = \left(S_l - S_{lr} \right) / \left(S_{ls} - S_{lr} \right) \qquad (5)$$

$$\hat{S} = \left(S_l - S_{lr} \right) / \left(1 - S_{lr} - S_{gr} \right) \qquad (6)$$

The van Genuchten (1980) characteristic curves are used to describe the capillary pressure functions:

$$P_{cap} = -P_0 \left(\left[S^* \right]^{-1/\lambda} - 1 \right)^{1-\lambda} \qquad (7)$$

where:

$$\frac{1}{P_0} = \frac{\alpha}{\rho_w g}$$

and:

$$-P_{max} \leq P_{cap} \leq 0$$

k_{rl} = relative permeability for aqueous phase
S_l = saturation of aqueous phase
S_{ls} = saturation of aqueous phase at fully saturated conditions
S_{lr} = residual saturation of aqueous phase
k_{rg} = relative permeability for CO_2-phase
S_l = saturation of CO_2-phase
S_{ls} = saturation of CO_2-phase at fully saturated conditions
S_{lr} = residual saturation of CO_2-phase
ρ_w = density of water, kg/m^3
g = acceleration due to gravity, m/s^2
λ = van Genuchten-Mualem parameter, m
α = van Genuchten parameter, 1/kPa

3.2 ECO2N

ECO2N is one of the modules describing fluid properties that can be used with TOUGH2. It is developed for simulation of geological storage of CO_2 in saline aquifers and contains descriptions of thermodynamic and thermo physical properties of mixtures with CO_2, H_2O and NaCl. When using ECO2N it is assumed that the fluids compose a two-phase system with one aqueous phase and one CO_2-rich phase, but it is possible to run simulations with only one phase present. During the calculations partitioning of H_2O and CO_2 between the phases takes place and a possible precipitation of halite with associated reductions in permeability and porosity is accounted for (Pruess, 2005). In the rest of this thesis these phases will be termed CO_2-phase and aqueous phase.

The module ECO2N (Pruess & Spycher, 2007) is an improvement of earlier modules designed for application to geothermal reservoir engineering. The main developments in ECO2N are that this module includes accurate descriptions of density, viscosity and specific enthalpy of CO_2 at the pressures and temperatures that will prevail at large depths. During the same temperature and pressure conditions this module also has a correct representation of thermophysical properties of brines and accurate partitioning of H_2O and CO_2 between the aqueous and CO_2 phases. ECO2N is however not able to distinguish between liquid and gaseous CO_2 and cannot model transitions between them. It is therefore not possible to use ECO2N for processes that involve two CO_2 phases. When using TOUGH2/ECO2N for modeling it accounts for single and multiphase flows with effects from capillary pressure and relative permeability as well as diffusion of all mass components. If not run in an isothermal mode the heat flow will include transport of sensible and latent heats, heat conduction and heat of dissolution effects. The user has the possibility to disable some processes; besides running in isothermal mode it is also possible to neglect diffusion and permeability change due to precipitation of halite.

4. MATERIAL AND METHOD

Injection of CO_2 was simulated with the numerical model TOUGH2/ ECO2N for two different cases of injection into crystalline bedrock and one case of injection into a saline aquifer. In the different scenarios simulations were run in three steps. The first run was done to obtain the boundary conditions and the second to attain the initial condition. The third and main simulation was run for fifty years with CO_2 injection during the first two years.

The capillary strength parameter α in the van Genuchten function for capillary pressure (equation 7) was determined with Leverett's (1941) scaling rule:

$$\frac{\alpha_{ref}}{\alpha} = \sqrt{\frac{K_{ref}}{K}} \tag{8}$$

Where α_{ref} is a reference value of α at saturated hydraulic conductivity, K_{ref}. The van Genuchten parameter λ was set to 0.457 in all scenarios since there was not enough information to vary this parameter. This value was chosen since it is used in the ECO2N user guide (Preuss, 2005) for simulations of both injection into a saline aquifer as well

as CO_2 migration through a fault zone. All simulations were run in isothermal mode without accounting for change in permeability due to precipitation of halite. The latter assumption was based on the low salinities in all simulations, much lower than brine, and therefore there will be little or no precipitation of halite. All simulations were run for slices of 1 m thickness and can therefore be considered as two-dimensional.

4.1 CRYSTALLINE BEDROCK

This scenario considered a fractured zone in crystalline rock overlaid by intact rock that could serve as a seal. Since the porosity and permeability are lower in fractured bedrock compared to a porous media the injectivity is also expected to be lower. The formation was situated at a depth of 1000 m. At these depths the water is expected to be saline and a salinity of 1.6% by weight was set to resemble conditions in Sweden at a site moderately far from the shore (Andersson et al, 2000; Byegård et al, 2006). The fracture zone was modeled as a homogenous matrix with hydraulic properties that were selected to represent a fractured crystalline rock typical for Sweden. The capillary strength parameters was obtained through scaling with eq 8 and K_{ref} was set to $5.7 \cdot 10^{-11}$ m/s and α_{ref} was chosen as $1.776 \cdot 10^{-3}$ from a faulted rock site (Rutqvist et al, 2006). The material properties are described in table 1.

Table 1: Material properties

Property	Fractured rock	Intact rock
Porosity	0.05^{*}	0.01^{**}
Permeability (m^2)	$4.68 \cdot 10^{-13*}$	$6.99 \cdot 10^{-17**}$
Irreducible gas saturation	$0.05^{\dagger}$	$0.05^{\dagger}$
Irreducible liquid saturation	$0.2^{\dagger}$	$0.2^{\dagger}$
van Genuchten parameter λ	$0.457^{\dagger}$	$0.457^{\dagger}$
van Genuchten parameter α	0.61	0.00744

* (Juhlin, personal communication 2007)

** (Niemi, personal communication 2007)

† (Pruess, 2005)

4.1.1. Crystalline bedrock, horizontal case

For the first scenario the fracture zone was 15 m thick, located at a depth of 1000 m and extending 4000 m in both directions from the injection point. Above and underneath the zone was intact rock that does not contain any fractures. The grid spacing was dense around the injection point and around the transitions from fractured to intact rock and coarser towards the boundaries. At the vertical boundaries a hydrostatic pressure profile was set as Dirichlet boundary condition to allow flow through the section. The injection took place in the middle of the fracture zone. An illustration of the conceptual model is shown in figure 1.
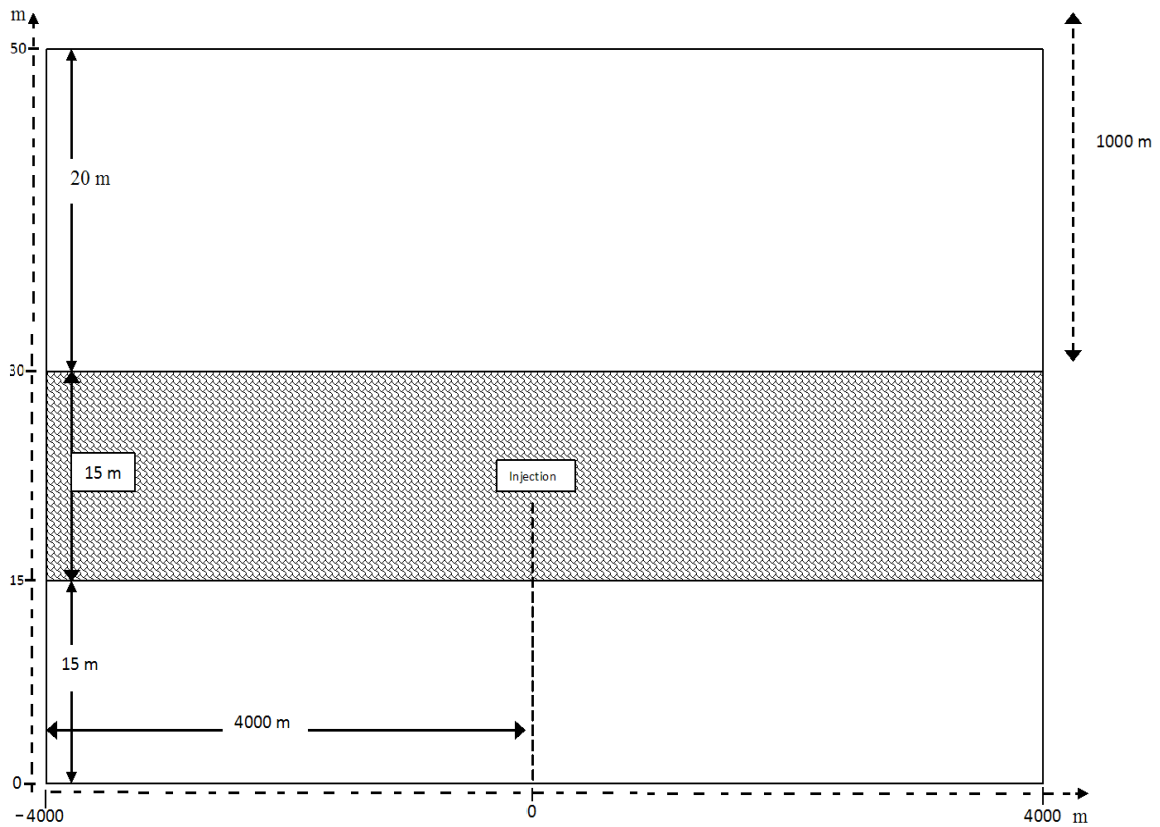
Figure 1 Illustration of the conceptual model of the horizontal fracture zone.

The injection causes pressure to rise in the formation, most evident and rapidly at the injection point. Since it was unknown which pressure increase that was acceptable without causing concern for geomechanical issues, the injection rate was set to a low value of about 315 ton per year or 0.01 kg/s. That is 1/30 of the injection in one 1 m slice of the horizontal injection well at Sleipner. In a well similar to the one at Sleipner this injection would be about 31.5 kton per year. Also the small thickness of the fracture zone forces the CO_2 to spread laterally and a high injection rate would generate an undesirable large CO_2 footprint.

4.1.2. Crystalline bedrock, sloping fracture zone

For the second scenario the profile was tilted so that the fracture zone had a slope of 3˚. As in the horizontal case there was intact rock without fractures above and underneath the fracture zone and all material properties were kept the same. An illustration of the sloping profile can be seen in figure 2. The injection rate was the same as for the horizontal case.
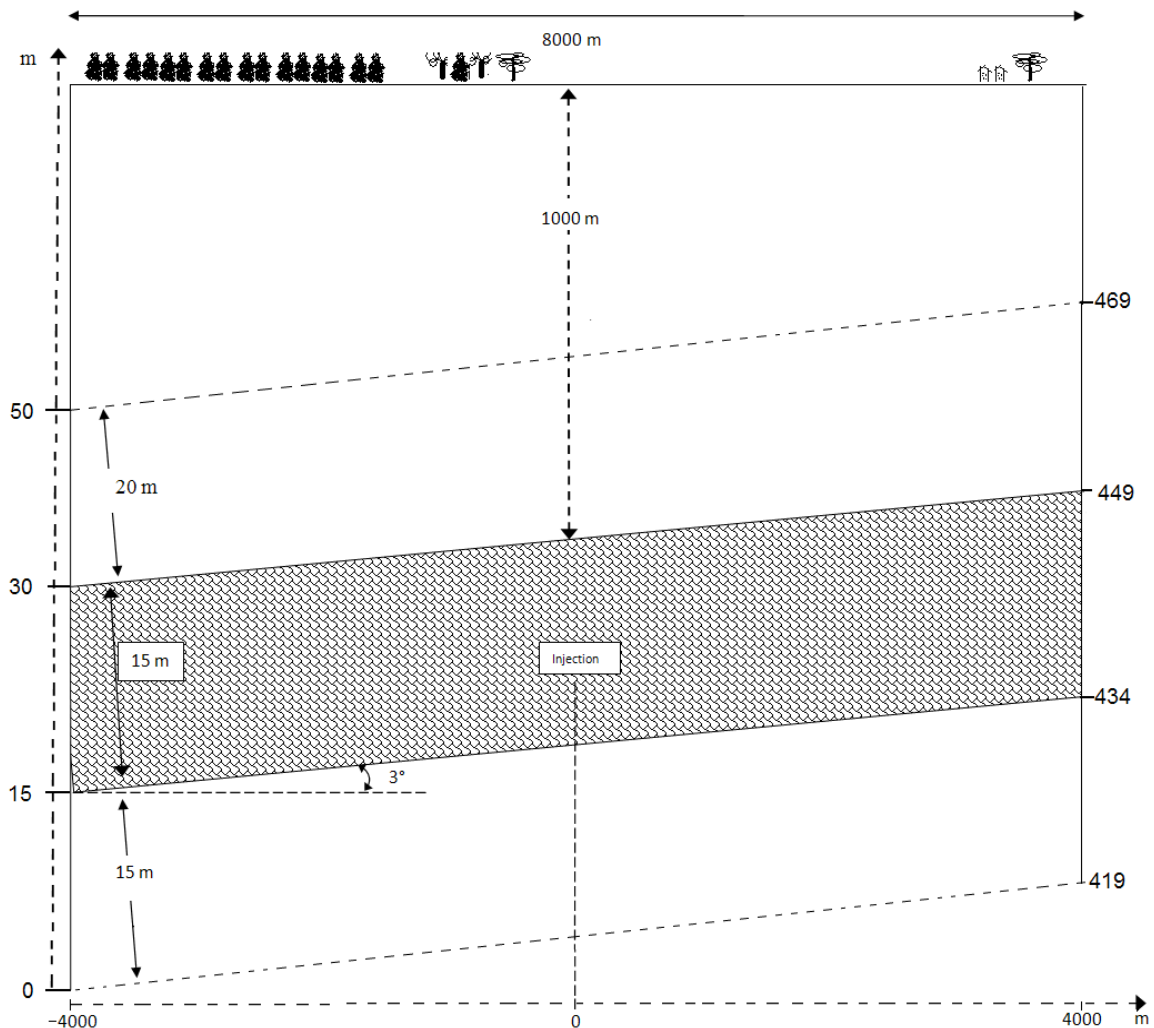
Figure 2 Illustration of the conceptual model of the sloping fracture zone.

The slope corresponds to a change in depth of about 5.24 m for a 100 m change in the horizontal direction.

4.2. DEEP SALINE AQUIFER

The aquifer in question is situated in Malmö harbor in south-west Sweden. All properties needed for the simulation were obtained from an investigation well in the area, with the exception of the van Genuchten parameters needed for the relative permeability and capillary functions. The latter had to be estimated based on a theoretical model. The aquifer is multilayered sandstone alternating with claystone and overlaid by a cap rock of dense limestone with high clay content. The horizontal permeability of the sandstone is slightly higher than the vertical due to layers of clay within the sandstone formation. The simulation was only run for the part of the aquifer with the highest permeability and the layers of claystone that are enclosing it. Figure 3 illustrates the upper part of the multilayered aquifer and the section of it that was included in the simulation. The injection rate was 0.1 kg/s for the 1-m thick section, which corresponds to about 1/3 of the injection in a 1-m section of the horizontal injection well at Sleipner. This means an injection of about 3.15 kton per year through the section or with an injection well similar to the one at Sleipner about 315 Mton per year.
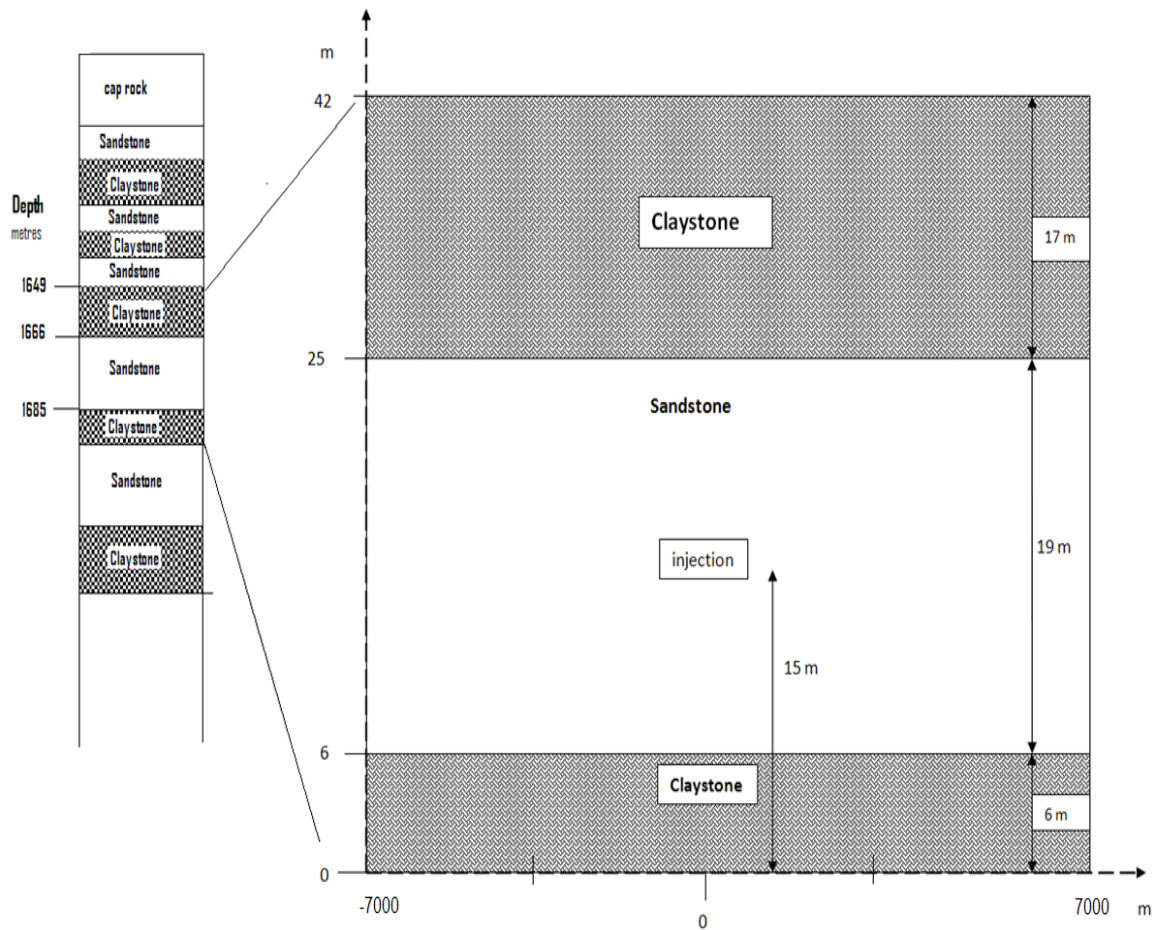
Figure 3 Illustration of the conceptual model of the aquifer.

The capillary strength parameters were determined through scaling with equation 8 and K_{ref} was set to $2.9 \cdot 10^{-5}$ m/s and α_{ref} was chosen as 2.73 (Pruess, 2005) from a layered aquifer. The salinity in the aquifer was set to 1.7 % by weight and the temperature at this section was 50 °C. The material properties are described in table 2.

Table 2 Material properties for the aquifer (Erlström, personal communication 2007) based on compiled data for Malmö boreholes.

Property	Sandstone	Claystone
Porosity	0.214	0.02
Horizontal permeability (m^2)	10^{-12}	10^{-16}
Vertical permeability (m^2)	$7 \cdot 10^{-13}$	10^{-16}
Irreducible gas saturation	0.05	0.05
van Genuchten parameter λ	0.457	0.457
van Genuchten parameter α	1.58	0.016
Irreducible liquid saturation	0.2	0.2

4.2.1. Sensitivity to changes in van Genuchten parameter α

In order to investigate how sensitive the simulations are to errors in the scaling parameter α, the simulation for the aquifer was run with variation of this parameter. The α corresponding to claystone was changed so that it instead of a permeability of 10^{-16} m^2 (see table 2) corresponded to a permeability of 10^{-15} m^2, which resulted in α = 0.0506, a value that was more than three times larger than the original α.

5 RESULTS

5.1 CRYSTALLINE BEDROCK, HORIZONTAL CASE

Two years after the injection start the CO_2 had spread more than 2000 m in each direction from the injection point. In figure 4 it can be seen that there at this point is no significant leakage of the CO_2 phase into the intact bedrock. Higher CO_2 saturations were located directly below the transitions from fractured bedrock to intact bedrock (located at 30 m in the coordinate system) and the highest saturation was to be found above the injection point. Five years after the injection start, three years after the end of the injection, the CO_2 had continued to migrate upwards (see figure 5) and the saturation of the CO_2 phase directly below the intact rock had increased even though there had been no additional injection. There was a small but visible amount of CO_2 that had entered the intact rock directly above the point of injection. Figure 6 illustrates the saturation of the CO_2 phase fifty years after the injection start. Here it can be seen that since the CO_2 was dissolving into the aqueous phase the saturation had started to decline. The leakage had also spread further in the horizontal direction but not as much in the vertical.
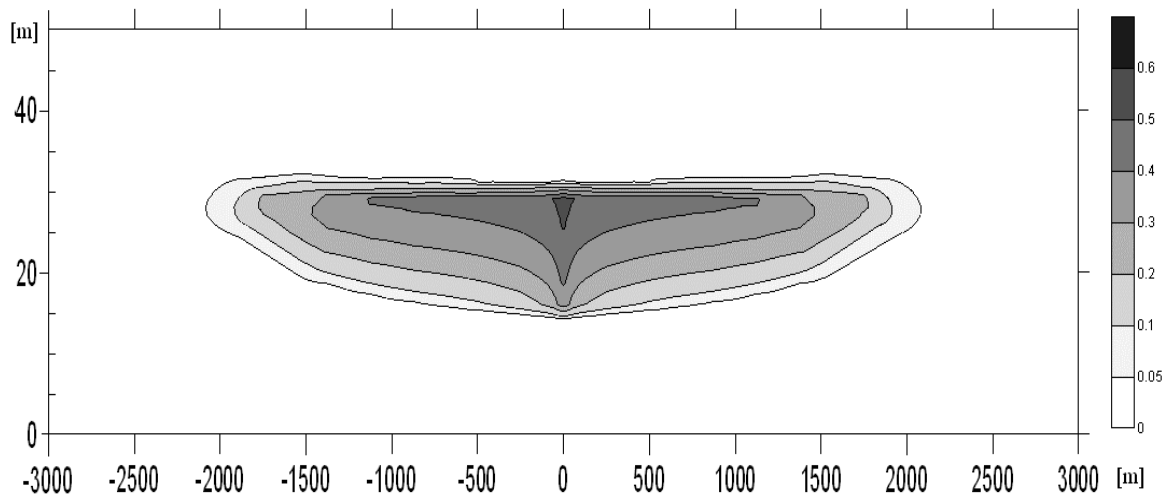
Figure 4 CO_2 saturation two years after the injection start in the horizontal fracture zone.
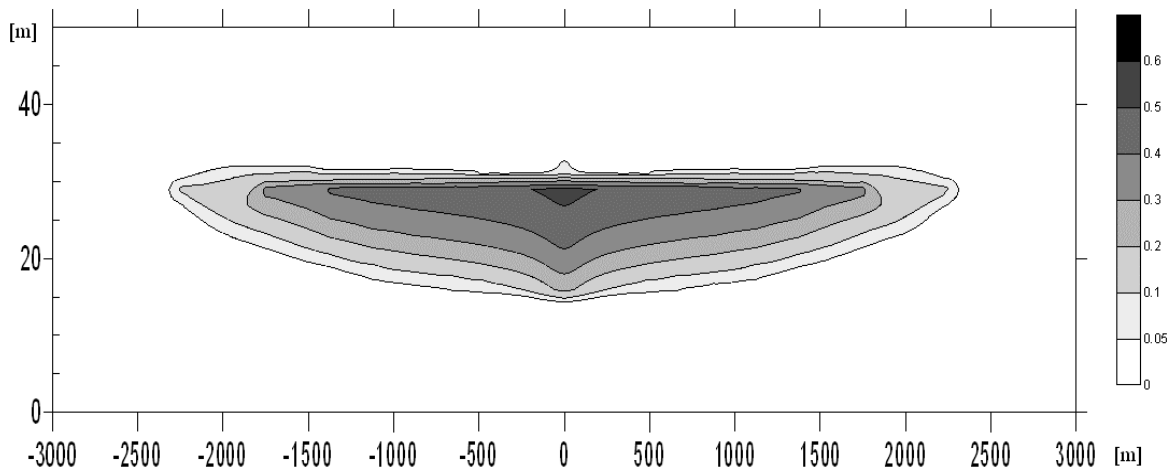

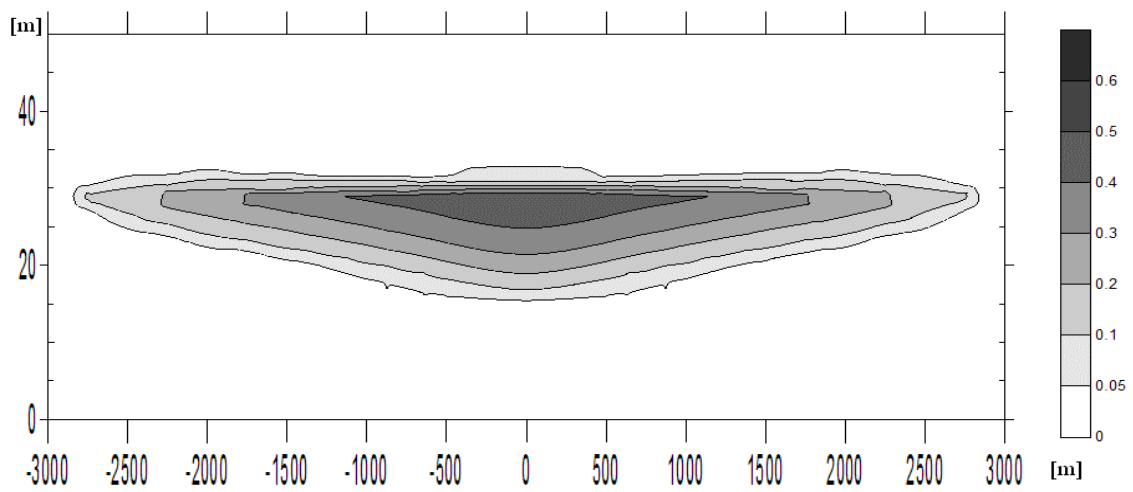**Figure 5** CO_2 saturation five years after the injection start in the horizontal fracture zone.

Figure 6 CO_2 saturation fifty years after the injection start in the horizontal fracture zone.

The aqueous phase containing dissolved CO_2 reached somewhat into the intact rock after two years. In figure 7 it can be seen that the leak was located directly above the point of injection. At this time leakage only occurred in the aqueous phase and there was no leak of CO_2 phase into the cap rock. CO_2 dissolved in the aqueous phase had after five years spread into the cap rock even further than directly after the injection (figure 8). It spread more in the vertical direction than the CO_2 phase, something that was even more apparent after fifty years (figure 9).

The pressure limit, 1.6 times the original hydrostatic pressure, is in this case about 16 MPa. After two years of injection the highest pressure in the profile is about 12.8 MPa and is thus well below the limit. The distribution of pressure in the profile two years after the injection start can be found in the appendix.
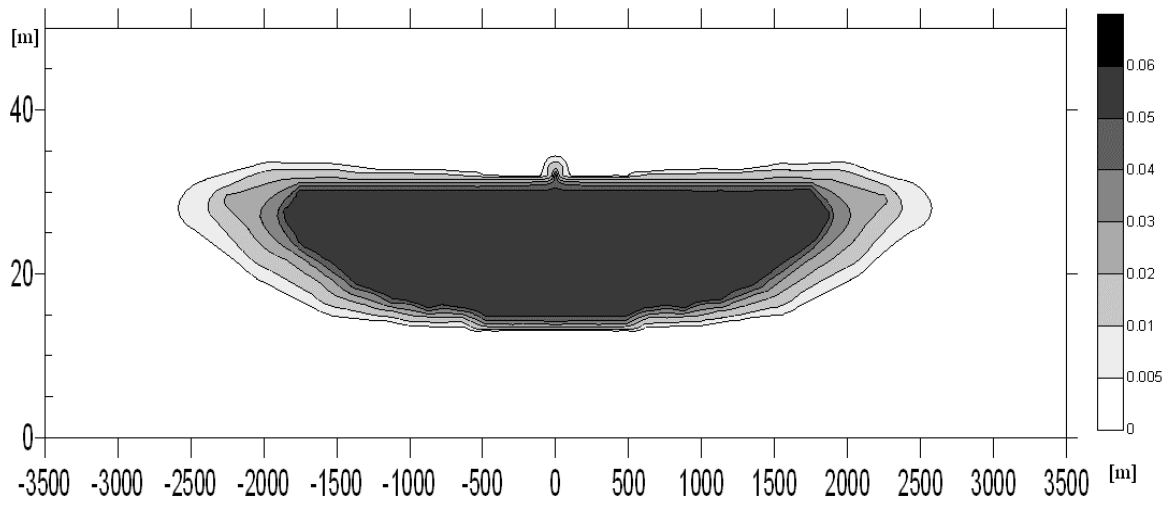
Figure 7 Mass fraction CO_2 dissolved in aqueous phase in the horizontal fracture zone, two years after the injection start.
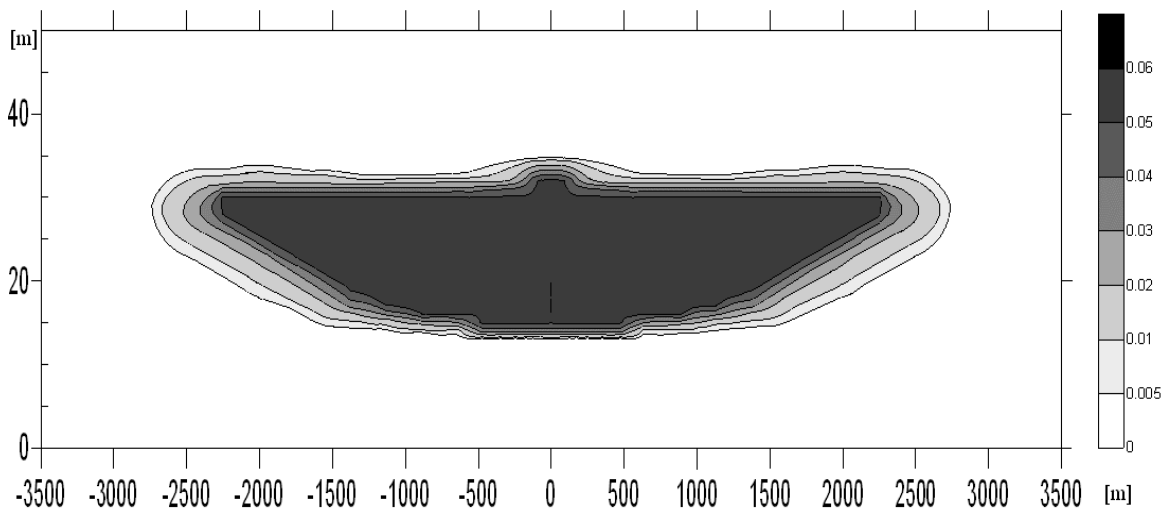
Figure 8 Mass fraction CO_2 dissolved in aqueous phase in the horizontal fracture zone, five years after the injection start.
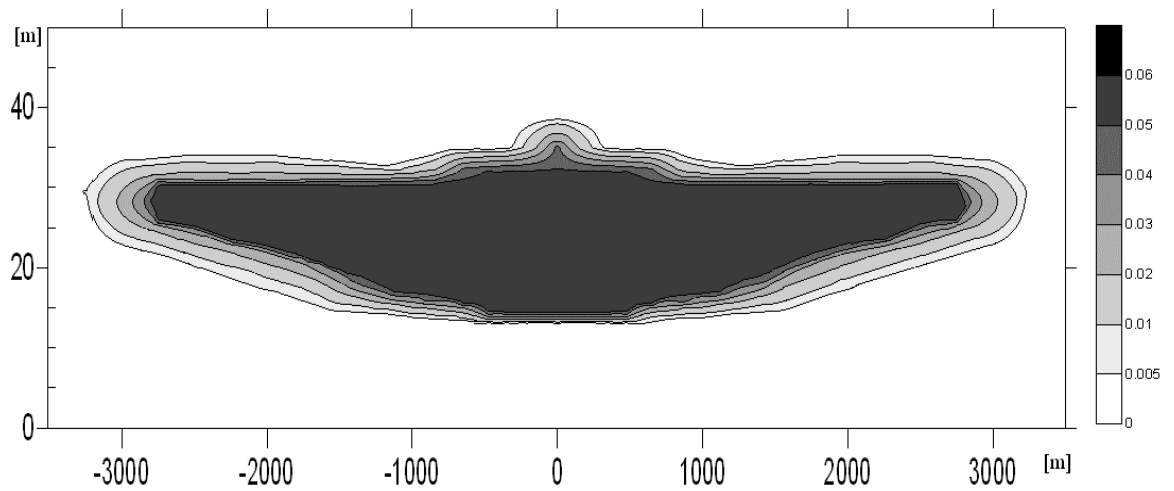

Figure 9 Mass fraction CO_2 dissolved in aqueous phase in the horizontal fracture zone, fifty years after the injection start.

5.2 CRYSTALLINE BEDROCK, SLOPING FRACTURE ZONE

When injected into a sloping fracture zone the CO_2 plume spread more up-slope than down-slope. The CO_2 phase saturation after two years is illustrated in figure 10 and there it can be seen that the plume had a horizontal spread on the upslope side that was about seven times larger than the spread on the down-slope side.
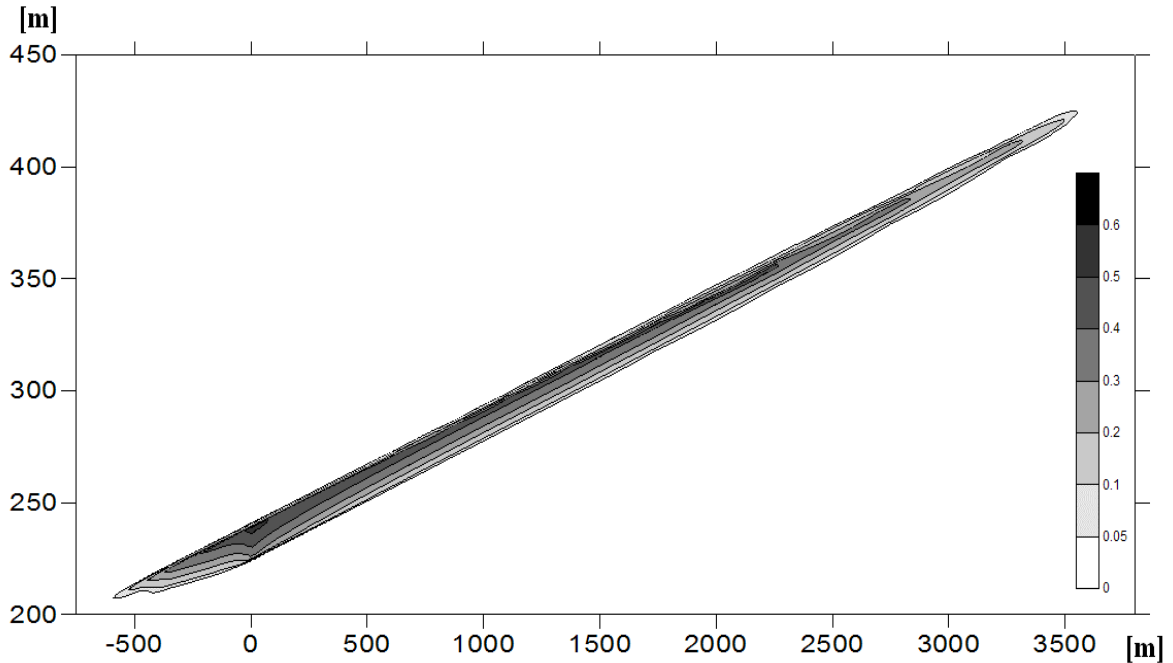
Figure 10 CO_2 saturation the sloping fracture zone, two years after the injection start.

Five years after the injection start, three years after the injection ended, the CO_2 plume had migrated upwards and was passing the boundaries of the system. The plume had partly migrated out of the system at this point and was leaving a trail of residual saturation behind (figure 11).
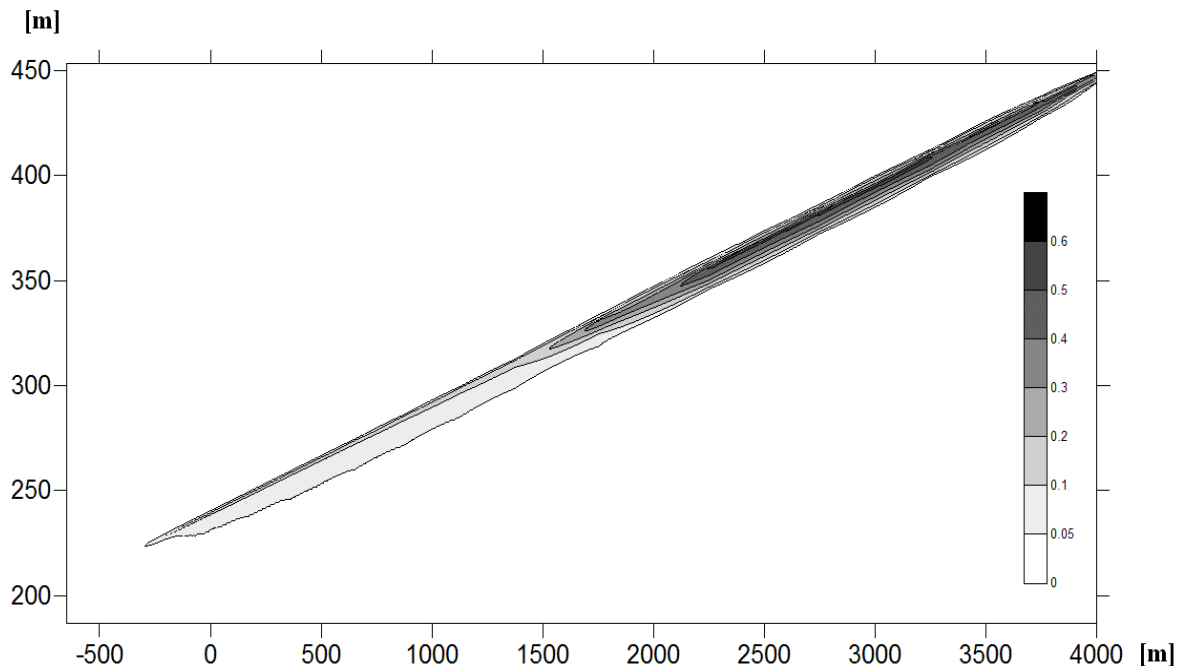

Figure 11 CO_2 saturation in the sloping fracture zone, five years after the injection start.

Ten years after the injection started most of the CO_2 plume had migrated out of the system (figure 12). The CO_2 dissolved in the aqueous phase did not migrate upwards in the way that the CO_2 phase did since it was not lighter than water. Instead the dissolved CO_2 remained in the system and the highest concentration of CO_2 dissolved in the formation water can be found in the lower part of the plume, see figure 13.

The entire plume did not disappear, however, but left a trail of residual saturation behind. The irreducible gas saturation was in the simulation set to 0.05 (table 1). In the 4000 m upslope of the injection point the fracture zone had a total volume of 63144 m^3. The remaining irreducible saturation in that volume should be about 158 m^3 CO_2. From figures 11 and 12 it however appears that saturation has at parts of the fracture zone fallen below the residual saturation. This may be due to that some of the CO_2 that remained as residual saturation has dissolved into the formation water thus reducing the saturation to levels below the residual saturation. As the limit for the lowest saturation visible in the figure is set to residual saturation it then appears as if the saturation is zero even in areas where it is slightly below residual saturation.
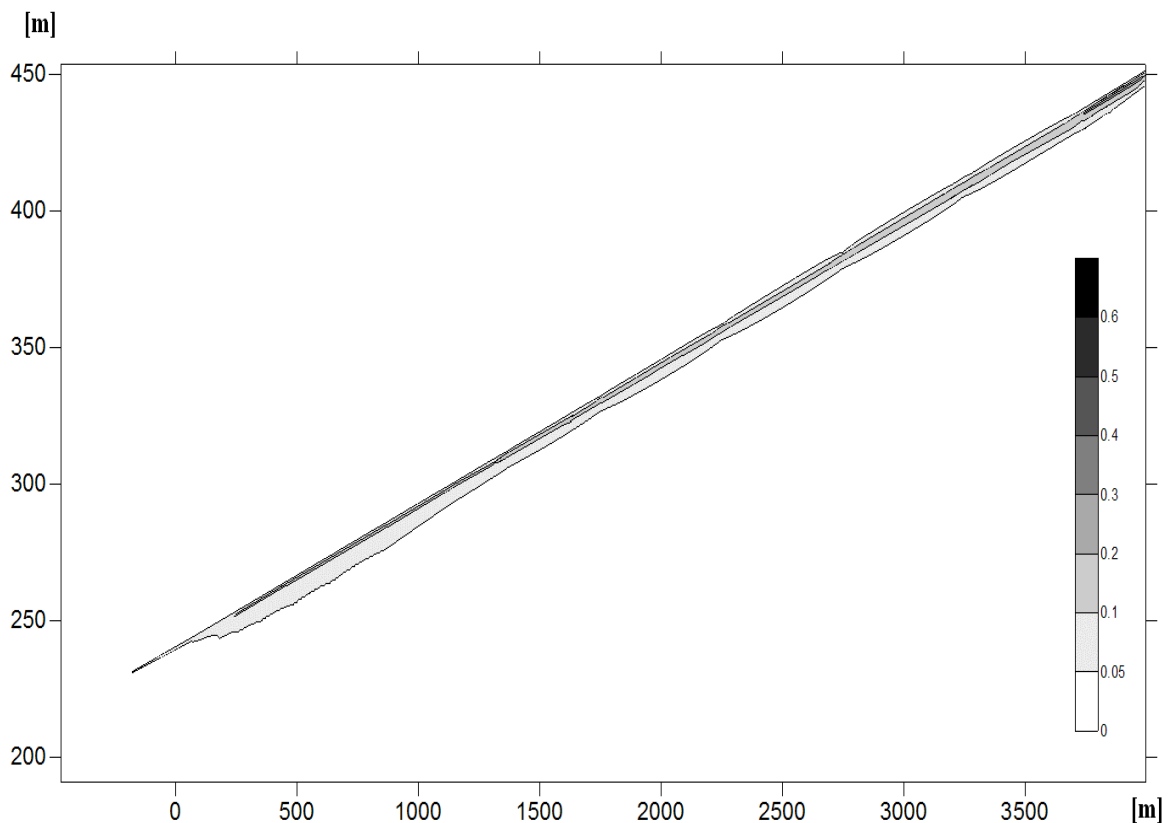

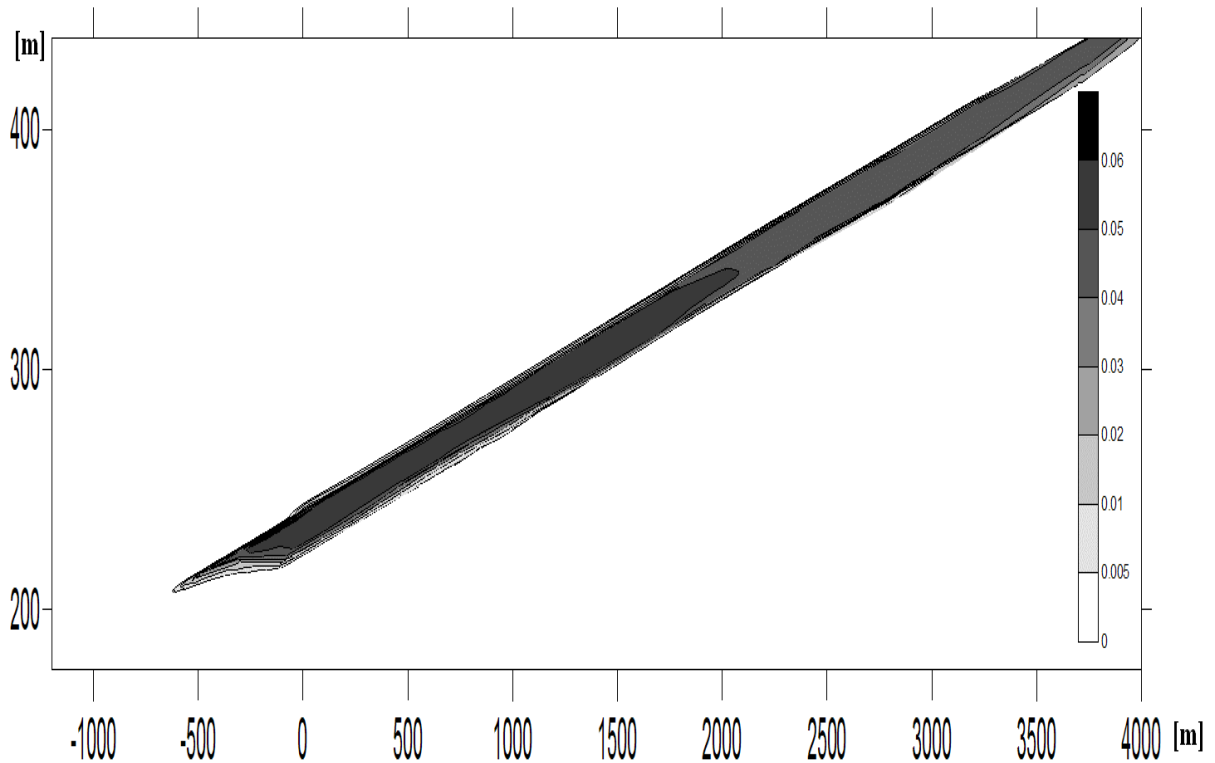**Figure 12** CO_2 saturation in the sloping fracture zone, ten years after the injection start.

Figure 13 Mass fraction CO_2 dissolved in the aqueous phase for the sloping fracture zone, ten years after the injection start.

5.3 DEEP SALINE AQUIFER

Two years after the injection start the CO_2 footprint extended about 2500 m in both directions from the injection point. The gas phase saturation was highest around the point of injection and also higher in the upper part of the sandstone layer. The overlying claystone extends from 25 m, and up to 42 m in the coordinate system and in figure 14 it can be seen that very little CO_2 had entered the layer of claystone after two years of injection. As in the horizontal case of crystalline bedrock it is apparent from figure 15 that the CO_2 migrated upwards and the saturation directly underneath the claystone was higher after five years than after two even though no further injection had been done. This was even more obvious after fifty years; the plume was spreading laterally, two years after injection start it reached 2500 m in each direction (figure 15) and fifty years from injection start it reached about 3800 m (figure 16).

The pressure limit, 1.6 times the original hydrostatic pressure, is in this case about 25.6 MPa. After two years of injection the highest pressure in the profile is about 28 MPa and is thus exceeding the limit. The distribution of pressure in the profile two years after the injection start can be found in appendix 2.
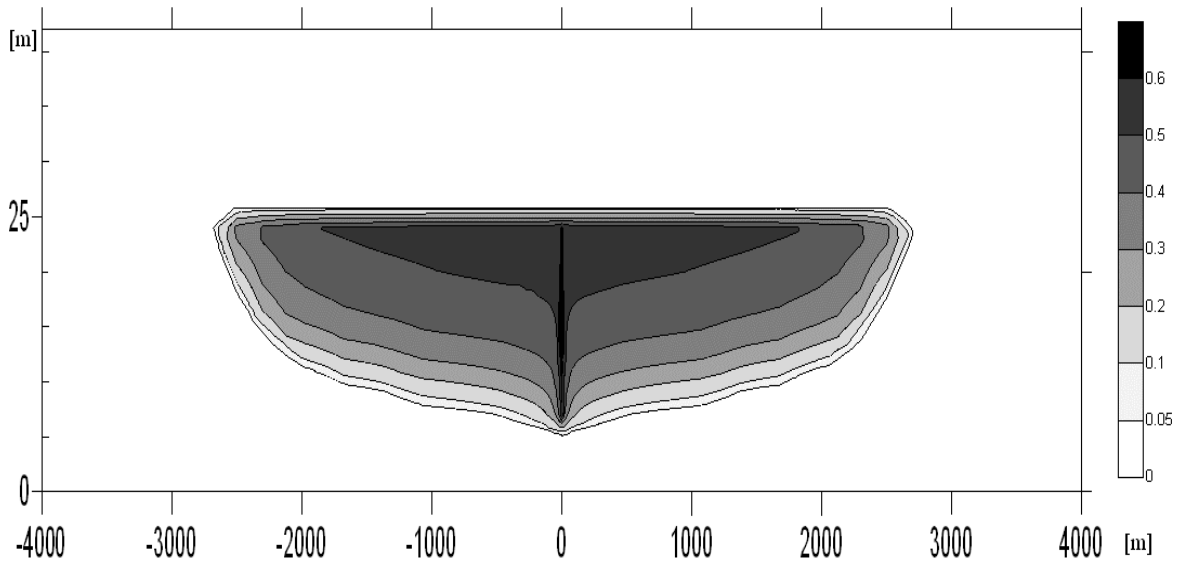
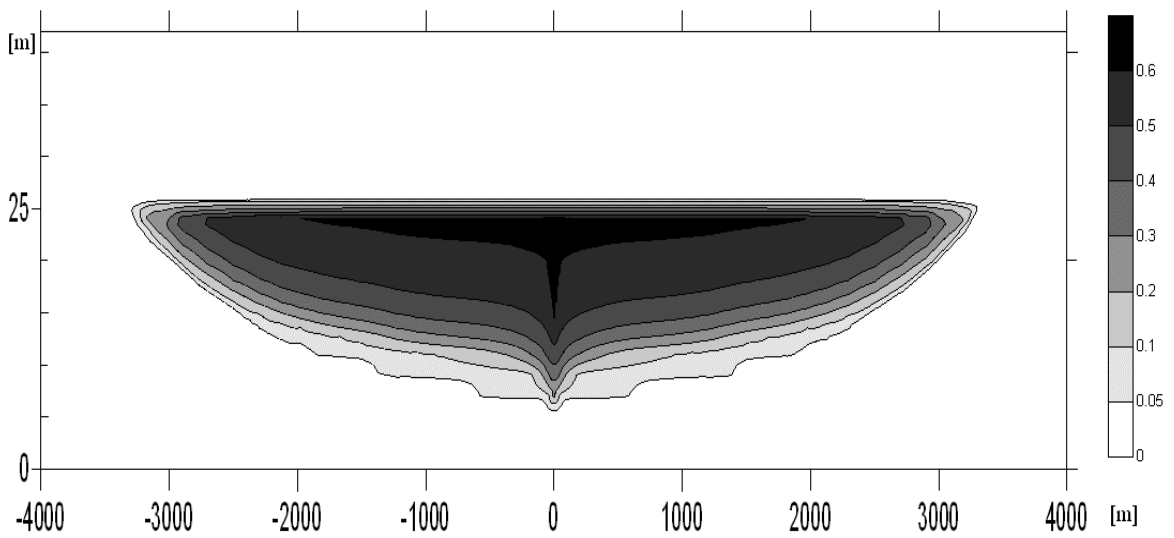**Figure 14** CO_2 phase saturation in the saline aquifer, two years after the injection start.

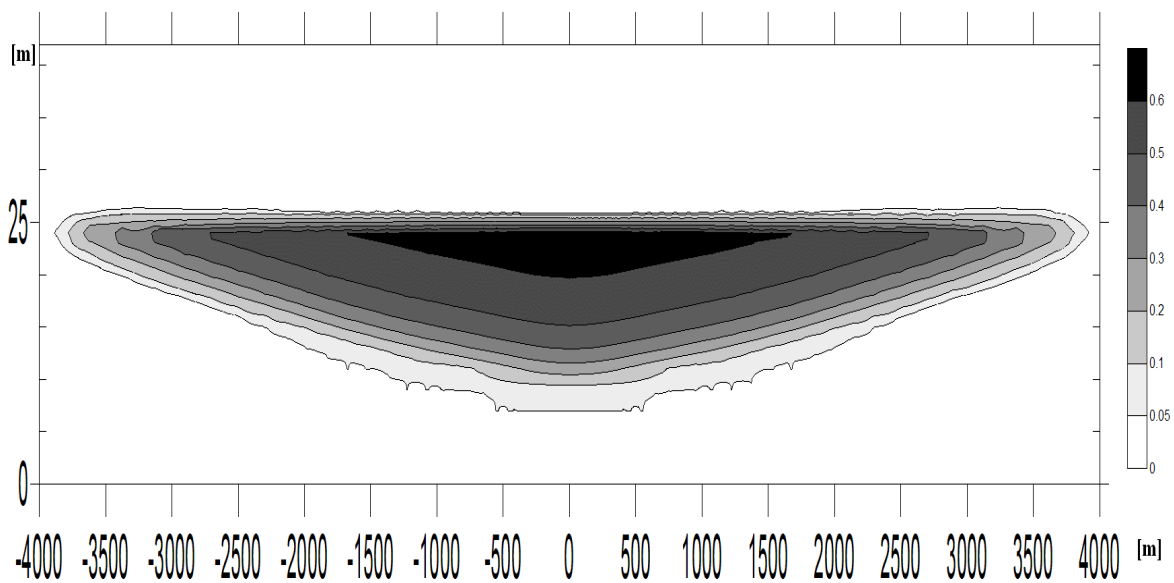**Figure 15** CO_2 phase saturation in the saline aquifer, five years after the injection start.

Figure 16 CO_2 phase saturation in the saline aquifer, fifty years after the injection start.

5.3.1 Sensitivity to changes in van Genuchten parameter α

When the α of the claystone layer corresponded to a permeability of $10^{-15}\,m^2$ there was a difference between the extension of the area with saturation in the range 0.005–0.01 compared to previous simulations (figures 14 and 17). Fifty years after the injection start there was a buildup in CO_2 saturation just below the transition from sandstone to claystone (figure 18). The CO_2 phase had however not migrated further into the claystone and the CO_2 that had done so in the earlier state had now dissolved into the aqueous phase (figure 19). Fifty years after the injection one can see that the CO_2 dissolved into aqueous phase had spread further into the claystone than the CO_2 phase had (figure 19). The spread was less than five meters into the upper layer.
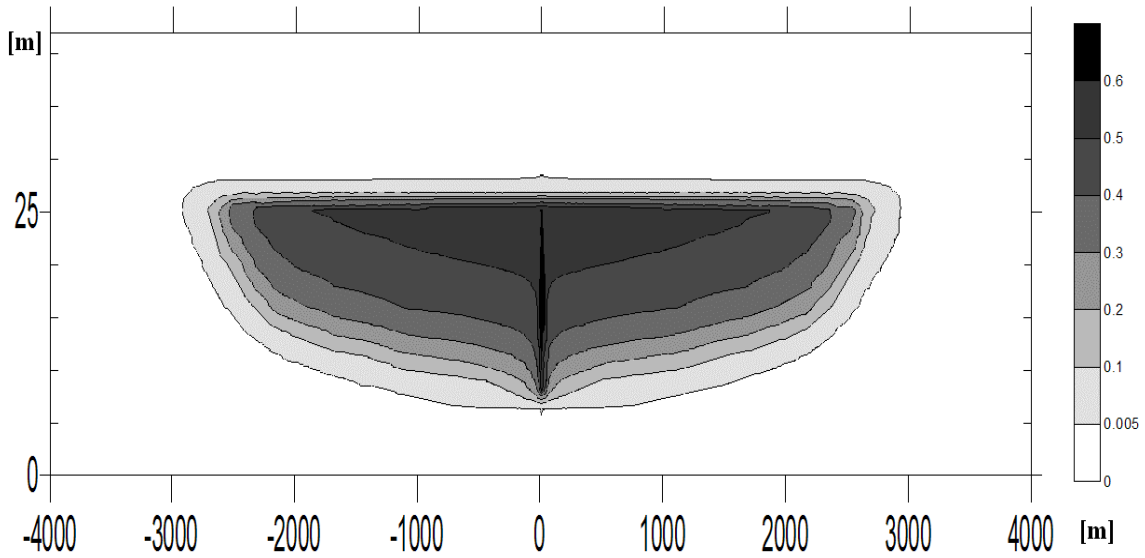

Figure 17 CO_2 saturation in the saline aquifer, two years after the injection start and corresponding to permeability of $10^{-15}\,m^2$.
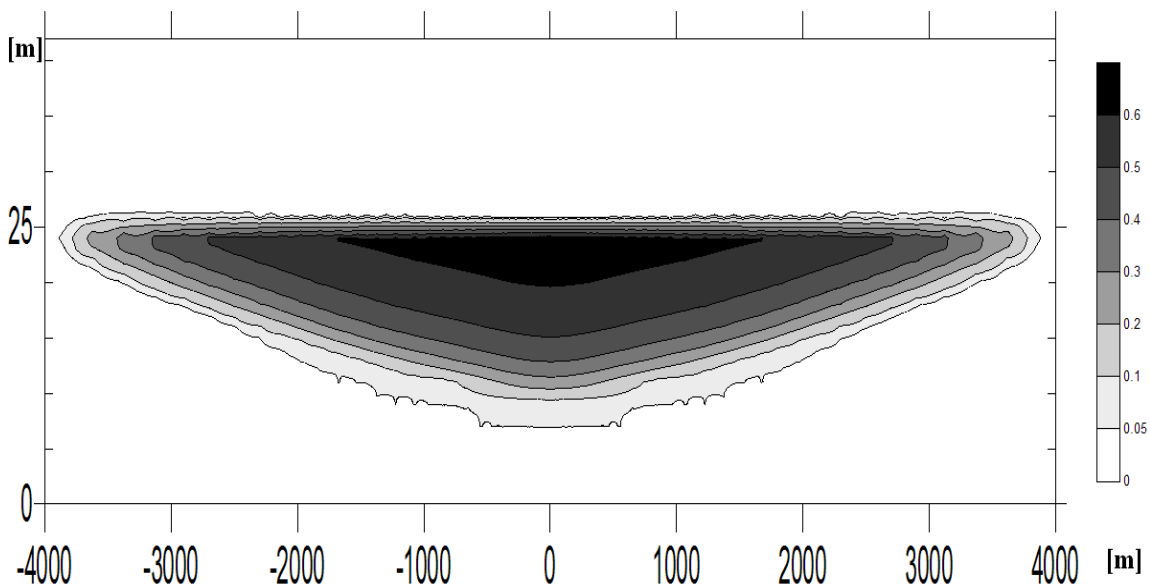

Figure 18 CO_2 saturation in the saline aquifer, fifty years after the injection start and corresponding to permeability of $10^{-15}\,m^2$.
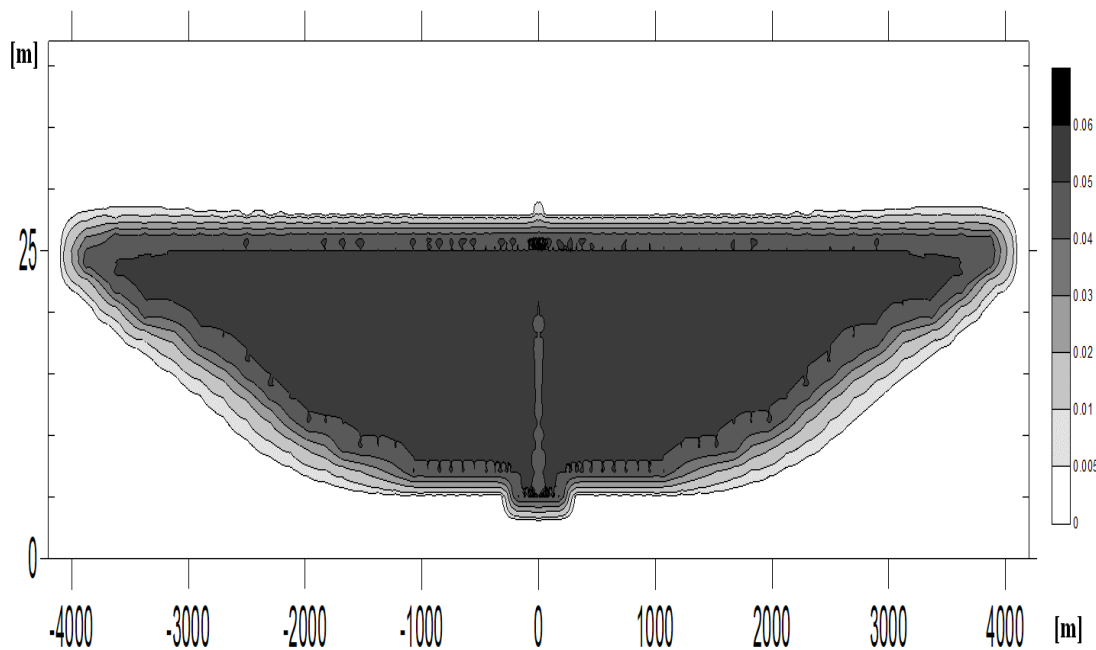
Figure 19 Mass fraction CO_2 dissolved in the aqueous phase in the saline aquifer, fifty years after the injection start corresponding to permeability of 10^{-15} m^2.

6. DISCUSSION AND CONCLUSIONS

In this study I have looked at possibilities of injecting CO_2 a saline aquifer in sedimentary rock, based on data from the Malmö aquifer. I have also studied CO_2 injections in a theoretical crystalline fracture zone with properties typical of crystalline rock in Sweden. While saline aquifers in sedimentary bedrock are considered a viable alternative for CO_2 storage are crystalline rock normally not considered. In Sweden can CO_2 storage in crystalline rock perhaps be an attractive alternative due to frequent occurrence of such sites. The thesis is entirely based on numerical simulations of CO_2 injections and has not considered data from actual CO_2 injections. The result can thus be only considered as preliminary in nature, and depending on the accuracy and representatively of the data available as well as the reliability of the model itself.

In the horizontal case of fractured bedrock there occurred seepage of CO_2 into the intact rock, despite the low permeability and porosity of the intact rock. It was unexpected since the pressure increase was low and should not cause this. It confirms the expectation that the injectivity in the fracture zone is low. The large storage footprint (in comparison to the injection rate) also needs to be taken into account since the effort and cost needed for monitoring of the injected CO_2 will increase with a larger area that needs monitoring. If fractured crystalline bedrock is to be used as storage of CO_2 it will probably only be possible with very small-scale injections since pressure buildup due to low injectivity and large storage footprint will make it unfeasible for storage of larger quantities.

It is also most unlikely that the fracture zone will be perfectly horizontal with no slope. A gentle slope of 3° caused the plume to migrate upwards rapidly and leave a trail of lower saturation and the CO_2 that had dissolved into the aqueous phase. The reason the

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area with residual saturation in the results did not cover the entire area where the plume had been present is that parts of the residual CO_2 had dissolved into the formation water. There is still a lot uncertainty in the role of residual saturation in geological storage and if CO_2 is injected into a fracture zone it will likely play a major part. It can perhaps be possible to store CO_2 in fracture zones as residual saturation and storage of CO_2 in fracture zones in Sweden could then perhaps be plausible. Since leakage can be expected from such storage it is important to ensure that there will be no damage at the surface. The role of residual saturation in geological storage of CO_2 is important and should be investigated further. The fractured crystalline bedrock was simulated as a homogenous media and that is a major simplification compared to the reality. Fractured systems are most complex and a reason to further investigate fractured rock's storage potential could be that CO_2 will probably behave somewhat differently in a fractured media compared to a porous media.

The sandstone aquifer is a viable alternative for geological storage of CO_2. At the simulated injection rate the storage footprint was large because the CO_2 did not seep through the claystone. It would have improved the storage capacity if the CO_2 had passed through the claystone since the increase in pressure due to injection then would be smaller and the plume would not spread as far laterally. The aquifer is multilayered and it is not the layers of claystone that are intended as cap rock but the upper layer of dense limestone. Still the simulations suggest that the site is interesting for storage and the option could be investigated further. data that I had access to were only from one well, but it is not likely that the thinner claystone layers will extend more than a few kilometers. There may be a connection between some of the sandstone layers that in the model were separated by thinner layers of claystone. Injection of CO_2 could then possibly be better at some other location in the aquifer. It would also be possible to inject CO_2 in several different sandstone layers. The layer chosen for injection in this simulation may not have been the best option. Further investigations and a simulation of the injection with much more detailed geological information included are called for in future studies. The simulations did however indicate that storage of CO_2 in this particular aquifer could be a possible alternative. More detailed geological investigations of the site and more detailed simulations of the injection need, however, to be carried out before any firm conclusions can be made. The pressure increase in the aquifer was too high in this simulation, something that needs to be carefully considered in order to decide a realistic injection rate if an injection project is to take place.

In both the case with the fracture zone and the sandstone aquifer the horizontal injection well at Sleipner was used as the example. A 2D simulation of a section through a horizontal well that extends for 100 m does give a reasonable representation of the spread and the possible injection rate at that section. But the reality is better represented by a 3D model, especially if the injection well does not extend far horizontally. The different geometry affects the pressure buildup and thereby it affects the possible injection rate. In an injection project this has to be taken into account.

A sensitivity study with varying the van Genuchten parameter α did have an impact, increasing with time, on the result. When simulations for the sandstone aquifer were run for an α more than three times larger than the original α, the impact on the result was, however, still small. The uncertainty in the parameter α seems thus to have had only a minor impact on the simulations for the Malmö aquifer. But, it is important in other cases to remember that α does influence the results and its effect should therefore be carefully estimated.

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APPENDIX 1

The governing equations in TOUGH2 for the fluid and heat flow are described by equations (1)-(5)

$$\frac{d}{dt}\int_{V_n} M^K dV_n = \int_{\Gamma_n} F^K \bullet n\, d\Gamma_n + \int_{V_n} q^K dV_n \qquad \text{(1) Mass and energy equation}$$

$$M^\kappa = \phi \sum_\beta S_\beta \rho_\beta X_\beta^K \qquad \text{(2) Accumulation of mass}$$

$$M^{NK+1} = (1-\phi)\rho_R C_R T + \phi \sum_\beta S_\beta \rho_\beta u_\beta \qquad \text{(3) Accumulation of heat}$$
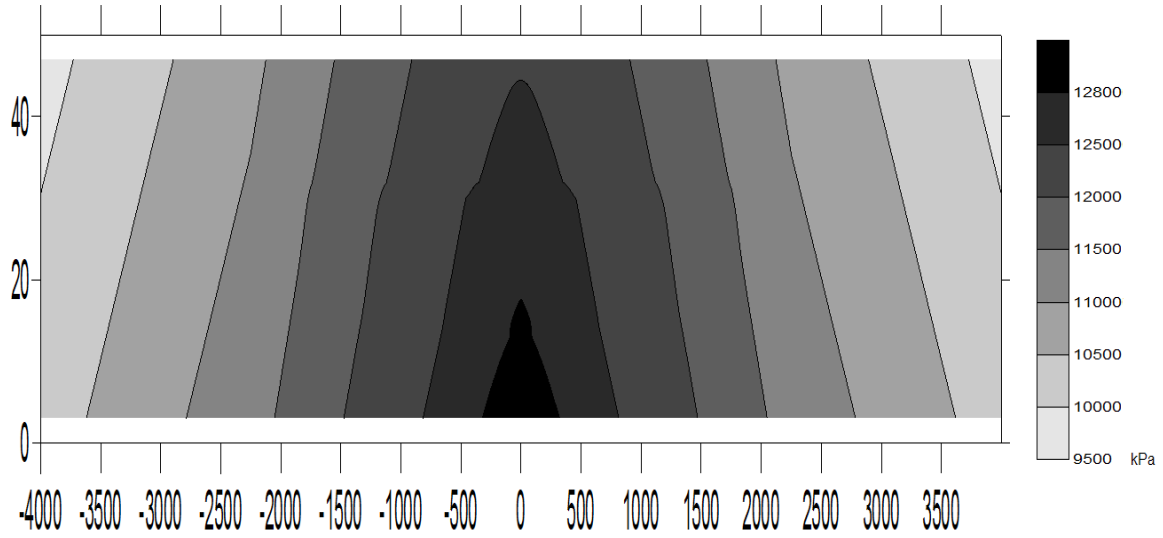
$$F_\beta = \rho_\beta u_\beta = -k\frac{k_{r\beta}\rho_\beta}{\mu_\beta}(\nabla P_\beta - \rho_\beta g) \qquad \text{(4) Mass transfer for individual phase}$$

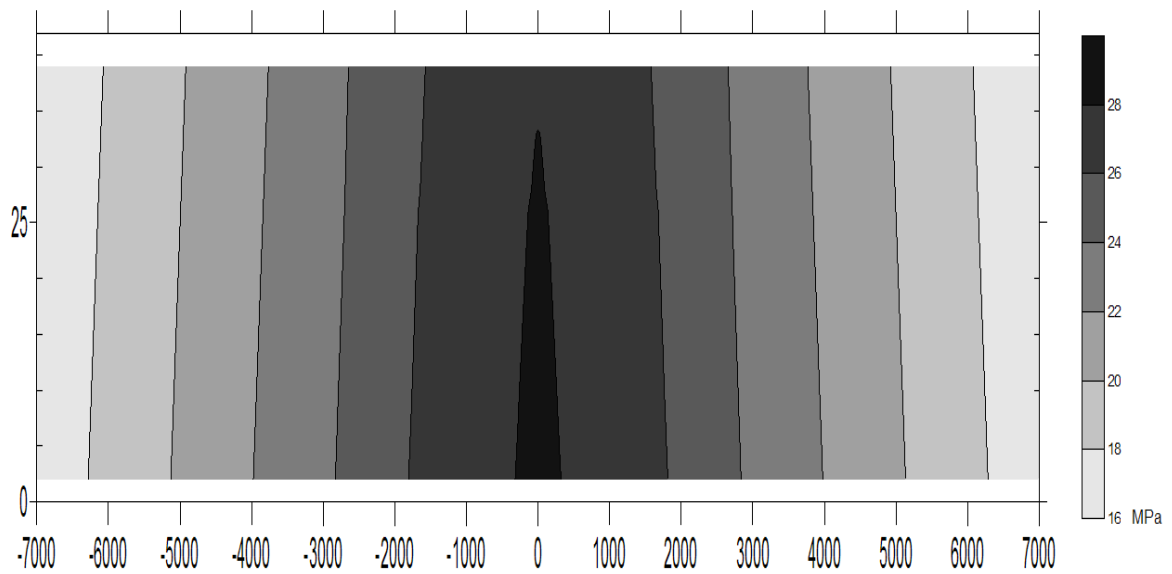$$F^{NK+1} = -\lambda \nabla T + \sum_\beta h_\beta F_\beta \qquad \text{(5) heat flux}$$

(Pruess et al, 1999)

APPENDIX 2

Pressure distribution 2 years after the injection start

Pressure in the horizontal case of fractured crystalline rock, 2 years after the injection start

Pressure in the sandstone aquifer, 2 years after the injection start