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Integrated simulations of CO$_2$ spreading and pressure response in the multilayer saline aquifer of South Scania Site, Sweden

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Abstract

An integrated modeling approach/workflow, in which a series of mathematical models of different levels of complexity are applied to evaluate the geological storage capacity of the Scania Site, southwest Sweden, is presented. The storage formation at the site is a layered formation limited by bounding fault zones, and injection is assumed to take place from one existing deep borehole into all layers. A semi-analytical model for two-phase flow is first used to evaluate the pressure response and related parameter sensitivity, as well as the first estimates of acceptable injection rates. These results are then used to guide the more detailed numerical simulations that address both pressure response and plume migration. The vertical equilibrium (VE) model is used to obtain a preliminary understanding of the plume migration with a larger number of simulations. Finally the full TOUGH2/ECO2N simulations are performed for the most detailed analyses of pressure responses and plume migration. Throughout, the results of the different modeling approaches are compared to each other. It is concluded that the key limiting factor for the storage capacity at the site in the injection scenario considered is the fast CO$_2$ migration within the high permeability layer. Future studies can address alternative injection scenarios, including using horizontal injection wells and injection to other layers than the high permeability layer.

Introduction

Carbon dioxide capture and geological storage is considered as a relevant technology to mitigate climate change, for example because of relative abundance of deep geological reservoirs and extensive knowledge from the oil and gas industry.[1], [2] There has been an increasing number of storage operations around the world, and deep saline formations especially are considered promising because of their volumetric abundance. The present study focuses on the storage capacity of a saline aquifer; storage capacity is defined here as the maximum amount of CO_2 that can be injected and securely stored under the given constraints.

Constraints for site-specific CO_2 capacity can be formulated into (i) the size of the geological containment domain,[1] i.e., the volume or area of review (AOR) where the movement of the fluids (e.g. brine leakage) may occur; and (ii) the sustainable pressure build-up[3], [4] beyond which irreversible geomechanical failure may be induced. The first constraint limits the duration of the injection for a given injection rate. The sustainable pressure build-up on the other hand defines the injectivity which is dependent on the hydrogeological properties of the formation (e.g. thickness, permeability, relative permeability, regional groundwater flow[1]). The capacity derived from the containment and the pressure constraints can be termed *migration‑limited capacity* and *pressure‑limited capacity*, respectively, as defined by Szulczewski *et al*.[5]

At the initial stage of a site screening, volume-based capacity calculation is usually used to estimate the *migration‑limited capacity*. The calculation is simply done by using the pore volume of the selected formation multiplied by one or a series of storage efficiency factors. The overall storage efficiency factor accounts for the variabilities and uncertainties of various physical parameters or processes, and thus varies over a wide range.[6]-[10] This range can be narrowed down with the availability of additional characterization data and better understanding of the involved processes.

Advanced estimations of CO_2 storage capacity conducted by using a variety of analytical or semi-analytical models are most suited when some additional site characterization data are available but still relatively sparse. These estimates usually focused on simplified systems (e.g. radially symmetrical systems) using different level of simplifications (e.g. sharp interface, zero compressibility) and often aimed at quick assessment or general discussions (i.e., not site‑specific).[11] For example, Okwen *et al*.[12] calculated CO_2 storage efficiency for a radial symmetric system with infinite areal extent based on an analytical model developed by Nordbotten *et al*.[13] Vilarrasa *et al*.[14] proposed a semi-analytical solution for the shape of the injected CO_2 plume with explicit accounting for CO_2 compressibility. These approaches, among

others,[15] can be categorized as focusing on the *migration-limited capacity*. In terms of the *pressure-limited capacity*, Zhou *et al*.[16] proposed a method to calculate the storage capacity based on the pressure build-up history over the injection period for closed and semi-closed systems. Mathias *et al*.[4] suggested a method to estimate injection-induced pressure build-up by analytically solving radially symmetric, two-phase two-component flow equations. Rutqvist *et al*.[3] further demonstrated a numerical approach to calculate the maximum sustainable injection pressure by using coupled multiphase fluid flow and geomechanical fault-slip analysis.

More advanced (i.e., for more site-specific) capacity estimates require extensive amounts of data, meaningful storage scenarios being formulated, and in most cases involve basin-scale three-dimensional numerical simulations.[17], [18] General-purpose numerical simulators are used in this regard, such as TOUGH2,[19] PFLOTRAN,[20] and Eclipse.[21] An alternative modeling approach includes the coupled numerical-analytical (hybrid) methods where analytical methods are integrated into numerical simulators to improve computational performance. One example is using analytical solution to provide multi-scale discretization correction to a numerical simulator whose resolution is dependent on grid refinement;[11] another example is using analytical solution to track the location of saturation front in a two-phase system at sub element scale under a finite element solution scheme.[22]

An approach that could be considered as falling in between the full-physics models and the analytical/semi-analytical models is the Vertical Equilibrium approach (VE),[23] that has been recently introduced to the CO_2 storage research community.[24]-[28] This approach assumes conditions of vertical equilibrium. It has been used to investigate the CO_2 storage potential in the Johansen formation, for example.[24] The VE model can explicitly address a variable thickness of the reservoir, an essential quantity for capacity estimation.

In this study a series of models of increasing accuracy and model complexity are used to evaluate the storage capacity of the South Scania site, Sweden. The site is presently not considered as a CO_2 injection site, but was carefully analyzed as one of the field sites of the EU FP7 project MUSTANG (www.co2mustang.eu) where the characteristics of a number of saline aquifers in Europe were studied in terms of geological storage of CO_2, their 3D geological models were constructed and related hydrogeological parameters for different reservoir units were determined.[29], [30] The goal of this overall work is to understand what kind of properties can be encountered and how they should be modeled. The objective of the current work is two-fold: first, to demonstrate the use of a multiple-step modeling approach for evaluating CO_2 dynamic behavior at a storage site; and second, to give site-specific predictions concerning CO_2 capacity of the South Scania site. By starting from a semi-analytical model with an order-of-magnitude of

the injection rates that can be used without exceeding the pressure threshold, we proceed to more detailed numerical models, first based on the VE approach, still being simplified, and finally based on a full three-dimensional numerical model (TOUGH2) of the site. The use of multiple modeling methods gives (i) more confidence in the model results, which is important in long-term model predictions, and (ii) a flexible procedure where output from the simpler models can be used (as inputs) for the more complicated ones.

South Scania site

The South Scania site is located in the province of Scania, Sweden (Fig. 1). The site has been studied for oil exploration and thermal energy productions with a relative abundant database available. In terms of geological storage for CO_2, the site has previously been reported by Chasset *et al*.[31] who looked at the data from borehole FFC-1 and focused on parameter sensitivity effects on CO_2 injection. In an earlier study we have used the site data for an up-scaling study, where a method of up-scaling heterogeneous data was introduced[32] as well as an injection potential estimation, with a focus on developing analytical models for injectivity.[33]The present study focuses on capacity estimation and is based on the extensive geological data and the geological model recently developed in the frame of EU FP7 project Mustang.[29], [30] Eight geological units have been mapped to the 3D geological model. The identified units are listed in top-bottom sequence in Table 1.

Table 1. Identified units in the 3D geological model of the South Scania site (letter C refers to sealing units and letter R to storage reservoirs)

	Lithology	Stratigraphy	Units	Depth of the unit top*
C2	Argillaceous limestone	Granvik Member	Primary seal	1115
C1	Silicified chalk	Arnager Limestone	Primary seal	1530
R1	Sandstone	Arnager Greensand	Secondary trap	1613
C3	Clays	Lower Cretaceous	Intermediate seal	1642

	Lithology	Stratigraphy	Units	Depth of the unit top*
R2	Sandstone	Jur.-Cret. Boundary	Primary trap	1673
R3	Fine sand	Lower Jurassic	Multi-layered alternative trap	1683
R4	Sandstone	Rhaetian	Alternative trap	1783
C4	Claystone	Lower Jurassic-Rhaetian	Intermediate seal	–

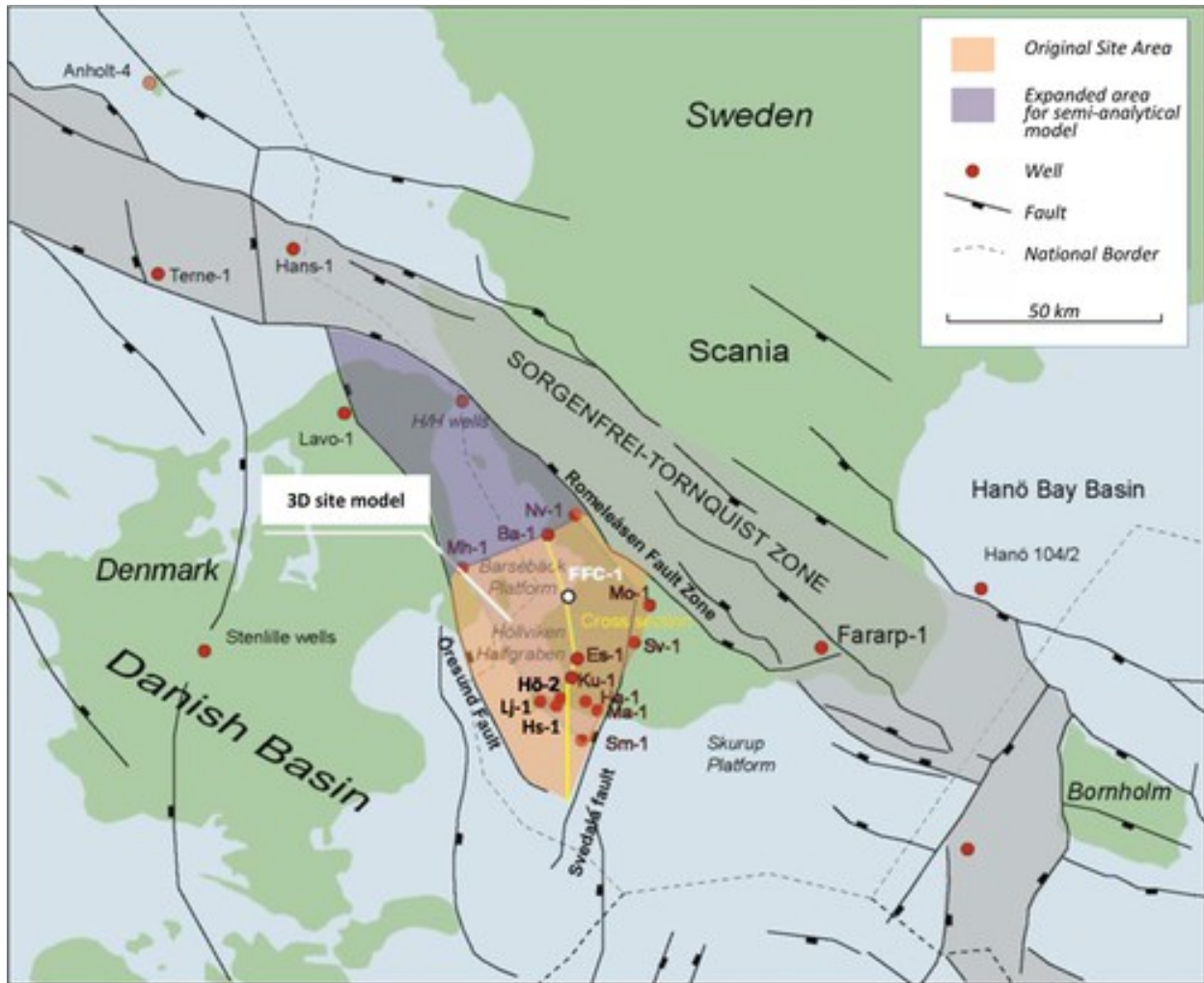- *Note: in meters below mean sea level; values are from FFC-1.

Figure 1
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Map of the Scania Site (after Erlström *et al*.29).
Caption

The primary cap-rock units C1 and C2 are relatively thick (total thickness ca. 250 ∼ 470 m) and the strata identified have a consistent thickness distribution. Their sealing ability is considered to be sufficient to prevent upward CO_2 migration. Therefore, C1 and C2 are excluded from this model for simplicity. Below these cap-rock units, the Lower Cretaceous Arnager Greensand is identified as a secondary trap, R1. Underlying R1 are a relatively thin (ca. 30 m), homogeneous intermediate seal C3 and the primary trap R2 which is a highly permeable aquifer, stratigraphically located at the Jurassic-Cretaceous transition interval. Below R2 follows a Rhaetian-Pliensbachian multilayered sequence of sandstone and claystone rendering two main traps, R3 and R4, separated by an intermediate seal, C4. The lateral distribution of C4 is highly uncertain, has not yet been resolved and thus is excluded from the current 3D model.30

The modeling domain in the present work thereby consists of a continuous sequence of R1, C3, R2, R3 and R4, and is considered to be sealed from the top and the bottom (Fig. 2). The possible leakage and pressure relief through the caprock and baserock are neglected, which leads to possibly overestimating the pressure build-up. The estimate is, however, conservative and therefore motivated in this preliminary evaluation of the reservoir's suitability for CO_2 storage. The hydrogeological properties compiled in Erlström *et al.*[29], [30] are listed in Table 2. It can be seen that the relatively thin reservoir unit R2 has an order-of-magnitude higher permeability than the other reservoir units, which have permeabilities that are commonly considered acceptable for CO_2 storage.

Table 2. Data-based parameters for CO_2 injection simulations (after Erlström *et al.*[29], [30])

	Unit	R1	C3	R2	R3	R4
Thickness	M	40	32	14	138	40
Permeability (horizontal)	mD	88	0.002	1800	160	200
Permeability anisotropy (horizontal to vertical)	–	1.5	1	3.5	7.5	3.5
Porosity	%	23	15	25	20	23
Salinity	NaCl g/l	125	125	125	125	125
Pore Compressibility	10^{-10} Pa^{-1}	4.50	-	4.50	4.50	4.50
Brine compressibility	10^{-10} Pa^{-1}	3.54	-	3.54	3.54	3.54
Temperature	ºC	55	55	55	55	55

	Unit	R1	C3	R2	R3	R4
Mean slope[*]	deg	0.86	0.83	0.81	0.74	0.66

- *Note: calculated along a horizontal straight line from FFC-1 to Kungstorp-1 (Ku-1).
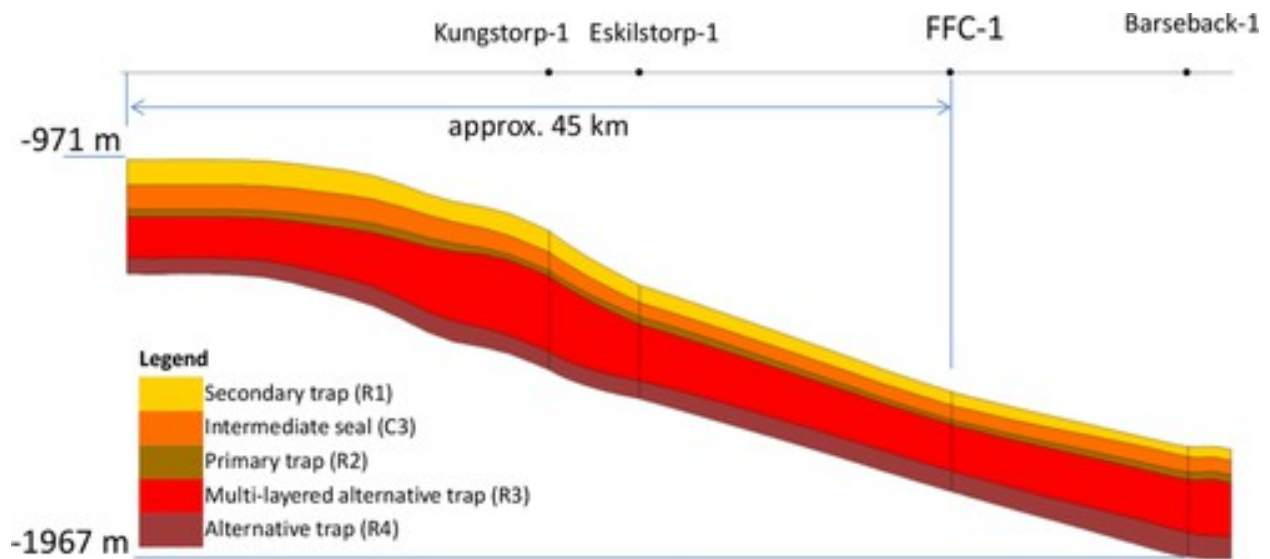

Figure 2

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Schematic of a vertical cross section of the 3D geological model (east-west view). The cross section is highlighted in Fig. 1 and passes through respectively Kungstorp-1 (Ku-1), Eskilstorp-1 (Es-1), FFC-1 and Barseback-1 (Ba-1). The scale in vertical direction is magnified by a factor of 25.

Caption

In all of the model analyses discussed below we assume CO_2 injection through the existing deep well FFC-1 whose extensive data are available.

Modeling approaches

The complexity level of site modeling is often limited by computational resources and data availability which make the most appropriate level of modeling ambiguous.[11] We want to select a group of models that are simple and ready to use while capable of capturing the essential physics. The idea has served as the philosophy for the selection of different modeling approaches where the use of the more demanding numerical approach is minimized.

Figure 3 presents a diagram of the workflow. We have used a similar procedure of models of increasing accuracy and complexity for analyzing the CO_2 storage capacity for the Dalders Monocline in the Baltic Sea.34 The actual models here are tailored for the South Scania site, whose storage formation is of multiple reservoir layers while the Baltic Sea formation is a single-layer reservoir. A brief summary of the main procedure is:

i.   Semi-analytical solution was first used for a wide range of injection rates to see the injectivity constraints and the parameter sensitivity under different boundary conditions.

ii.   For all the viable injection rates, we used a VE model (based on Nordbotten *et al*.35) to check the migration limits, and select an injection rate that can meet both injectivity and migration constraints.

iii.   Then, full three-dimensional simulations were performed using a TOUGH2 simulator for the selected injection rate and the results were compared with the VE ones.
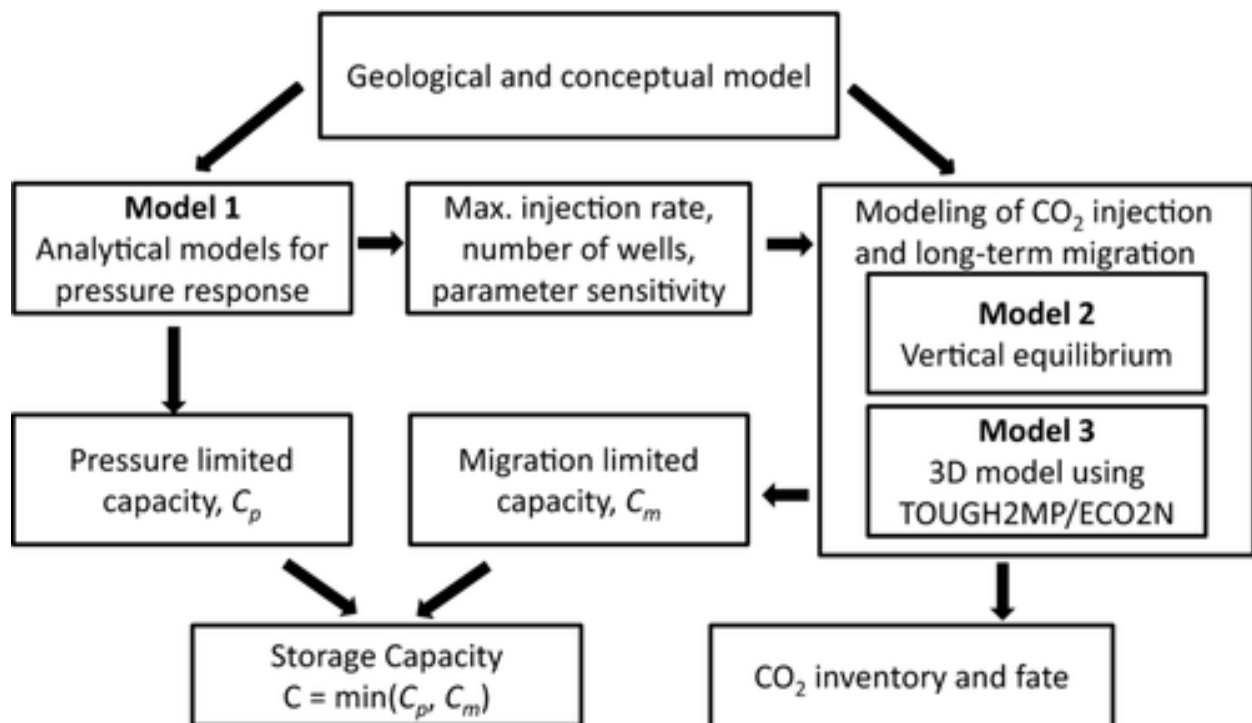

Figure 3
Open in figure viewerPowerPoint
Order of analyses and modeling methods used (after Yang *et al*.34).
Caption

To summarize, in this stepwise approach, the semi-analytical solution was used to screen the possible injection rates that meet the injectivity, then the VE model was used to down-select the injection rate for migration limits, and finally TOUGH2 with greater complexity (solubility and

capillary trapping) was used for the most detailed predictions of the long-term CO_2 evolution and detailed inventory for the selected injection scenario.

The semi-analytical approach

We use a semi-analytical model[33], [36], [37] to obtain pressure build-up estimation. The solution is obtained through analytically solving the radially symmetric, two-phase two-component flow equations.[36], [37] The solution assumes a horizontal formation, impermeable caprock and baserock, vertical pressure equilibrium, homogeneous fluid and formation properties and negligible capillary pressure effect. The solution takes into account the effect of CO_2 compressibility by iteratively calculating the CO_2 density based on the actual near-well pressure build-up. It can also take into account the effect of impervious fault boundaries by including superposition of pressure response from image wells.[33] The semi-analytical solution is described in more detail in the Supporting Information (SI).

The lateral extent of model domain was chosen to coincide with three bounding faults (i.e., Romeleåsen, Svedala, and Öresund; Fig. 1). The overlying and underlying formations were assumed to be impermeable. The four reservoir units (R1-R4; Fig. 2) were assumed non-interfering and considered each as individual single layer model at their respective depths with uniform thickness, and homogeneous permeability and porosity. This first part of the study focused on the near-well pressure response for the four reservoir units.

As usual for the type of large-scale fault zones, their hydraulic (boundary condition) characteristics as the bounding faults are poorly known. We have used the best geological considerations and ended up with the possible boundary-condition scenarios (BS) summarized in Table 3. The first two boundary scenarios (BS1 and BS2) present the extreme cases. The third scenario, however, is the more probable presentation for the site according to the available geological information. In all three boundary condition scenarios, we have considered one injection well at the well location of FFC-1.

Table 3. Scenarios for boundary condition sensitivity

	Romeleåsen Fault	Svedala Fault	Öresund Fault
BS1	Close	Close	Close

	Romeleåsen Fault	Svedala Fault	Öresund Fault
BS2	Open	Open	Open
BS3	Close	Open	Open

The vertical equilibrium approach (VE)

An in-house VE simulator with a multi-layer feature (refer to SI) was developed for CO_2 injection and migration in geologic formations, based on the general mathematical/numerical procedures suggested by Gasda *et al.*,[24], [27] and was validated by comparing results with other implementations[25] using a benchmark problem designed by Dahle *et al.*[38]

A 3D model is created for the southern part of the study region with an area of about 1800 km² (Fig. [1]). The hydrogeological units R1, C3, R2, and R3-R4 are modeled separately and coupled through interlayer fluid fluxes calculated by one-dimensional multiphase version of Darcy's equation. In each unit the VE model assumes homogeneous permeability and porosity (Table [2]). R3 and R4 are lumped together due to the similarity in medium properties. The capillary pressure, residual trapping and the mutual dissolution between CO_2 and brine with a convective dissolution process were not considered in this model. The model, along with the most realistic boundary conditions, is illustrated in Fig. [4]. Romeleåsen fault (NW-SE) was considered as closed boundary. All other boundaries were considered open and permitting fluid flow.
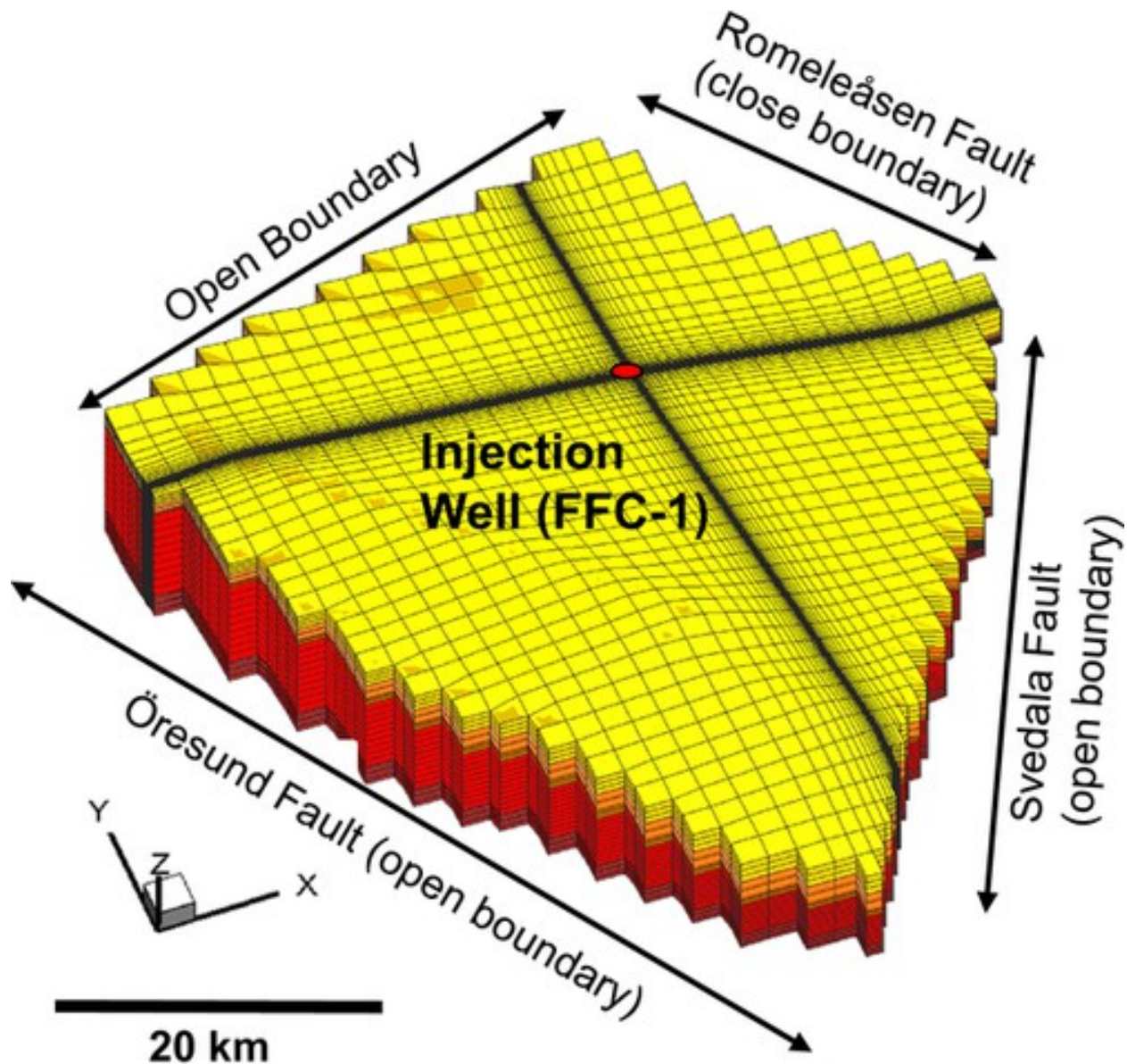
Figure 4

Oblique view of the 3D model for numerical simulations. The different colors represent units R1, C3, R2, R3 and R4 (the color of the units correspond to the legend in Fig. 2).

Caption

TOUGH2 simulation

Most comprehensive modeling simulations were carried out by using the massively parallel version of TOUGH2 code TOUGH2-MP[39] with a parallel version of ECO2N[40] (short for T2MP in the following text).

A 3D model was constructed including R1, R2, C3, R3 and R4 (Fig. 4). The medium properties for each unit were homogeneous and according to Table 2, the top and bottom elevation for each hydrogeological unit was based on linear interpolation of the surface data in the 3D geological model (after Erlström *et al.*[30]). The detail of the implementation is described in SI.

Due to the lack of experimental data on the two-phase flow characteristic functions, these parameters were taken from the literature (Table 4, after Pruess *et al.*[40]). Capillary pressure and the relative permeability of the liquid phase were described with van Genuchten function.[41] Corey function[42] was used for the relative permeability of the gaseous phase. The capillary entry pressures (P_c) for each unit were scaled according to the Leverett scaling:[43]

$$P_c = P_{c,ref}\sqrt{\frac{k_{ref}}{k}}$$

(1)

where $P_{c,ref}$ is the reference capillary entry pressure, k_{ref} [mD] is the reference permeability.

Table 4. Parameter values used for numerical simulations based on literature.[40]

Parameters	Values
Irreducible water saturation, $S_{1,r}$ [-]	0.300
Residual gas saturation, $S_{g,r}$ [-]	0.050
Van-Genuchten parameter, m [-]	0.457
Reference for Leverett scaling on capillary pressure, P_{ref} [Pa]	1.98×10^4
Reference permeability, k_{ref} [mD]	100
Pore compressibility [Pa^{-1}]	4.5×10^{-10}

Results

Following the modeling workflow, we first present estimation of the well injectivity by means of the analytical modeling based on which a viable injection scenario for the more detailed modeling can be determined. We then present the simulated pressure response due to the CO_2 injection as well as the CO_2 migration during and after the injection, as obtained with the two numerical models.

Injectivity estimation

Injectivity characterizes the ease with which the CO_2 can be injected into a target formation.[1] A constant rate injection was considered and the injectivity was evaluated by looking at the pressure response.

We chose the pressure build-up threshold to be 50% of the initial hydrostatic pressure.[3] At the center of the injection well where the hydrostatic pressure is 1.7×10^7 Pa, a pressure build-up of 50% gives a threshold (pressure increase) of 0.85×10^7 Pa. Pressure increase with different injection rates after 50 years of injection was determined (Fig. 5). For the most realistic boundary condition scenario BS3, a total injection rate of about 15 Mt (million metric tons) CO_2 per year from one well can be realized during the 50-year injection period. This high injection rate indicates that the pressure build-up may not be the dominant constraint for the Scania Site in this injection setting. The maximum allowed injection rate for the different reservoir units can be estimated from Fig. 5 and are summarized in Table 5. Note that the assumption of non-interference of pressure between the different reservoir units may affect the total maximum allowed injection rate, but the effect is expected to be relatively small because at the injection well, all pressure changes are the same for different reservoir units.

Table 5. Estimated maximum CO_2 injection rates (Mt CO_2/year) based on results shown in Fig. 5

Reservoir units	BS1	BS2	BS3	Used in numerical simulations*
R1	0.75	1.2	1.1	0.17
R2	2.5	>6	6	1.23

Reservoir units	BS1	BS2	BS3	Used in numerical simulations*
R3	4.0	>6	6	1.03
R4	1.5	2.5	2.2	0.60
Total	7.75	>15.7	15.3	3.00

- *Note: based on preliminary modeling with VE model assuming the same distribution of flow as obtained with semi-analytical model.
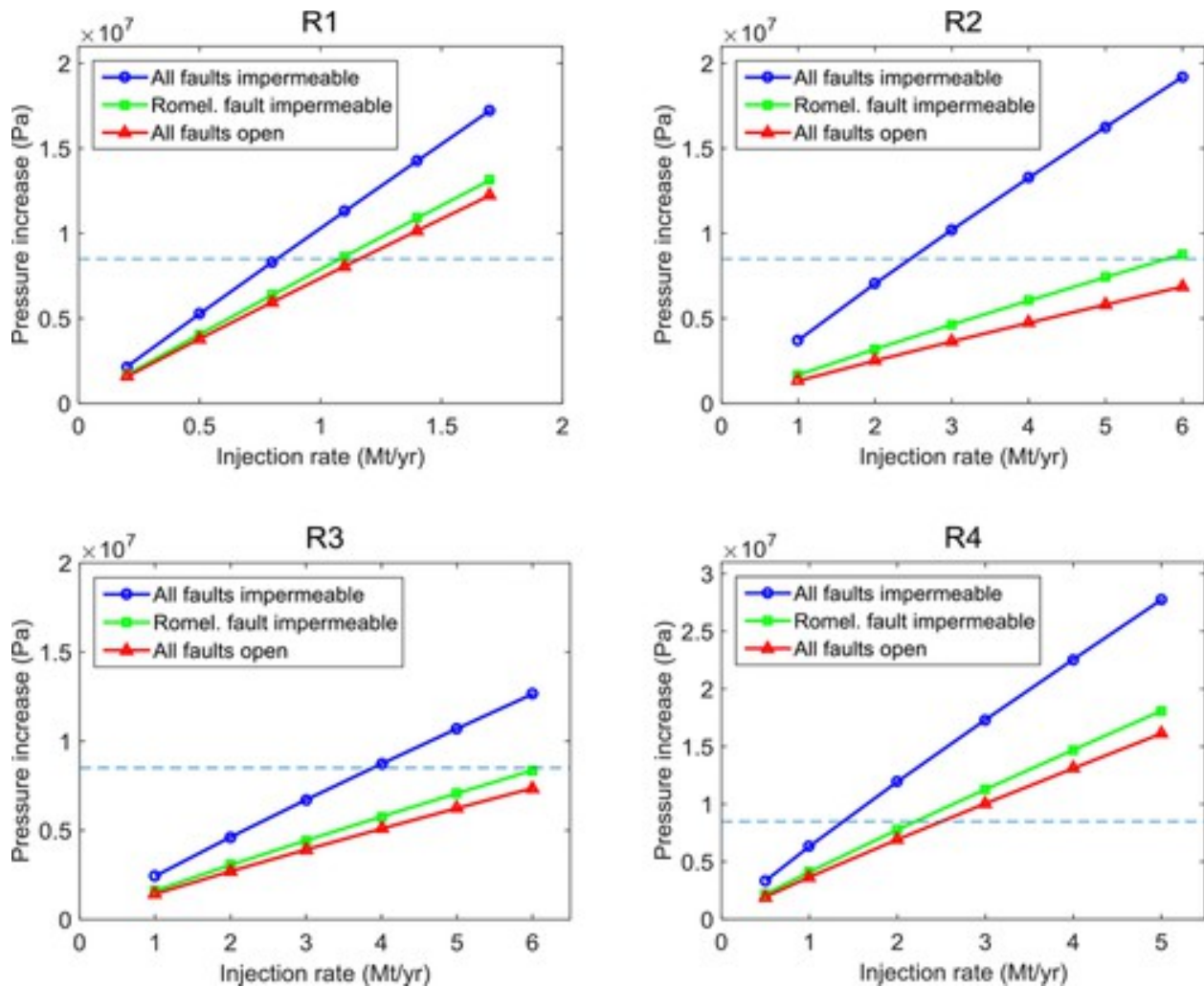
Figure 5
Pressure increase in the vicinity of the injection well as a function of the CO_2 injection rate as estimated with the semi-analytical solutions (Model 1). Horizontal dashed line indicates the pressure increase cut-off value of 50% overpressure.
Caption

Preliminary estimate of plume spreading

The next step was to estimate if the limitation imposed by CO_2 migration becomes a dominant storage capacity criterion. For preliminary estimation of plume migration several different injection rates were tested, starting from the estimates from the injectivity analyses (section on Injectivity estimation), using the computationally more efficient but less accurate VE approach. We simulated CO_2 injection through the existing vertical borehole FFC-1 at a constant injection rate for 50 years. This was followed by simulation of the post-injection CO_2 migration over a duration of 950 years. The total simulation time was 1000 years. The CO_2 injection rate for each unit was calculated according to its permeability and thickness. The results indicate that a total

injection rate of 3 Mt CO_2 per year (Table 5) may already result in significant CO_2 plume spreading at the end of 750 years of simulation. Note that the VE approach used here has no dissolution included and thus likely leads to an overestimation of CO_2 plume size. This total injection rate of 3 Mt/year was also chosen as the injection rate for the subsequent simulations carried out with the TM2P code.

Pressure build-up

More detailed estimates of the pressure evolution were made with the numerical VE and T2MP models. The injection-induced pressure build-up was defined through an overpressure factor (F_{op}) as

$$F_{op}(\%) = \frac{P_F - P_H}{P_H} \times 100 \qquad (2)$$

where F_{op} is overpressure ratio in percentage, P_F is pore fluid pressure, and P_H is hydrostatic pressure. Following the injection scenario formulated in the previous section, we preceded the injection simulations using both the VE approach and T2MP. An injection rate of 3 Mt/year for a time of 50 years as described earlier was used, and the plume spreading and pressure evolution over 1000 years (including the injection and post-injection periods) was simulated with both models. With this injection scenario we do not expect unacceptable overpressures (Fig. 5). Figure 6(a) shows results from the VE simulation at the end of the injection. The pressure build-up is seen mainly in the vicinity of the injection blocks. The overpressure increases gradually from the beginning and then reaches a maximum value (~8%) at the end of injection. For T2MP simulation, the maximum overpressure is seen in R2 at about 7% (Fig. 6(b)). Note that in both VE and T2MP modeling, the pressure interference between different reservoir units was inherently considered.
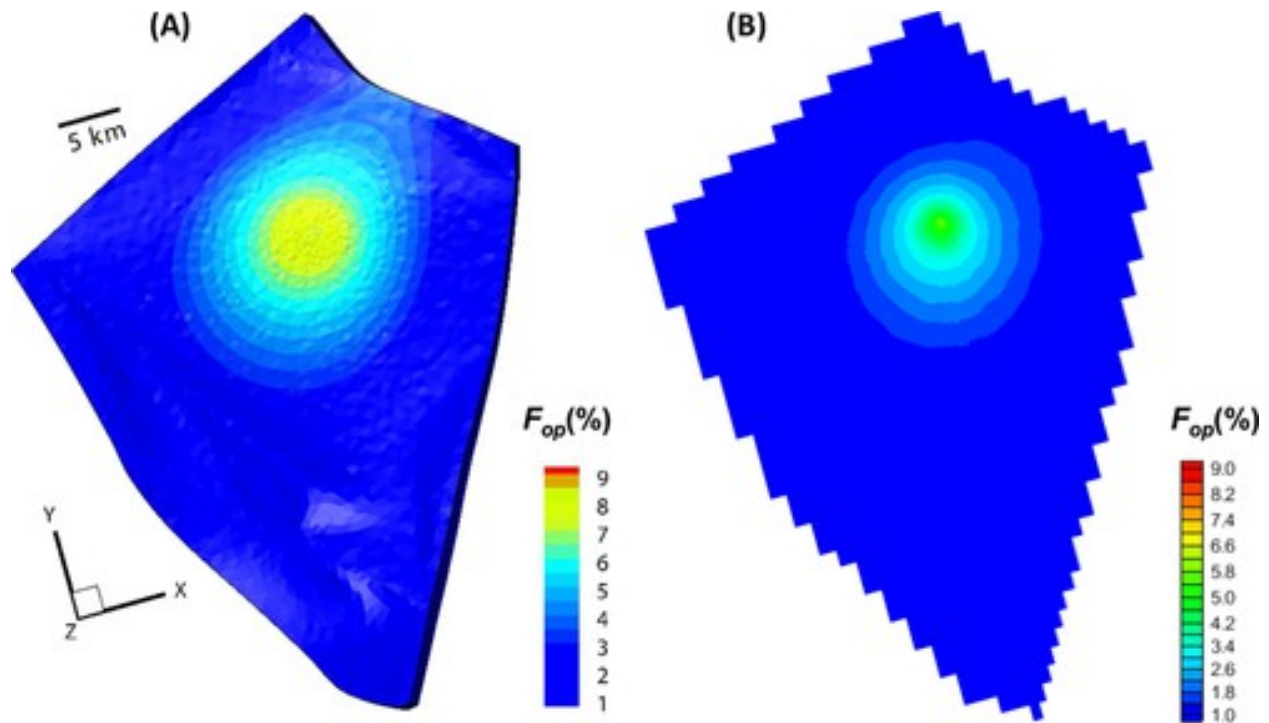
Figure 6
Pressure build-up (showing R2) at the end of 50-year CO_2 injection. The injection rate is 3 Mt CO_2/year. Boundary condition is according to BS3. (A) Result from VE. (B) Result from T2MP.
Caption

The pressure response is mainly determined by the intrinsic reservoir parameters namely permeability, porosity, compressibility, and reservoir thickness. All of this information has been maintained and adequately addressed in both VE and T2MP simulations. The CO_2 dissolution can contribute to the dissipation of pressure but the effect is small, and this effect is different in the two models as T2MP does take dissolution into account while our VE model does not.[37] The results from the two numerical simulations are similar and confirm the results from the semi-analytical calculation that only a small pressure build-up would occur with the selected injection rate. It can be concluded that with the current injection configuration, the injection-induced pressure build-up is not a limiting factor for the storage capacity at the South Scania site. The limitation imposed by CO_2 migration will be explored next.

CO_2 plume migration

Figure 7(a) shows the CO_2 plume thickness at the end of 50-year injection simulated with the VE model. It should be noted that due to the structure of the VE-model (vertical averaging over the thickness of the layer) CO_2 spreading in this model is measured in plume thickness rather than in

gas saturation. We can see that for the lower units (R2, R3, and R4) the spreading has not reached far while the plume thickness is quite high (partly due to the greater thickness of R3 and R4). The most dominant spreading is in R2 where CO_2 migrates up-dip about 10 km in 50 years. R2 is a thin layer with high permeability. The plume in R1 in comparison shows similar shape, but smaller thickness due to the smaller thickness of the unit.
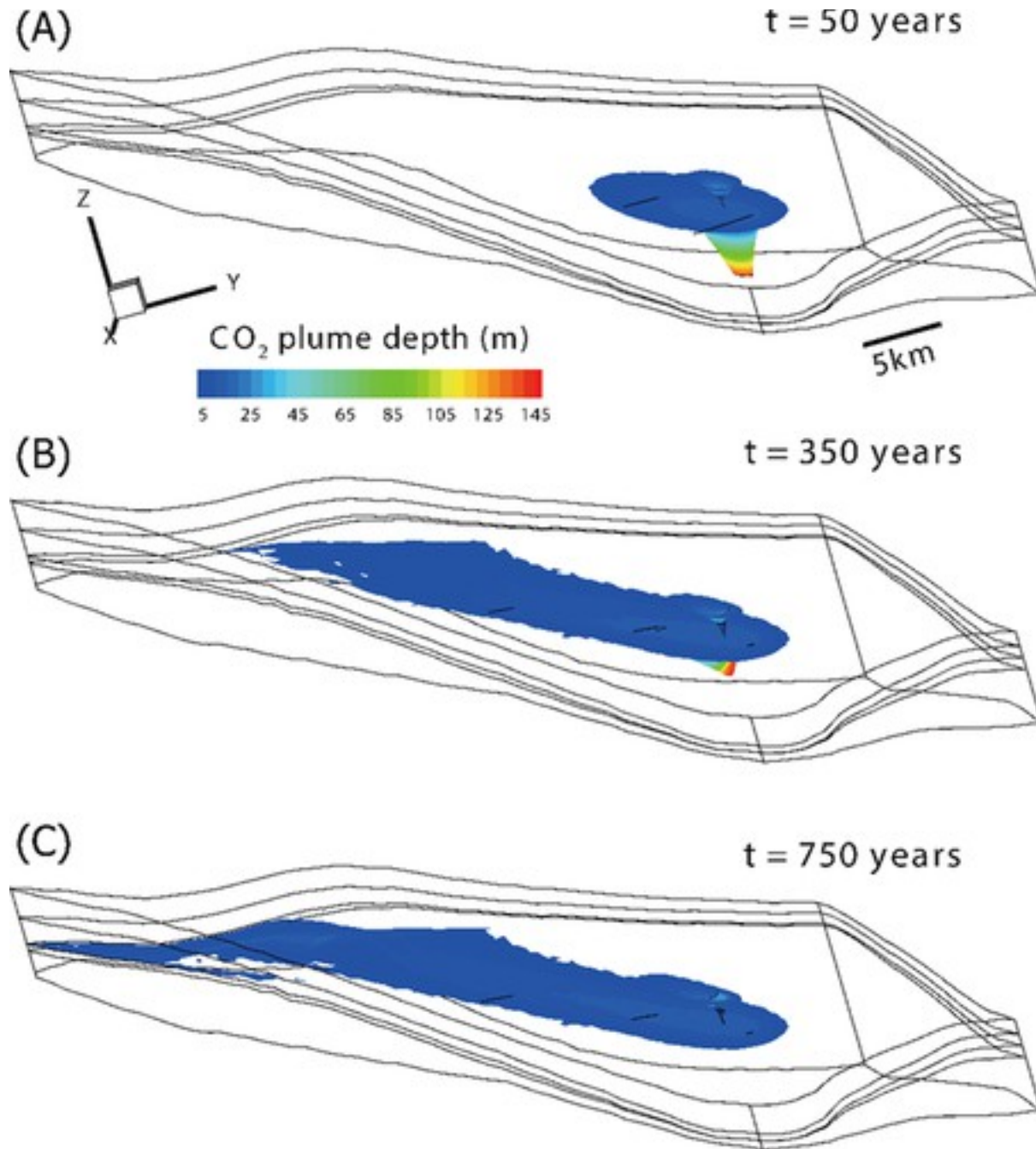

Figure 7

CO$_2$ plume migration predicted by VE model. (A) 50 years, (B) 350 years, and (C) 750 years after injection. CO$_2$ thickness less than 1m was eliminated from the color.

Caption

At the end of year 350 (Fig. 7(b)), CO$_2$ has migrated notably in the up-dip direction towards the south of the model domain. Its pattern follows the topography and the thickness of the CO$_2$plume tip is at the order of 10 meters. In the most permeable unit R2, the front of the plume has moved about 29 km from the injection well. The plume continues to move underneath the caprock, and eventually reaches the Öresund and Svedala faults (Fig. 7(c)), to which the total travel distance from the injection well is about 35 km. Focusing on unit R2 where the significant migration would have occurred, an injection rate of 3 Mt CO$_2$ per year over 50 years can lead to a CO$_2$ flow distance of 35 km in 750 years. This relatively fast migration indicates that the migration can be a limiting factor to the CO$_2$ storage operation at the Scania site.

For the T2MP simulation results, the CO$_2$ plume migration is plotted in terms of CO$_2$ saturation (Fig. 8). The spatial distribution shows two up-coned plumes: one in R1 and the other one in R2, R3, and R4 that act together. The most significant lateral spreading is seen in R2 where the front of the CO$_2$ plume moved about 8 km at the end of the 50-year injection period. From year 350 to year 750, the plume front moves about 5 km. At the end of year 1000 (Fig. 9), the front is about 31 km from the injection well in the up-dip direction. Comparing this with the VE result, the upslope extent of the plume is not as far while an identical lateral spreading of the CO$_2$ is realized in R2. The end-of-simulation saturation pattern agrees with the caprock topography which is an indication of structural trapping (Fig. 10). This result is very similar to the one produced by the VE approach. Since C3 has a very low permeability which can work as a perfect seal, the effect of the caprock in T2MP is effectively equivalent to the confined aquifer assumption made in VE.
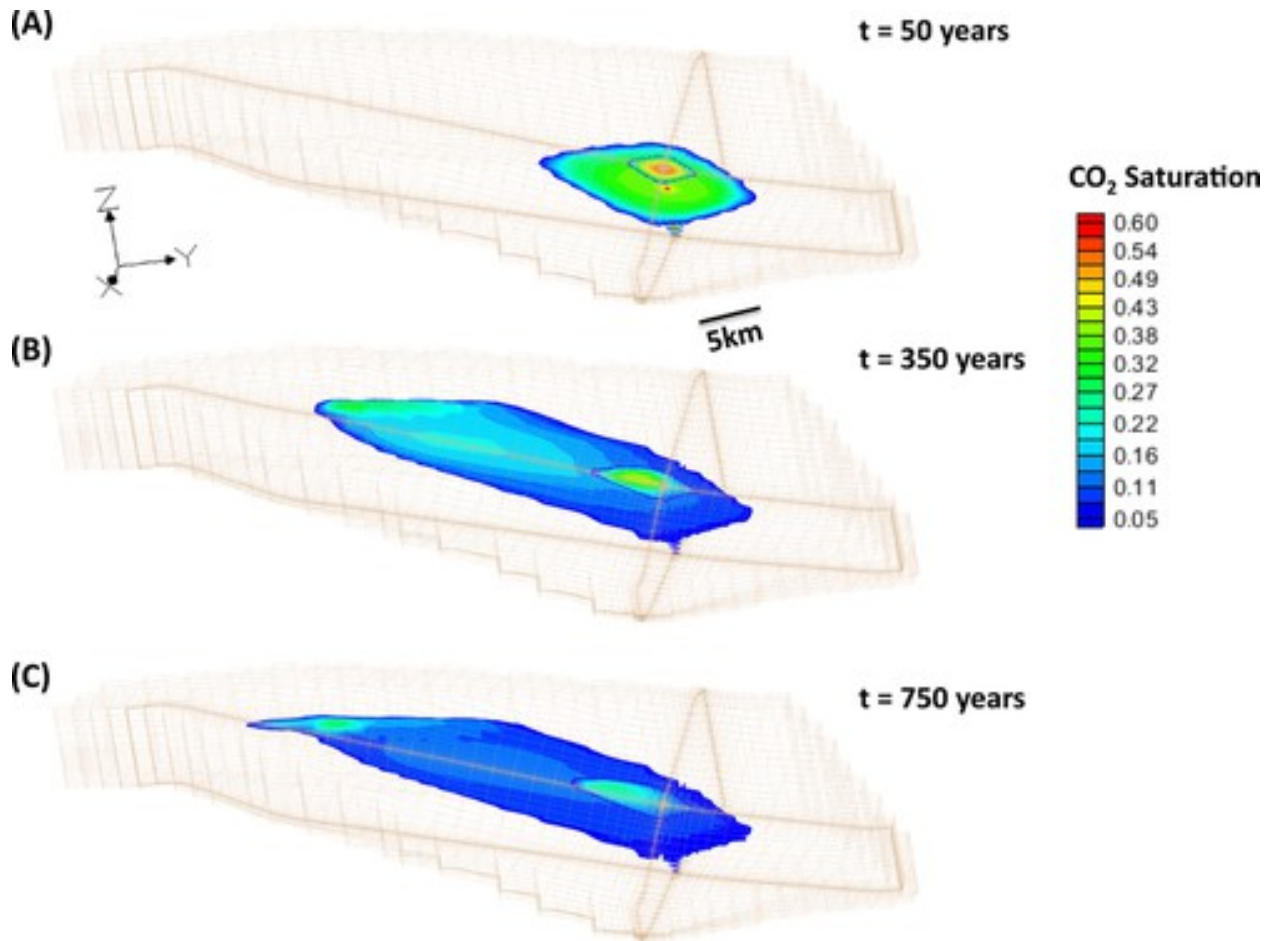
Figure 8
CO_2 plume migration from the T2MP simulation runs at (A) 50 years (cease of injection), (B) 350 years, and (C) 750 years.
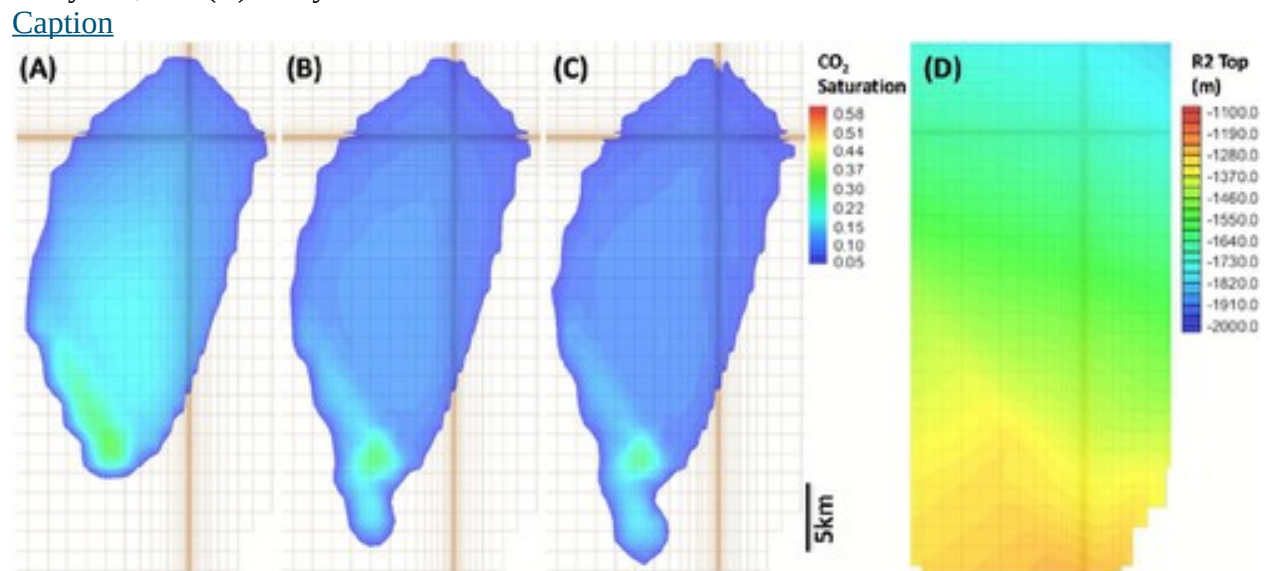Caption

Figure 9

CO₂ saturation in R2 from T2MP (showing the top of R2). (A) t = 350 years; (B) t = 750 years; (C) t = 1000 years. (D) R2 top elevation.
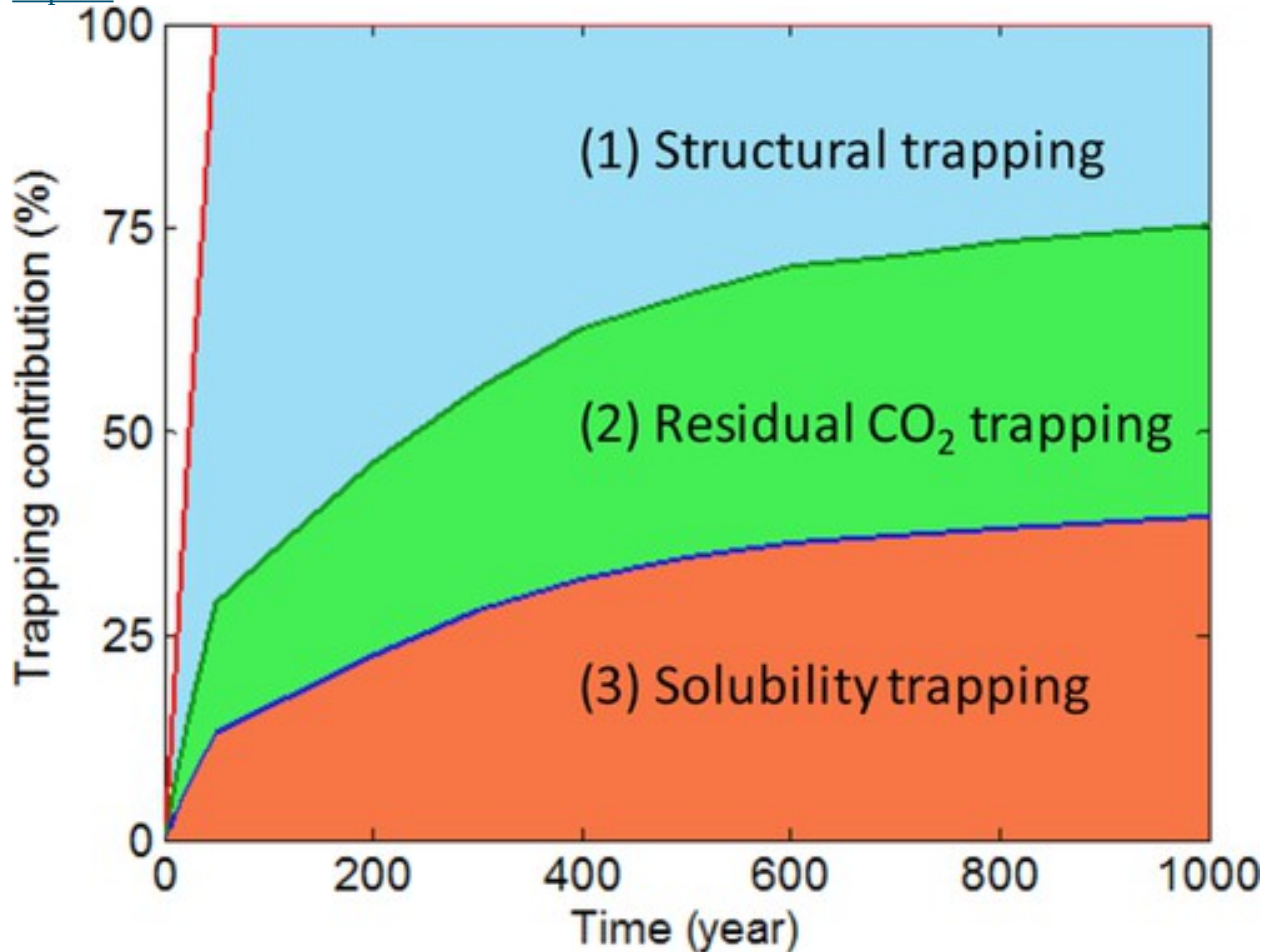
Figure 10

CO_2 trapping contribution (percentage of the total mass) as a function of simulation time using T2MP. The total 150 Mt CO_2 stored at the South Scania Site consists of three components: (1) Structural CO_2 trapping, the injected CO_2 with saturation greater than the residual ($S - S_{gr}$); (2) Residual CO_2 trapping, i.e. the trace CO_2 saturation ($S = S_{gr}$) if gaseous CO_2 has visited a certain pore volume; (3) Solubility trapping, i.e. the CO_2 dissolved in the aqueous phase.

Discussion

A detailed comparison focusing on the two numerical approaches is given in the following section. The limiting factors for the CO_2 storage at the South Scania site are then identified and followed by a perspective for the use of the integrated workflow.

Indication from numerical simulations

We take R2, the most permeable unit, as an example and compare the simulation results from the three different approaches. At an annual injection rate of 1.23 Mt, the semi-analytical approach gives a pressure build-up of 10% (Fig. 5). It can be seen that the pressure responses from the two numerical models are quite similar (Fig. 6) and also in reasonably good agreement with those from the semi-analytical model. Note that although the near wellbore pressure increase exhibits a seemingly linear relationship with the mass injection rate, it is actually a non-linear relationship due to the effect of CO_2 compressibility.

The pressure build-up is most sensitive to the transmissivity of the reservoir layers. The effect of the chosen boundary condition is most significant in R2 where the boundary condition change from BS1 (all fault zones closed) to BS2 (all fault zones open) allows for a doubled injection rate.

The plume migration on the other hand is clearly faster in the VE model than that from T2MP. The reason for this is the lack of the retardation mechanisms of CO_2 dissolution and residual trapping in our current implementation of the VE model which causes the model to overestimate the CO_2 migration. Therefore, the results of the VE model should be taken as indicative and serving as guidance for the 3D T2MP modeling.

It is of interest to look at the mass distribution in different trapping states as a function of time based on a comprehensive T2MP simulation. The CO_2 inventory is given as contributions (percentage of the total mass) from the different trapping mechanisms (structural trapping, residual trapping and solubility trapping; Fig. 10). After the end of the injection both the residual and the dissolution trapping continue to increase gradually while the proportion of structurally trapped CO_2 decreases. After 350 years, more than 50% of the injected CO_2 is already in residual or dissolved state. At around year 500, the three trapping mechanisms give almost equal contributions and at the end of year 1000, more than two thirds of the total CO_2 has been trapped residually or by dissolution. A follow-up T2MP run indicated that the system will stabilize at around year 1400. The results are identical to Fig. 9(c) and thus not included for space consideration.

It can be inferred that the VE approach with the sharp interface assumption can be used reasonably well to predict the spatial distribution of the plume if the structural trapping is the prominent mechanism or otherwise to present a somewhat exaggerated yet indicative scenario of the migration, due to the lack of physical/geo-chemical retardation mechanisms. On the other hand, the capable but computationally more demanding T2MP should be used when a viable

injection scenario has been formulated and CO_2 migration is understood to be a limiting factor for the storage capacity.

The integrated modeling

We started the South Scania site modeling with a relatively simple semi-analytical model (Model 1) and concluded the modeling with the comprehensive T2MP (Model 3). The flexible VE approach (Model 2) was used to bridge the two. The VE model produced reasonably good result for the CO_2 footprint, compared to the 3D T2MP model, despite the fact that it does not include residual and dissolution trapping (in current work).

From the computational perspective, the implementation of VE is noticeably less demanding than the T2MP approach. For the current problem configuration (SI), the VE simulation took roughly 1 h (1 CPU) while the time needed by T2MP was at the order of 30 h using 16 CPUs on a cluster. The computational advantage of VE made it possible to conduct several trial runs to test the range of injection rates. We deliberately put aside the couplings of geochemistry and geomechanics which are even more computational demanding. The combination of VE and T2MP enables interpretation of the trapping caused by, for example, residual and dissolution. If the CO_2 migration following caprock topography is the main concern then the VE approach can be used individually to predict the CO_2 migration.

In this work, the complexity level of the modeling increased alongside with gradually improved/more detailed understanding of the site properties, as the more complex models require and/are capable of incorporating more data detail. It is to be noted that the level of complexity can be further increased by, for example, including the permeability or porosity heterogeneity within the individual layers. More advanced coupling, for example the use of TOUGHREACT[44] (geochemistry) and TOUGH-FLAC[45] (geomechanics), is beyond the scope of this study. The idea of integrated modeling using various approaches can be further extended to serve different modeling objectives.

Conclusions

The overall objectives of this work have been (i) to get first estimates of CO_2 storage capacity in the South Scania site in a specific scenario where injection takes place from one existing vertical well into the layered formation and, (ii) to present a modeling framework where models of increasing complexity are successively employed to carry out such an estimation. In this framework the simpler models are first used to make a larger amount of scoping simulations (semi-analytical and VE models) that help to design the exact model scenarios for the more

detailed and computationally more demanding models (T2MP). Throughout, the results of the different models are compared against those of each other. In terms of the pressure response, the results of all three methods can be compared while the migration behavior can be compared based on the two numerical models. The successive use of multiple models also provides increased confidence in the overall model results, which is important for long-term model predictions.

It is identified that the limiting factor for the CO_2 storage at the South Scania site is the CO_2 migration within the high permeability unit (R2). This CO_2 containment limitation gives a maximum injection rate of about 3 Mt CO_2 per year during a 50-year injection operation through a vertical borehole at FFC-1. The site is thus adequate for storing a total of 150 Mt CO_2 given the current injection scenario and hydrogeological parameters. This capacity estimate is subject to variations due to the uncertainties and heterogeneities in the permeability,[46] porosity, and layer thickness. An evaluation of the uncertainty bounds of the capacity estimates can be carried out when more detailed (hydro)geological information is available.

Alternative injection scenarios that can more efficiently use the total capacity of the site include injecting, for example, through horizontal or vertical wells into the lower units (R3 and R4) only, where the permeability is not as high but the total thickness considerable. These alternative scenarios should be tested in future studies.

Acknowledgments

Biographies

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