Model complexity and choice of model approaches for practical simulations of CO_2 injection, migration, leakage and long-term fate

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Abstract

This report documents the accomplishments achieved during the project titled "Model complexity and choice of model approaches for practical simulations of CO_2 injection, migration, leakage and long-term fate" funded by the US Department of Energy, Office of Fossil Energy. The objective of the project was to investigate modeling approaches of various levels of complexity relevant to geologic carbon storage (GCS) modeling with the goal to establish guidelines on choice of modeling approach. To achieve this objective, a thorough literature review was undertaken and the following five modeling approaches were identified as being relevant to GCS modeling: (1) fully coupled three-dimensional models, (2) simplified three-dimensional models, (3) vertical equilibrium models, (4) single-phase models, and (5) macroscopic invasion percolation models. In order to fill gaps in the model complexity spectrum, two new modeling approaches were developed. The newly developed vertical dynamic reconstruction approach couples vertical segregation dynamics with vertically-integrated equations, thereby eliminating the need for the vertical equilibrium assumption in vertically integrated models. This new approach lies between simplified three-dimensional models and vertical equilibrium models on the model complexity spectrum. The second approach couples viscous effects with macroscopic invasion percolation models, and thus lies between simplified three-dimensional models and macroscopic invasion percolation models. In order to determine the applicability of the modeling approaches to different types of storage formations and GCS related questions, the modeling approaches were applied to five example sites (Sleipner, In Salah, Basal Cambrian Aquifer, Ketzin, and Kimberlina), and a set of guidelines were established based on the modeling results for these cases, as well as other modeling results reported in the literature. Single-phase models are the appropriate choice for basin-wide pressure response modeling. For cases where multi-phase flow effects cannot be neglected and vertical segregation of CO_2 and brine is fast (i.e., vertical permeability higher than 100 mD), vertical equilibrium models should be used. If vertical segregation dynamics need to be included and vertical flow due to heterogeneity in formation parameters is low, the newly developed vertical dynamic reconstruction approach is the most appropriate modeling approach. Simplified three-dimensional models are the approach of choice for circumstances with complex three-dimensional flow dynamics, for instance close to an injection well or in formations with significant three-dimensional heterogeneity. The most complex approach – fully coupled three-dimensional models – should only be used if there is significant two-way coupling between flow and geochemistry or geomechanics. Lastly, it appears that macroscopic invasion percolation models are not appropriate for GCS modeling except under specialized circumstances.

Table of contents

1 Executive summary

The main goal of this project was to assemble a set of modeling approaches relevant to geologic carbon storage (GCS) across the spectrum of model complexity, and to determine the applicability of these modeling approaches to different conditions and questions relevant to GCS. In addition to five existing modeling approaches, two new modeling approaches were developed during this project to fill in gaps in the model complexity spectrum. The following five existing modeling approaches were considered in this project: (1) fully-coupled models (include three-dimensional multi-phase flow as well as geochemistry and/or geomechanics and two-way interactions between flow, geochemistry and geomechanics), (2) simplified three-dimensional models (include three-dimensional multi-phase flow, but neglecting geochemistry and geomechanics), (3) vertically-integrated vertical equilibrium models (two-dimensional vertically-integrated flow with the assumption of vertical pressure equilibrium of CO_2 and brine), (4) single-phase models (include only brine flow, neglecting multi-phase flow effects), and (5) macroscopic invasion percolation models (three-dimensional migration of CO_2 governed by successive invasion of grid cells based on capillary invasion criteria; this approach neglects viscous resistance to flow).

In addition to the five existing approaches, two new modeling approaches were developed during this project: (1) a vertically-integrated approach that takes the vertical dynamics of CO_2 and brine segregation into account, and (2) an approach based on macroscopic invasion percolation that takes viscous effects into account. In vertically-integrated approaches, the three-dimensional governing equations of multi-phase flow are integrated over the thickness of the formation, and vertical pressure equilibrium of CO_2 and brine (i.e., no vertical flow) is usually assumed to reconstruct the saturation profiles. In the newly developed approach, termed dynamic vertical reconstruction (Guo et al., 2014), instead of assuming vertical equilibrium, the segregation dynamics are included by coupling one-dimensional (vertical) models of counter-current vertical flow with the two-dimensional vertically-integrated flow equations. While the new approach adds the need to solve many one-dimensional systems along with the two-dimensional system, the overall computational cost increases only slightly, because solving one-dimensional systems requires relatively little computational time. The dynamic reconstruction approach has been shown to compare well to simplified three-dimensional models, both for homogeneous formations (Guo et al., 2014) and for layered formations such as sedimentary basins (Guo et al., 2016a).

Two improvements to the macroscopic invasion percolation approach were investigated in this project: the use of capillary pressure – saturation relationships to allow partial filling of grid cells and the incorporation of viscous effects to represent flow resistance and to enable post-injection modelling. Comparisons to experimental data did not show any advantages of the newly developed enhanced macroscopic invasion percolation algorithms over simplified three-dimensional models. These algorithms were therefore not included in model applications at the example sites.

In order to investigate the applicability of the modeling approaches to issues related to GCS, the following five example sites were chosen: (1) the Basal Cambrian Aquifer in Canada, (2) the Sleipner CO_2 injection site in Norway, (3) the In Salah site in Algeria, (4) the Ketzin site in Germany, and (5) Kimberlina site in California. The Basal Cambrian Aquifer was chosen due to its large spatial extent, and vertical equilibrium models and single-phase models (numerical and semi-analytical for both approaches) were run to investigate the basin-wide pressure response. The results showed that the numerical single-phase and the numerical two-phase vertical equilibrium models gave very similar results, while the semi-analytical models were not able to match those results, suggesting that at the basin scale large-scale lateral heterogeneity is important while multi-phase flow effects are not (Huang et al., 2014). The Sleipner CO_2 injection site was chosen, because both a geologic model for the site and plume monitoring data are available, and because CO_2 has been injected at an industrial scale for over a decade. Vertical equilibrium, dynamic reconstruction and simplified three-dimensional models were run for this site, and all three approaches gave comparable results, suggesting that vertical equilibrium models are the appropriate choice for this site, due to the high vertical permeability (Bandilla et al., 2014). The In Salah site was included in this project, because surface uplift was used for monitoring and fully-coupled models (flow and geomechanics) were used to interpret the surface uplift. A literature review showed that fully-coupled models were best able to match the measured surface uplift (Rinaldi & Rutqvist, 2013), while decoupled models (i.e., models where fluid flow is solved first and surface uplift is modeled afterwards) were not sensitive enough to estimate the location of some of the important geological features (Morris et al., 2011). The Ketzin site is characterized by channelized heterogeneity in the injection formation, due to its fluvial deposition history. Simplified three-dimensional and vertical equilibrium models were applied to a set of synthetic models with relatively simple channel geometries to determine if vertical equilibrium models are able to predict CO_2 and brine migration for geologic conditions such as found at the Ketzin site. The results show that vertical equilibrium models are able to accurately predict the CO_2 plume for many channel configurations, if there is a significant difference in capillary entry pressure between the channel and background materials. The impact of modeling approach choice on optimization studies was investigated using geologic data from the Kimberlina site. Vertical equilibrium and simplified three-dimensional models were used in an optimization framework, to determine optimal active pressure management operations to protect a fault adjacent to the CO_2 injection. Both approaches lead to similar results, however the optimal locations of the production wells were different due to high sensitivity of the well location to the predicted CO_2 plume.

Based on modeling results from this project and from the literature a set of guidelines for the choice of modeling approach for GCS simulations has been assembled. Single-phase models are the appropriate choice when investigating basin-wide pressure response, where the CO_2 plumes are small compared to the overall model domain. Vertical equilibrium models are applicable at both the site and basin scales, if the vertical permeability is above 100 mD and if vertical heterogeneity in the injection formation is not expected to lead to complex three-dimensional CO_2 migration. For sites with vertical permeability of less than 100 mD dynamic reconstruction models are the appropriate modeling approach, unless permeability patterns leads to significant three-dimensional flow. Simplified three-dimensional models are able to accurately represent complex three-dimensional flow, and are therefore the appropriate modeling approach at the site scale for cases with significant vertical flow (e.g., close to the injection well) and strong change in fluid properties (e.g., density change due to pressure change). Fully-coupled models should only be used if there is a significant feedback between formation properties (e.g., porosity and permeability) and geochemistry and/or geomechanics.

2 Report details

2.1 Introduction

Geologic carbon storage (GCS) is the storage component of the climate change mitigation technology called carbon capture and storage (CCS). In CCS carbon dioxide (CO_2) is captured at large stationary CO_2 sources such as coal fired power plants. The captured CO_2 is then injected into the deep subsurface for permanent storage. While different types of storage complexes have been investigated, deep saline aquifers are the most likely storage reservoirs due to their large storage capacity and relatively wide distribution throughout the world (Metz et al., 2005). In order to achieve the goal of safe and permanent storage, the injected CO_2 needs to remain in the storage complex. Computational modeling is usually necessary to predict the migration of CO_2 in the subsurface. In addition, the injection-induced migration of the resident brine also needs to be modeled, as brine may have deleterious impacts on underground sources of drinking water (USDW) should it migrate into shallow subsurface zones.

The migration of CO_2 and brine is usually modeled using multi-phase flow models. Due to the high density difference of CO_2 and brine (on the order of 250 - 750 kg/m^3), CO_2 has a strong buoyant drive in the vertical direction, along with a pressure drive due to injection-induced pressure gradients. In addition to the multi-phase flow effects many other processes may impact the migration of CO_2 and brine. For instance, CO_2 may dissolve into brine, increasing the density of the brine and thus leading to convective mixing (e.g., Emami-Meybodi et al., 2015; Riaz et al., 2006). Having CO_2 and brine co-occupy the pore space leads to the possibility of a number of chemical reactions with the potential to alter the pore space through dissolution and/or precipitation of minerals. While the precipitation of carbon minerals is advantageous, as it immobilizes the injected CO_2, the pore space alteration may also impact the intrinsic permeability of the formation, potentially leading to preferential flow paths or loss of injectivity (Gaus, 2010). CO_2 injection alters the stress state of the subsurface, potentially triggering seismic events. While the majority of seismic events are too weak to have an impact at the surface, they may increase permeability by creating new fractures or reactivating existing fractures. Larger seismic events may be problematic for a GCS operation, as large-scale faults may be reactivated, creating conduits for the injected CO_2 to the shallow subsurface or even the atmosphere (Zoback & Gorelick, 2012). If the seismic events are felt at the surface, they will also decrease public acceptance of GCS projects.

CO_2 and brine migration related to GCS operations involves several different spatial scales, ranging from the pore scale to the basin scale. Many questions, such as storage security or operational scheduling, are investigated at the site scale – typically hundreds of meters to tens of kilometers. At this scale multi-phase flow (pressure drive, buoyancy drive) tend to be the dominant processes, although smaller-scale processes may also be important. For instance, pore space alteration due to dissolution/precipitation of minerals occurs at the pore scale, but can have an impact on the flow at the site scale. Convective mixing, driven by dissolution of CO_2 into brine, is caused by vertical viscous fingering with finger diameters on the order of tens of centimeters. The impact of these smaller-scale processes are often represented as up-scaled parameters in site-scale models, for instance as changes in permeability for the case of dissolution/precipitation or enhanced dissolution rates for convective mixing. Other processes, such as flow along concentrated leakage pathways (e.g., faults or abandoned wells), cannot be as easily up-scaled, and have to be directly represented in site-scale models. While many GCS related questions are answered at the site scale, some questions need to be investigated at other scales. For example, the degradation of well cement in the presence of CO_2-saturated brine or pure CO_2 occurs at the pore scale where some processes (e.g., buoyancy, convective mixing) do not play a significant role. On the other hand, questions about the impact of industrial-scale deployment of CCS need to be addressed at the basin scale (hundreds of kilometers). In this case many of the processes (e.g., buoyancy, pore-space alteration) are not as important and questions posed at the very large scale are often answered adequately by single-phase flow models.

Due to the multitude of processes and scales, there are many different approaches to model CO_2 and brine migration. In this project we examined a variety of modeling approaches with complexity ranging from three-dimensional models coupling multi-phase flow, geochemistry and geomechanics to two-dimensional single-phase models. These modeling approaches have in common that they are based on a combination of mass balance equations and Darcy flux equations. For the multi-phase flow approaches a set of constitutive relationships also needs to be included. Depending on the complexity of formation geometries and fluid properties, the set of governing equations are solved numerically or semi-analytically. More details on the governing equations can be found in Nordbotten and Celia (2012) and Bandilla and Celia (2016), and are thus not presented here.

The goal of the project presented here was to investigate the impact of modeling approach complexity on GCS modeling results and how to identify the most appropriate modeling approach for a given combination of site parameters and questions asked. To accomplish these goals a literature review was conducted to identify modeling approaches used for GCS modeling. In addition, two new modeling approach were developed. A set of five example GCS sites (Sleipner, In Salah, Basal Cambrian Aquifer, Ketzin and Kimberlina) were chosen to compare different modeling approaches for realistic conditions, and based on those comparisons – and others from the literature – a set of modeling approach guidelines was formulated.

In this report we first summarize a literature review of GCS modeling approaches, and then discuss the two new modeling approaches developed during this project. This is followed by the comparisons of the different modeling approaches at the five example site. Finally, a set of guidelines for choice of modeling approach are formulated.

2.2 Existing methods

The first step in assessing the appropriateness of complexity level for different modeling approaches was to identify the modeling approaches that have been applied to investigations related to GCS. The following section is a summary of a literature review on modeling approaches used for GCS modeling; for the full literature review the reader is referred to Bandilla et al. (2015). The literature review identified the following modeling approaches as relevant to GCS modeling:

- Fully-coupled three-dimensional: in this approach three-dimensional multi-phase flow is coupled to geochemical and/or geomechanical models, so that impacts of changes to flow-related properties (e.g., porosity, permeability) due to feedback from pressure changes (geomechanics) or reactive solute transport (geochemistry).
- Simplified three-dimensional: where the three-dimensional governing equations of multi-phase flow are solved to simulate migration of CO_2 and brine in the subsurface. While this approach neglects the impacts of geochemistry and geomechanics on flow, the flow solution can be used as a basis for decoupled geochemical (e.g., solute transport for monitoring analysis) and geomechanical modeling (e.g., for surface uplift).
- Vertically-integrated: here, the three-dimensional governing equations of multi-phase flow are integrated over the thickness of a formation, leading to set of two-dimensional (parallel to the bedding plane) governing equations in terms of reference phase pressures and depth-averaged phase saturations. In order to calculate the integrated phase mobilities – important parameters in the two-dimensional integrated equations – the relative permeability profiles need to be reconstructed along the direction of integration (perpendicular to bedding). The vertical equilibrium assumption is commonly invoked to reconstruct the saturation profiles from which the relative permeability profiles are calculated. Under certain conditions (e.g., homogeneous formation properties, sharp interface between CO_2 and brine), the resulting vertically-integrated governing equations can be solved analytically.
- Macroscopic invasion percolation: in this approach CO_2 migration is modeled through a series of invasion events where the invasion is based on considerations of capillary entry pressure. The domain is discretized into cells, and once a particular cell is filled, CO_2 invades an adjacent cell depending on capillary invasion criteria. Unlike the approaches described above, viscous forces are neglected in the macroscopic invasion percolation approach, and transient behavior is only introduced if a specific-flux source term drives the flow.
- Single-phase: for single-phase models only the governing equations for one phase (brine) are solved, essentially neglecting any multi-phase flow effects. In the context of GCS, the single-phase governing equations are usually solved in their vertically-integrated form.

In the context if GCS, fully-coupled three-dimensional models are considered the most complex modeling approach, because all relevant processes and their interactions are represented. For cases where the impacts of geomechanics and geochemistry on multi-phase flow can be neglected, simplified three-dimensional models can be used; the modeling is simplified by reducing the represented processes, focusing on flow dynamics only. Simplified three-dimensional models can be further simplified, if the vertical segregation of CO_2 and brine occurs fast relative to the model time-scale. The three-dimensional governing equations can then be integrated over the thickness of the formation, leading to a set of two-dimensional governing equations which are the basis for vertical equilibrium models; simplification comes in the form of reducing the dimensionality of the problem. If the formation can be assumed to be homogeneous, vertical equilibrium models can sometimes be solved analytically, resulting in simplified vertical equilibrium models. A second approach to simplify the simplified three-dimensional models is to neglect multi-phase flow effects while retaining the three spatial dimensions. The resulting single-phase models are simplified by reducing the represented processes. Macroscopic invasion percolation models take a different simplification approach. Viscous effects (that is, flow dynamics) are neglected while maintaining a two-phase system, and fluid migration is determined by capillary-based invasion criteria where capillary pressures are based on density differences and formation topography. I these models, the three-dimensional structure of the domain is retained and can be represented at fine scales due to the computational simplicity of the approach.

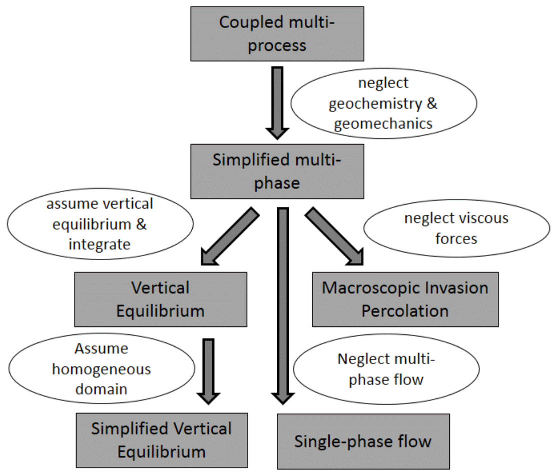


Figure 1: Model complexity hierarchy taken from Bandilla et al. (2015). Coupled multi-process models are referred to as fully-coupled models in the text; simplified multi-phase models are referred to as simplified three-dimensional.

The above modeling approaches have been applied to GCS modeling, both for real sites and for hypothetic domains. The majority of studies have used simplified three-dimensional simulators – such as TOUGH2, MRST, Eclipse or CMG-GEM – to simulate CO_2 and brine migration at both the site and basin scale. Simplified three-dimensional simulators appear to be the preferred approach when designing injection operations and interpreting monitoring data. The use of fully-coupled models is fairly limited, with usually only geochemistry or geomechanics being considered. For instance, a model coupling flow with geochemistry was used to investigate the impact of precipitation/dissolution at the Sleipner site (Audigane et al., 2007), while models coupling flow and geomechanics were used to explain the dual-lobe surface-uplift at the In Salah site (e.g., Rinaldi & Rutqvist, 2013). Due to their computational efficiency, vertical equilibrium models have mainly been applied at the basin scale to address questions of long-term storage safety (e.g., Gasda et al., 2012) and dynamic storage capacity estimates (e.g., Bandilla et al., 2012). Celia et al. (2011) used a simplified vertical equilibrium model to conduct a study of basin-wide leakage along abandoned wells, taking into account the uncertainty of well permeability. The use of single-phase models is mainly restricted to the study of large-scale pressure response to CO_2 injection (e.g., Huang et al., 2014; Nicot, 2008), where CO_2 plumes are very small compared to the model domain. Macroscopic invasion percolation models have seen very limited application in GCS modeling. Cavanagh (2013) used a macroscopic invasion percolation model to history-match the CO_2 plume in the 9^{th} layer of the Utsira formation at the Sleipner site.

Exploration of the existing approaches for GCS modeling pointed to two gaps in the modeling approaches spectrum. First, all vertically-integrated multi-phase flow models relied on the vertical equilibrium assumption for reconstruction of the saturation profiles. However, vertical equilibrium is not a requirement for vertically-integrated models, and therefore vertically-integrated models incorporating the vertical dynamics of CO_2 and brine segregation would fall between simplified three-dimensional and vertical equilibrium models on the complexity spectrum. Second, an approach that uses the conceptual approach of macroscopic invasion percolation models, while incorporating the resistance to flow due to viscosity, would fill the gap between simplified three-dimensional and macroscopic invasion percolation models. The investigation and development of such approaches is discussed in the next section.

2.3 Newly developed approaches

2.3.1 Dynamic vertical reconstruction

Vertically-integrated modeling approaches are derived by integrating the three-dimensional governing equations of multi-phase flow (i.e., phase mass conservation, Darcy phase mass fluxes) over the thickness of the formation. The integration results in a set of two-dimensional governing equations parallel to the bedding plane of the formation. While the structure of the governing equations does not change with integration, the primary unknowns of the vertically-integrated equations are the depth-averaged phase saturations and phase reference pressures (e.g., defined as the pressure at the bottom of the formation), instead of three-dimensional saturation and pressure fields. Also, parameters such as porosity and intrinsic permeability change from point values to integrated values. Integrating the phase relative permeabilities is more problematic, as the relative permeability profiles depend on the saturation profiles, instead of on the depth-averaged saturation given by the vertically-integrated equations. This means the vertical saturation profiles need to be reconstructed based on the depth-averaged saturation. The common approach is to take advantage of the density difference between CO_2 and brine (250 – 750 kg/m^3), which means that vertical segregation occurs relatively quickly. In vertically-integrated models it is commonly assumed that the segregation time scale is much shorter than the time scale of lateral migration, so that it can be assumed that the two fluids have completely segregated and no more flow occurs in the vertical direction. In this case the fluids are at pressure equilibrium (i.e., both are at “hydrostatic” pressure), and therefore the assumption of fast segregation is termed the *vertical equilibrium assumption*. Based on the vertical equilibrium assumption, closed-form algebraic expressions are used to reconstruct the saturation profiles needed for the integrated relative permeabilities. Court et al. (2012) found that the vertical equilibrium assumption is usually valid if the vertical permeability is higher than about 100 mD (10^{-13} m^2). Therefore, vertical equilibrium models are not appropriate at GCS site with low vertical permeability.

As part of the project reported on here, Guo et al. (2014) developed a new vertically-integrated modeling approach, that does not rely on the vertical equilibrium assumption, and thus extends the applicability of vertically-integrated models to cases with lower vertical permeability. The new approach directly represents the vertical segregation dynamics of CO_2 and brine, and is thus termed the *vertical dynamic reconstruction* approach. The general idea of the approach is to model the segregation of CO_2 and brine as one-dimensional (vertical) counter-current flows, instead of assuming vertical equilibrium. The overall solution approach remains the same as for vertical equilibrium models, with the same vertically-integrated equations being solved numerically on a two-dimensional grid. However, instead of using algebraic equations to reconstruct the saturation profile at the end of each time step, one-dimensional numerical models of CO_2 and brine flow are solved to simulate flow dynamics in the vertical direction. The one-dimensional column models are independent of each other, as the inter-column fluxes are lagged by one time step. The additional computational cost of the new approach compared to the vertical equilibrium approach is the numerical solution of a set of small one-dimensional models. A comparison of the dynamic reconstruction approach to a fully discretized model and a vertical equilibrium model for a case with a permeability of 10 mD shows, that the dynamic reconstruction model is able to represent the segregation dynamics, while the vertical equilibrium model fails (Figure 2). For a more detailed derivation of the dynamic reconstruction model and for additional test cases the reader is referred to Guo et al. (2014).

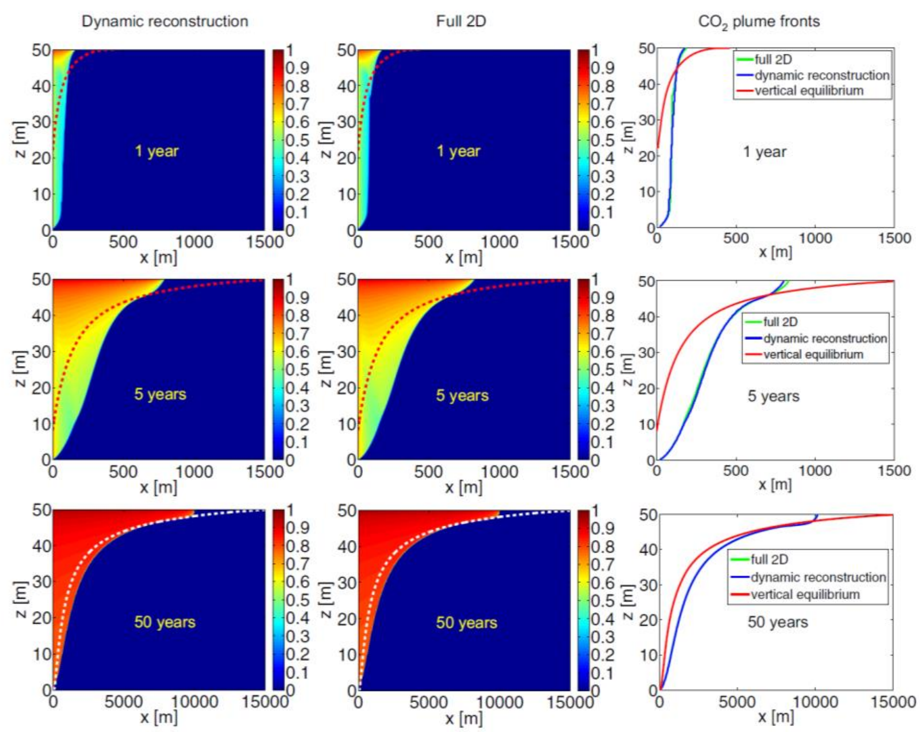


Figure 2: Comparison of a dynamic reconstruction model, a fully-discretized model (Full 2D) and a vertical equilibrium model (dashed lines) for a homogeneous formation with a permeability of 10 mD. Taken from Guo et al. (2014).

An additional limitation for vertical equilibrium models are formations with significant heterogeneity in vertical permeability, such as in layered sedimentary systems. While vertical equilibrium models have been applied to cases of alternating high and low permeability formations (Bandilla et al., 2012; Gasda et al., 2009), significant layering within a formation poses problems for vertical equilibrium models, because vertical permeability is not represented. Based on the dynamic reconstruction approach, Guo et al. (2016a) developed a multi-layer approach, termed *multi-layered dynamic reconstruction* that extends the applicability of vertical equilibrium models to cases with layered formations. Each layer in the formation is represented by a vertically-integrated model with vertical dynamic reconstruction, and the stacked models are coupled through vertical CO_2 and brine fluxes based on the pressure difference between adjacent layers. In the limit, as the number of layers is increased (i.e., the vertical resolution), the multi-layered dynamic reconstruction approach resembles a simplified three-dimensional model. A comparison of the multi-layered dynamic reconstruction model to a simplified three-dimensional model shows good agreement between the two models for a case with four layers based on formation parameters of the Mount Simon Sandstone (Figure 3). More details on the approach and additional test cases are presented in Guo et al. (2016a).

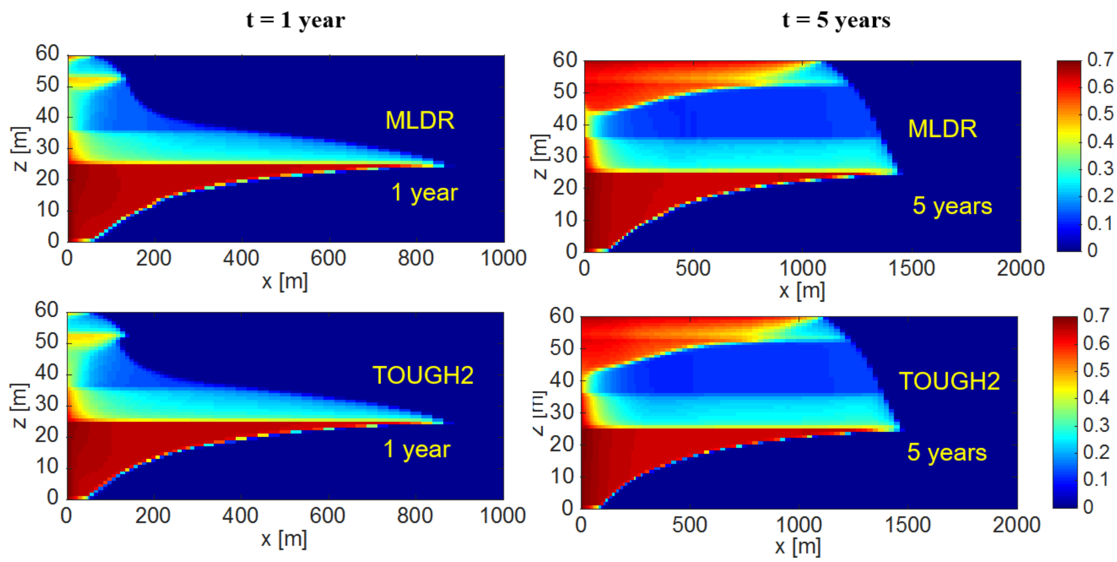


Figure 3: Comparison of a multi-layered dynamic reconstruction model (MLDR) to a simplified three-dimensional model (TOUGH2) for a test case with four layers based on the Mount Simon Sandstone and injection into the lowest layer. Taken from (Guo et al., 2016a).

The development of the vertical dynamic reconstruction approach closes the gap in the modeling approach complexity spectrum between simplified three-dimensional models and vertical equilibrium models by extending the applicability of vertically-integrated models to formations with lower vertical permeability and formations with vertical layering in permeability. It should also be noted that the computational cost of solving the one-dimensional column models is small compared to the solution of the vertically-integrated equation, which means that the vertical dynamic reconstruction approach retains the computational efficiency of other vertically-integrated modeling approaches.

2.3.2 Invasion percolation with viscosity

As shown by several studies in the literature (Cavanagh, 2013; Cavanagh & Ringrose, 2011), invasion percolation (IP) models are computationally very efficient due to the underlying relatively simple algorithms. Both Darcy's law and the gravity-capillary balance solved by IP approaches can be derived from the same multiphase continuum momentum equation under different limiting conditions (Oldenburg et al., 2016). Oldenburg et al. (2016) presented a detailed review for the degree of capability of Darcy's law and IP approaches for various large-scale GCS driving forces and processes. In the IP approach, gravity and capillarity are assumed to be the dominant driving forces in a quasi-static two-phase system. The computational efficiency of the IP-based simulators allows use of very fine grids that honor fine-scale stratigraphic details of the storage reservoir. This makes these IP models suitable for analyzing the impact of small-scale heterogeneities on flow. However, the neglect of viscous effects and the lack of time-dependence in the IP models are significant disadvantages in comparisons to the Darcy's law based models that can simulate single-phase and multiphase flows with viscous, gravitational and capillary forces included.

A variation of the IP approach was used by several researchers (Braun et al., 2005; Glass et al., 2001; Glass & Yarrington, 2003; Ioannidis et al., 1996; Kueper & Mcwhorter, 1992; Yortsos et al., 1993) in large domains where each lattice site represents a macroscopic domain defined by local effective properties (i.e., equivalent pore size or equivalent entry pressure, or local capillary pressure-saturation and relative permeability functions). This approach, referred to as the Macroscopic IP (MIP) was also used to develop upscaled relationships for two-phase flow parameters in large domains with sub-grid scale heterogeneities (e.g., Yang et al., 2013).

As a part of this project, we developed new MIP modeling approaches and tested their capabilities using some experimental data and traditional two-phase flow models. As described in the following sub sections, we first developed an enhanced MIP model including buoyant and capillary forces only. This new model can be useful for quick rough estimates of plume migration and distribution during CO_2 injection. Secondly, we developed a continuum MIP model to include dynamic and viscous effects for simulating post-injection plume migration.

The macroscopic invasion percolation model developed in this work builds upon the earlier MIP modeling approaches with capillary and buoyancy effects (Carruthers, 2003; Ioannidis et al., 1996; Kueper & Mcwhorter, 1992; Yortsos et al., 1993) with a few improvements. Unlike the approach presented by Carruthers (2003) that assumed that invaded cells can be either at a critical non-wetting phase saturation or at a connate wetting phase saturation, this new model can allow fluid saturations at invaded cells to vary based on capillary pressure-saturation curves assigned to each cell that represent macroscopic distribution of fluids. A short description of the algorithm is presented below.

As in the IP approach, the domain is represented by a lattice and each lattice cell represents a macroscopic domain defined by local effective properties (i.e., equivalent pore size or equivalent entry pressure, or local capillary pressure-saturation and relative permeability functions).The algorithm employs an inequality based on the gravity-capillary force balance to simulate the migration of CO_2 expressed as $\Delta P_i + \Delta\rho\, g\, h_i > P_{d,i}$, where ΔP_i is the pressure difference (macroscopic capillary pressure) between the two fluid phases which initially are assumed to be equal to a capillary pressure corresponding to critical non-wetting saturation (or percolation threshold) at injection points. The second term represents the buoyant force; $\Delta\rho$ is the density difference, g is the gravitation acceleration and h_i is the vertical distance from cell i to the continuous bottom of the invading fluid. $P_{d,i}$ represents the entry pressure at cell i. Steps of the algorithm, termed *enhanced MIP*, during injection are given as follows:

1) Assign critical non-wetting saturations and associated macroscopic capillary pressure to injection points.
2) Calculate the total driving force, $\Delta P_i + \Delta\rho\, \boldsymbol{g}\, h_i$, at all faces between non-wetting and wetting fluid phase cells.
3) Select a cell for invasion next to a non-wetting invaded cell where $[\Delta P_i + \Delta\rho\, \boldsymbol{g}\, h_i - P_{d,i}]$ is positive and maximum. If there is positive value (i.e., the driving force is not sufficient to overcome resisting capillary force), the macroscopic pressure difference (Pc) is incrementally increased at all the cells unless the end of injection has been reached.
4) Update saturations from Pc-S functions at each cell involving non-wetting fluid.
5) Calculate time by dividing the total volume of the invaded non-wetting fluid to the injection rate.
6) Go to step 2 if the calculated time in (5) is less than the total injection duration. Otherwise, stop the computation.

In this second step we developed a continuum macroscopic invasion percolation model considering viscous forces in addition to capillary and buoyancy forces. The fluid-fluid interfaces move based on the solution of the pressure equation and a level-set equation in terms of a phase indicator function for two fluid phases, $\Phi \in [0,1]$. The level-set equation is represented as $\partial\Phi / \partial t + \nabla.(\boldsymbol{u} / \phi\Phi) = Q$, where $\boldsymbol{u}$ is the velocity of the interface obtained from a momentum balance equation, given by $-\mu / k\, \boldsymbol{u} = \nabla P + \rho g \nabla z + \nabla(P_d \Phi)$. ϕ is the porosity, and viscosity and density are defined respectively as $\mu = \mu_w + (\mu_n - \mu_w)\Phi$ and $\rho = \rho_w + (\rho_n - \rho_w)\Phi$. This model removes the limitation of the traditional MIP modeling approach by defining a time-scale when there is no injection, and as a result, it can simulate the post-injection plume distribution and viscous effects. However, as in the traditional two-phase flow model, there are still two coupled equations that need to be solved, but the equations of the continuum MIP model are simpler that those of the traditional two-phase flow model. Based on the results of our analyses, although the computational efficiency of the continuum MIP model is slightly higher than the traditional two-phase flow model, the continuum MIP model is still much less efficient than the MIP model. Thus, we did not further pursue testing and applying the continuum MIP modeling approach in this project as this model will not be preferred over more accurate traditional two-phase flow modeling approaches in GCS modeling applications.

In order to test the accuracy of the MIP and the traditional two-phase flow models, we simulated a laboratory experiment conducted by Trevisan et al. (2015). We used a uniform grid size of 0.5cm×0.5cm in a 2D domain, representing a synthetic aquifer (70cm×16cm) with an inclination of 2° (Figure 4a). Figure 4b shows the packing configuration used in one of the heterogeneous experiments. Fluids are assumed to be incompressible and immiscible. For the wetting fluid (glycerol-water 80-20% mixture), the density and viscosity values are 860 kg/m^3 and 4.9 mPa s, respectively. The surrogate fluids mimic the density and viscosity contrasts of supercritical CO_2 and brine under a deep reservoir condition. Figure 4a shows location of the injection zone and boundary conditions used in the simulations. No-flow conditions are set at the top, bottom and left boundaries, and constant pressures are kept at the right (outlet) boundary, modeld by very coarse sand in the experiments by Trevisan et al. (2015). More details on the experimental conditions and the properties of the materials can be found in (Trevisan et al., 2015) and (Cihan et al., 2016). The injection occurred at a rate of about 0.7 mL/min for 5.5 hours.

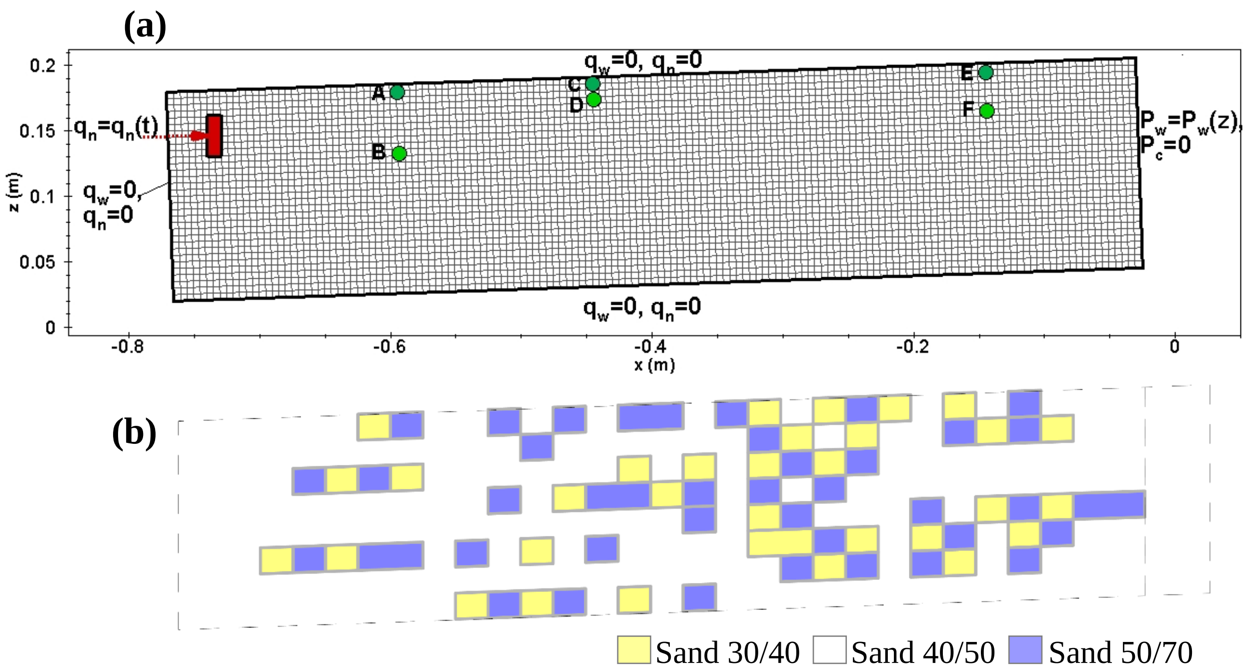


Figure 4: (a) The synthetic aquifer (70cm×16cm) with an inclination of 2° is represented in a 2D numerical domain by a uniform grid with cell sizes of 0.5cm×0.5cm. (b) Packing configuration. (adapted from Cihan et al., 2016).

A comparison of both a MIP model and a traditional two-phase flow model to experimental results – in terms of visual observations of spatial distribution of injected fluid saturation at different times – is presented in Figure 5. The MIP algorithm is extremely efficient compared to the numerical two-phase flow solver. However, the macroscopic invasion percolation model appears to overestimate plume migration and shape close to the injection zone, while at later times and farther away from the injection well the MIP model better represents the migration path of the injected fluid. However, the MIP model can only simulate the two-phase flow displacements during injection, due to quasi-static nature of the model. The two-phase model (based on the Finite-Volume method, using the same grid system as in the MIP model) represented the initial plume migration and saturation distribution much better than the MIP model as quantitatively shown by Figure 6, but at later times, the two-phase flow model appeared to overestimate the plume size and migration observed in the experiment. However, including a hysteretic model into the two-phase flow simulator (Cihan et al., 2016) significantly improved the predictions during the post-injection period (Figure 6). Based on the results, we conclude that Darcy's law-based models should be the preferred approach over MIP models for GCS simulations.

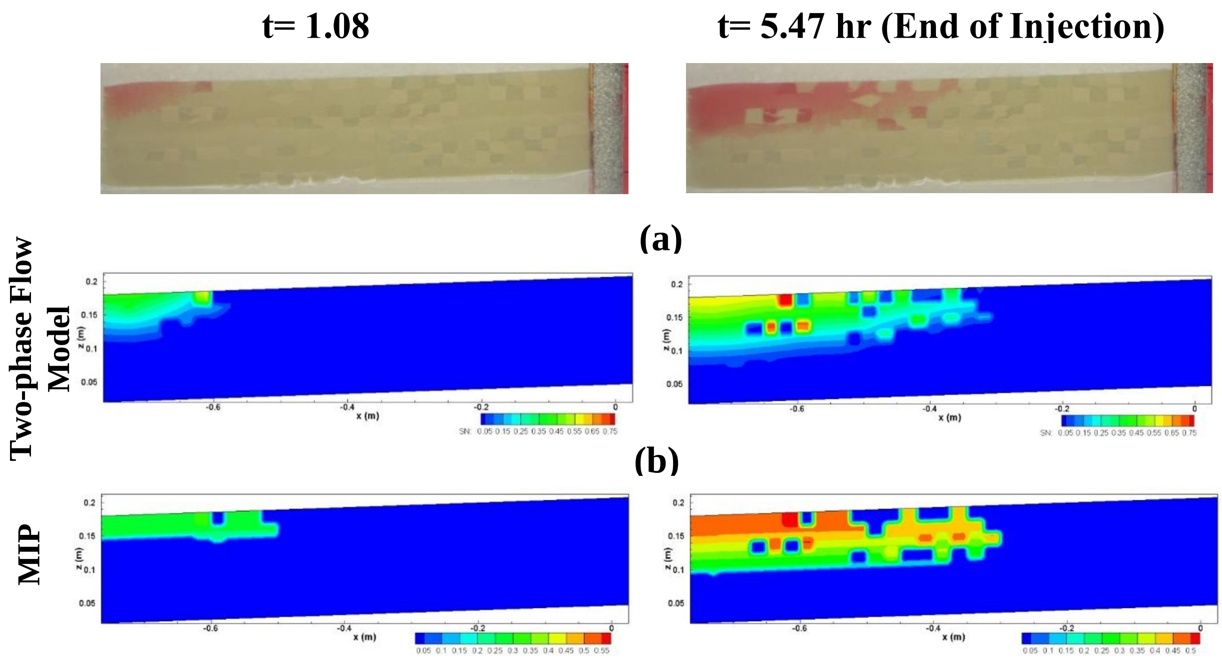


Figure 5: Comparison of the numerical model results for nonwetting fluid phase saturation distribution to experimental data under a heterogeneous sand packing condition. The figures show the results at 1.0 hr and 5.5 hrs for (a) the traditional two-phase flow model and (b) the MIP model. The heterogeneous packings include three sands: Accusands 30/40, 40/50 and 50/70. The fluids are Soltrol 220 (nw) and glycerol-water (80-20%) mixture (w).

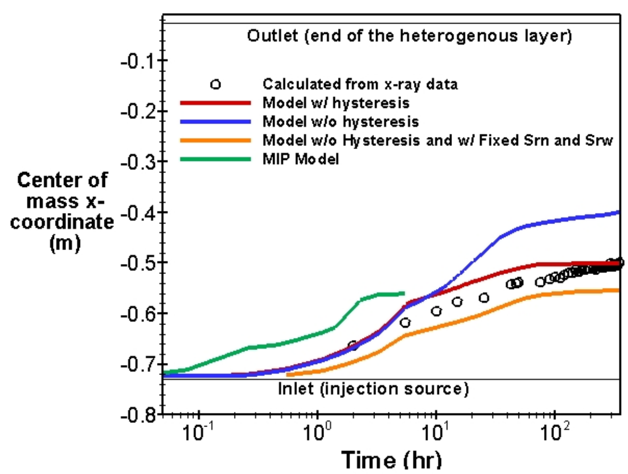


Figure 6: Temporal changes of the horizontal component of the plume centroid. The experimental spatial moment results are based on the x-Ray measurements of saturation at discrete points. The MIP model (green line) can represent the two-phase displacements only during the injection.

2.4 Application of models

2.4.1 Example site selection

As part of this project GCS modeling approaches were compared at five example GCS sites. The sites were chosen to represent a wide range of injection formation conditions, with each site highlighting a particular feature important to GCS modeling. The Cambrian Basal Aquifer was chosen as example of a domain with large spatial extent, where multiple CO_2 injection operations may access the same formation. The high permeability and long injection history coupled with extensive CO_2 plume monitoring make the Sleipner site interesting for site-scale modeling of CO_2 migration. The In Salah site is unique in that surface uplift was used for monitoring, and that coupled multi-phase flow and geomechanics models were necessary to interpret the uplift pattern. The Ketzin site was chosen due to the heterogeneity patterns based on the fluvial deposition history of the formation. The vicinity of several faults to the formerly proposed Kimberlina site, make it an interesting example to study optimal pressure management options. The following subsections discuss modeling studies at each of the five example sites.

2.4.2 Basal Cambrian Aquifer

The Basal Cambrian Aquifer is a spatially extensive saline aquifer system located in the northern Great Plains – Prairie region of North America (Peck et al., 2013), and covers an area of about 1,320,000 km^2 in three US states (North Dakota, South Dakota and Montana) and three Canadian provinces (Alberta, Manitoba and Saskatchewan). The formation properties (e.g., permeability, thickness, depth) are generally favorable for GCS, although the properties vary significantly spatially. For instance, the formation is very deep along the western boundary (up to 4500 m) and outcrops on the eastern boundary. There are also several large stationary CO_2 sources related to coal-fired power plants and oil and gas production in the vicinity of the Basal Cambrian Aquifer, and GCS operations are currently ongoing in the northeastern part of the Basal Cambrian Aquifer as part of the Shell Quest Carbon Capture and Storage Project (Bourne et al., 2014).

Huang et al. (2014) conducted a modeling study based on the Canadian portion of the Basal Cambrian Aquifer, with the goal of investigating the impact of modeling approach complexity on the basin-wide pressure response to industrial-scale CO_2 injection. The model covered an area of 811,000 km^2 and CO_2 was injected at nine sites over a period of 50 years at a combined rate of 62.7 Mt of CO_2 per year. Three numerical modeling approaches (vertically-integrated vertical equilibrium multi-phase with capillary transition zone, vertically-integrated vertical equilibrium multi-phase with sharp interface, and vertically-integrated single-phase) and two semi-analytical modeling approaches (vertically-integrated vertical equilibrium multi-phase with sharp interface and vertically-integrated single-phase) were used in the study. The authors found that the three numerical models agreed well with each other, both in terms of pressure distribution and area of significantly elevated pressure, while the two semi-analytical solutions were not able to capture the pressure accurately (Figure 7). These results suggest that vertically-integrated single-phase models are sufficient to simulate the basin-wide pressure response induced by GCS operations, because the CO_2 plumes are small compared to the size of the model domain and thus multi-phase flow effects can be neglected. The second conclusion based on these results is that superimposing results from homogeneous domains – as is done for the two semi-analytical models – is insufficient to capture the spatial heterogeneity of the domain. Finally, the authors found that injecting CO_2 at the sites of the sources may not be feasible due to poor injectivity (i.e., low permeability and low thickness) at several of the source sites in the western part of the basin. The authors present an alternative injection scenario where CO_2 is transported to sites with more favorable injectivity. For more details on the modeling conducted for the Basal Cambrian Aquifer the reader is referred to Huang et al. (2014).

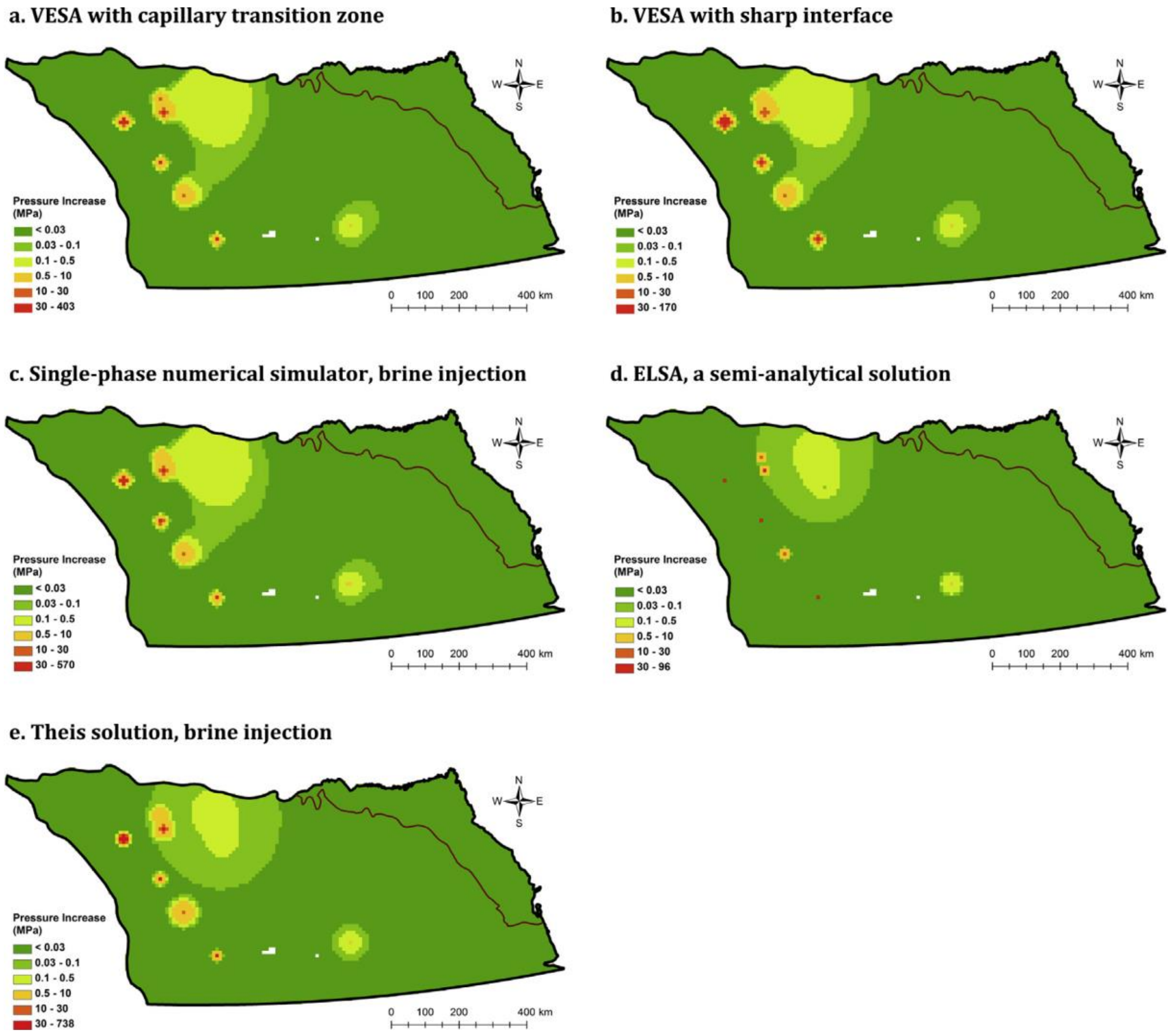


Figure 7: Comparison of basin-wide pressure response due to 50 years of CO_2 injection into the Canadian portion of the Basal Cambrian Aquifer based on five vertically-integrated modeling approaches: a) numerical multi-phase vertical equilibrium with capillary transition zone, b) numerical multi-phase vertical equilibrium with sharp interface, c) numerical single-phase, d) semi-analytic multi-phase vertical equilibrium with sharp interface, and e) semi-analytic single-phase. Taken from Huang et al. (2014).

2.4.3 Sleipner CO_2 injection site

The Sleipner CO_2 injection site located in the North Sea off the coast of Norway is the longest operating industrial-scale GCS operation in the world. Since the project's inception in 1996, approximately 1 Mt of CO_2 are injected every year into the Utsira Sand formation (Torp & Gale, 2004). CO_2 is being injected into the bottom of the Utsira formation, a Pliocene sandstone formation characterized by high permeability (1-3 Darcy) and porosity (35-40%) (Chadwick et al., 2004). While the permeability and porosity in the Utsira Sand are considered to be homogeneous, low permeable mudstone lenses act as baffles impeding the upward migration of CO_2. However, the mudstone lenses are horizontally discontinuous, allowing CO_2 to eventually reach the top of the Utsira formation. The lenses lead to a distinct vertical structure of the CO_2 plumes, where mobile CO_2 collects under a mudstone lens until it reaches a spill point and CO_2 migrates upward to the next overlying lens (Bickle et al., 2007). The CO_2 plume has been delineated using multiple seismic surveys, leading to the conceptualization that the Utsira sand is divided into nine layers which are separated by impermeable mudstone layers (Cavanagh & Haszeldine, 2014). The sandstone layers are connected to each other through openings in the mudstone layers. The injection induced pressure increase in the Utsira Sand is insignificant, due to high permeability and large lateral extent of the aquifer.

Several simulation studies have been conducted at the Sleipner site to investigate the migration of CO_2 in the Utsira Sand (e.g., Cavanagh, 2013; Lindeberg et al., 2001). To facilitate the modeling of CO_2 migration in the uppermost part of the Utsira Sand (termed the *9^{th} layer*), for which the most detailed plume delineation exists, IEAGHG published a geologic model of the 9^{th} layer and adjacent mudstone layers (Singh et al., 2010). As part of the project reported on here Bandilla et al. (2014) used the 9^{th} layer geologic model to compare a simplified three-dimensional model with three vertically-integrated models: vertical equilibrium with sharp interface, vertical equilibrium with capillary transition zone, and vertical dynamic reconstruction. Initial tests with simplified geometries showed that the vertical dynamic reconstruction model and the vertical equilibrium models gave very similar results, suggesting that the vertical equilibrium assumption is valid in the 9^{th} layer at Sleipner; this was expected due to the high permeability at the site. The vertical dynamic reconstruction model was therefore not applied at the full site geometry. A comparison of plume cross-sections and plume outlines for the simplified three-dimensional model, the vertical equilibrium model with sharp interface and the vertical equilibrium model with capillary transition zone shows that the three models agree very well with each other (Figure 8). These results suggests that a vertical-equilibrium with sharp interface model is the most appropriate modeling approach for CO_2 migration modeling at Sleipner. These results also confirm results of an earlier study by Nilsen et al. (2011). It should however be noted, that none of the results presented here or in other modeling studies, matches the CO_2 plume extent particularly well, suggesting that either the geologic model is not accurate or additional processes need to be included in the modeling.

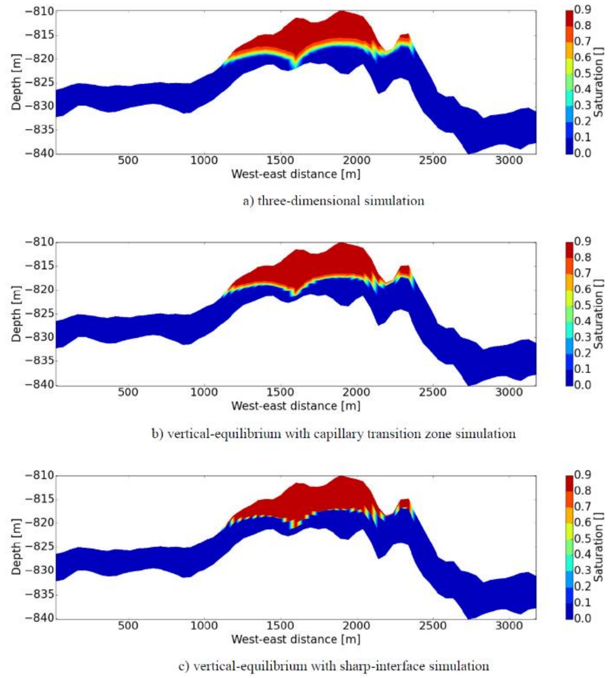


Figure 8: Cross-section CO_2 saturations in the 9th layer of the Utsira Sand at the Sleipner CO_2 injection project based on three modeling approaches: a) simplified three-dimensional, b) vertical equilibrium with capillary transition zone, and c) vertical equilibrium with sharp interface. Taken from Bandilla et al. (2014).

2.4.4 In Salah

At the In Salah site in central Algeria CO_2 from a natural gas processing plant was injected into the water-leg of an active natural gas field (Wright, 2007). Over an eight year period (2004 – 2011) between 0.5 and 1 Mt of CO_2 were injected per year into a carboniferous sandstone at a depth of about 1800 m; a total of about 8 Mt. The injection formation is 20 m thick and has average permeability and porosity of 10 mD and 0.15, respectively (Ringrose et al., 2009). To increase injectivity, CO_2 was injected in three horizontal wells over a length of 1 to 1.5 km. The main goals of the injection were to prove the feasibility of an industrial-scale CO_2 injection, demonstrate plume monitoring techniques, and set precedents for future GCS regulations (Wright, 2007). Due to the site's location in the Algerian desert, satellite-based land surface uplift measurements were used for site monitoring (Vasco et al., 2010). While the uplift at two of the injection wells is dome shaped, the uplift at the third well has a "dual-lobe" shape. Several computer models that include both multi-phase flow and geomechanical effects have been used to interpret the uplift data.

Rutqvist et al. (2010) coupled the flow simulator TOUGH2 and the geomechanics simulator FLAC to investigate if the dome-shaped uplifts could be explained by deformations in the injection formation alone, or if deformation of the caprock had to be included as well. The three-dimensional model covered an area of 100 km^2 and included the rocks from the land surface to a depth of 4000 m. The two simulators were sequentially coupled at each time step; the flow simulator (TOUGH2) produced pressures, which were turned into deformations by the geomechanics simulator (FLAC). The deformations were then translated into changes in porosity and permeability and fed back into the flow simulator for the next time step. Rutqvist et al. (2010) found that while the uplift at two of the wells could be explained by deformation of the injection zone alone, the uplift at the other well required that the lower part of the caprock deformed as well. This lead to the conclusion that the lower part of the caprock had to be permeable enough to allow for limited fluid flow.

Morris et al. (2011) used a different approach to determine why the uplift patterns were different at the three wells (i.e., dome-shaped vs. dual-lobe shaped). They coupled the flow simulator NUFT to the geomechanics simulator SYNEF by assuming that the feedback from the deformation to the flow field was negligible. This allowed them to first model the flow over the entire simulation period, and then use the resulting pressure evolution to predict the rock deformation and surface-uplift. The model included a set of faults that acted either as enhanced flow paths or flow barriers. Morris et al. (2011) found that a fault intersecting the well needed to be extended into the caprock to explain the dual-lobe pattern. However, their model was not sensitive to the vertical extent of the fault, and therefore the authors could not determine if the fault extended into the overlying aquifer.

In order to determine if the fault mentioned in the previous paragraph reached the aquifer Rinaldi and Rutqvist (2013) refined the Rutqvist et al. (2010) TOUGH2-FLAC model, increasing the model domain, creating a finer mesh, and adding a vertical fracture zone in the vicinity of the injection well. The fracture zone location and properties were based on seismic surveys and model calibration. To best fit the measurements, the authors assumed time-dependent permeability and fracture zone activation. The model was able to predict the dual-lobe surface uplift in both magnitude and pattern, confirming the conceptual model of a fracture zone intercepting the horizontal injection well. Based on a sensitivity analysis of fault geometry and properties, the authors concluded that the fault was confined in the caprock and did not reach the overlying aquifer.

Preisig and Prevost (2011) used a model of the In Salah injection site to study the impact of temperature on the creation and reactivation of fractures. Unlike the modeling approaches used in studies discussed earlier, the authors used a fully-coupled model where the governing equations for flow and geomechanics were solved simultaneously, instead of sequentially. To reduce the computational effort, only a two-dimensional slice perpendicular to the horizontal well was modeled. The authors found that a temperature difference between the host rock and injected CO_2 of 20 °C is sufficient to create fractures in the caprock that are similar to the ones observed at In Salah.

Computer modeling has also been used to predict the CO_2 plume migration at In Salah. For instance, (Ringrose et al., 2009) reported on a modeling effort to explain the sooner than expected arrival of CO_2 at near-by monitoring well. However, the strong impact of geomechanics at the In Salah site is unique among the example sites discussed here, and therefore the In Salah flow models are not discussed here.

2.4.5 Ketzin

A pilot-scale CO_2 injection was conducted at the Ketzin CO_2 injection site in Brandenburg, Germany (Martens et al., 2012). Approximately 70,000 tonnes of CO_2 were injected over a four year period into the Stuttgart Formation at a relatively shallow depth of 630 – 650 m. Injection occurred through a single vertical well, and two adjacent wells, located 50 m and 112 m from the injection well, were used for monitoring. The Stuttgart formation was deposited under a fluvial environment (Norden & Frykman, 2013), and therefore consists of coarse-grained material (termed *sand* due to its depositional origin) in former stream channels imbedded in a fine-grained background material (termed *clay*). The injection well intersected several such channels, and it is expected that CO_2 mainly migrated along those channels. CO_2 breakthrough occurred after 22 days at the closer monitoring well (50 m) and after 217 days at the farther monitoring well (112 m).

Unfortunately, the exact location of the stream channels at the Ketzin injection site is unknown, so that geological models of the site rely on distributions for parameters such as channel width, amplitude and frequency. Values for these distributions are based on regional values taken from the literature (Norden & Frykman, 2013). Kempka and Kühn (2013) used a simplified three-dimensional model to simulate the pilot-scale CO_2 injection at Ketzin, based on the geologic model developed by Norden and Frykman (2013). They were able to history match the bottom hole pressure in the injection well and the CO_2 arrival times at the two monitoring wells by adjusting permeability values and constraining the stream channel locations with additional seismic data. However, the geologic model used by Kempka and Kühn (2013) was not available to this project, so that simpler stream geometries are used here.

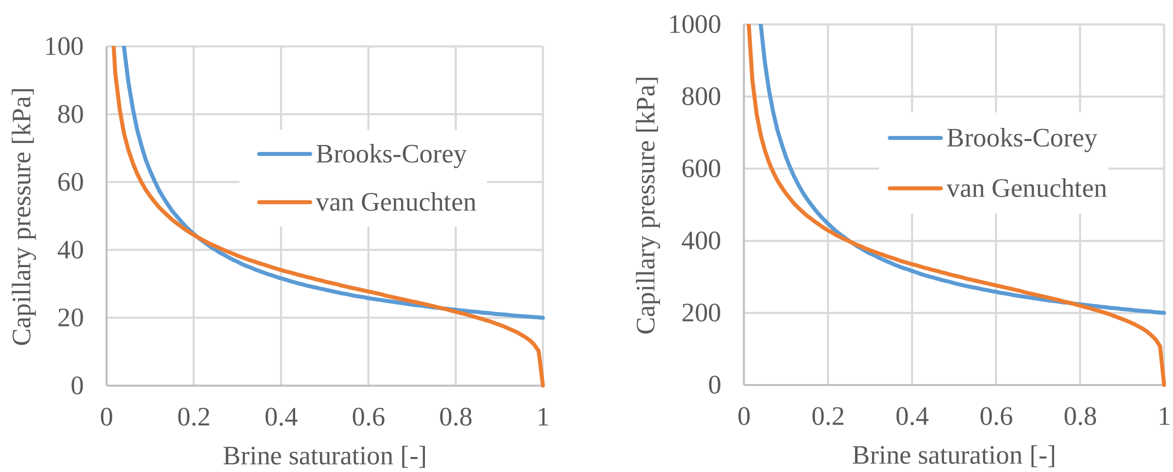
In most implementations of vertical equilibrium models parameters are assumed to be constant over the formation thickness, while they may vary in the other two spatial dimensions. This assumption is not valid for the case considered here where the sand and clay facies may have significantly different permeability and capillary entry pressure. Not only are the formation properties heterogeneous, but the injected CO_2 is expected to remain mainly in the high permeability sand facies. It is important to predict the vertical saturation profiles accurately, because the mobility of CO_2 is different if the CO_2 is residing in sand or clay. In other words, if the CO_2 were mainly residing in the sand facies, the integrated CO_2 mobility should be higher than if the CO_2 were residing in the clay. In order to reconstruct the saturation profiles correctly, we have developed an iterative approach where the bottom of the plume is moved up and down until the appropriate depth-averaged saturation is reached. While this is based on the same approach as for other vertical equilibrium models with capillary transition zones, the saturation reconstruction is more complicated for this fully heterogeneous case, because differences in capillary entry pressure lead to discontinuities in saturation at facies transitions. Unlike for vertical equilibrium models for vertically homogeneous formations, the highest CO_2 saturation is not necessarily at the top of the formation; this is due to variations in capillary entry pressure. Once the vertical saturation profiles are known, the integrated mobilities can be calculated based on the saturation profiles and the permeability profiles.

In order to investigate if vertical equilibrium models are applicable to domains with such channelized heterogeneities, results from the simplified three-dimensional simulator TOUGH2/ECO2N (Pruess et al., 1999; Pruess & Spycher, 2007) are compared to the vertically-integrated simulator VESA (developed at Princeton University). The model domain is rectangular, measuring 13 km in the lateral directions with a thickness of 50 m. The top and bottom boundaries are assumed to be no-flow boundaries and the lateral boundaries are held at constant pressure. Initially, there is no CO_2 in the domain and the brine pressure is hydrostatic throughout. The model grids used in the two simulators have the same horizontal discretization, with a cell size of 25 x 25 m at the injection well increasing to 250 x 250 m at the outer edge of the domain. The three-dimensional grid for TOUGH2 has a vertical resolution of 1 m. CO_2 is injected into the center of the domain at a rate of 1 Mt (=10^9 kg) per year for a duration of 1 year.

Table 1: Formation parameters for the two facies

parameter	unit	sand	clay
permeability	mD	100	10
porosity	-	0.2	0.18
Brooks-Corey λ	-	2	2
Capillary-entry pressure	kPa	20	200

The model contains two facies termed *sand* for the coarser-grained stream channel material and *clay* for the finer-grained floodplain material. The formation parameters are uniform for each of the two facies, and values for the parameters are given in Table 1. Due to implementation restrictions of the two simulators, different capillary pressure – saturation relationships are used for the two simulators: TOUGH2 uses van Genuchten expression, while VESA uses a Brooks-Corey expression. The van Genuchten parameters are chosen so that the two expressions give close to identical capillary pressure – saturation relationships (Figure 9). The relative permeability – saturation expressions are equivalent in the two simulators.

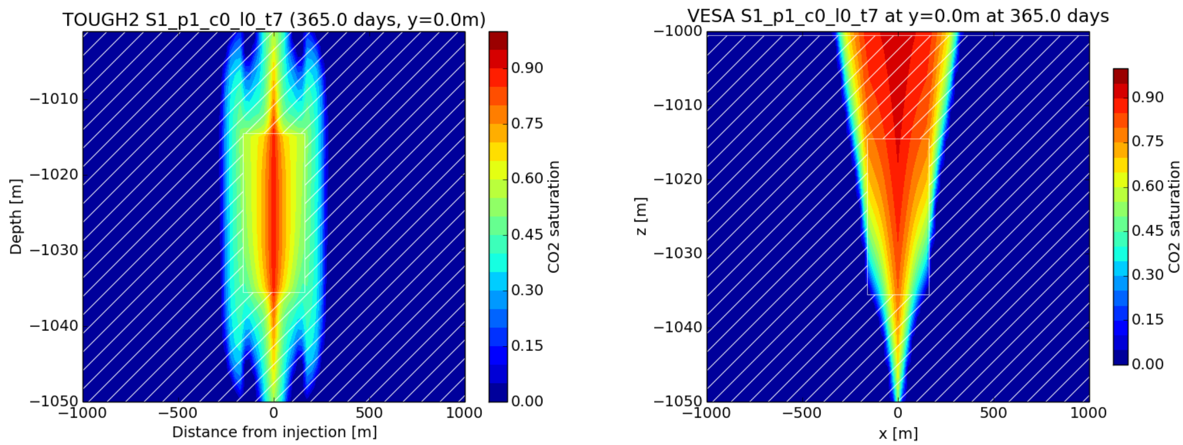


a) sand facies

b) clay facies

Figure 9: capillary pressure – saturation relationships for the sand (a) and clay facies (b).

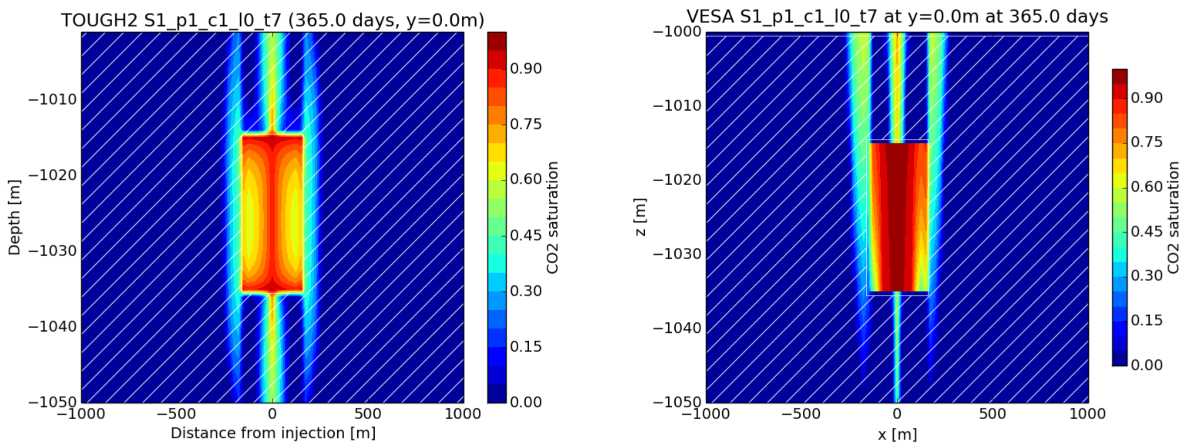
The first set of comparisons investigates the impact of heterogeneity in capillary entry pressure on the vertical equilibrium model performance. A straight 300 m wide and 20 m high sand channel is placed into the domain, so that the channel center line goes through the injection well. For the first model run the same capillary pressure – saturation relationship is used for both the sand and clay facies. The results are as expected for the TOUGH2 simulation, with the majority of CO_2 remaining in the sand channel, due to the much lower permeability of the clay facies. For the vertical equilibrium model, on the other hand, most of the CO_2 migrates into the clay facies, because vertical equilibrium models have no representation of vertical permeability.



a) simplified three-dimensional b) vertical equilibrium

Figure 10: Cross-sections of CO_2 saturation profiles at the injection well after 1 year of injection for a model with a single channel for a clay capillary entry pressure of 20 kPa using a simplified three-dimensional model (a) and a vertical equilibrium model (b).

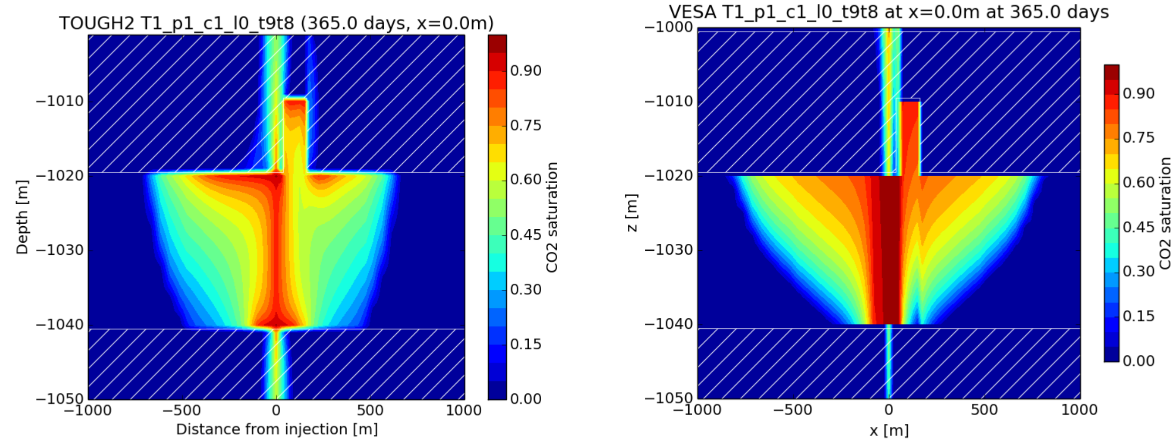
When the models are run using the original capillary pressure – saturation relationships for the two facies (entry pressures of 20 kPa for sand, 200 kPa for clay), the saturation profiles predicted by the vertical equilibrium model are much more realistic, with the majority of CO_2 remaining in the sand channel. The two modeling approaches agree well with each other, although the CO_2 plume extends slightly farther in the vertical equilibrium model. This difference is likely due to the CO_2 plume thickness being constrained by the vertical resolution in the simplified three-dimensional model, while no such constraint exists in the vertical equilibrium model.



a) simplified three-dimensional b) vertical equilibrium

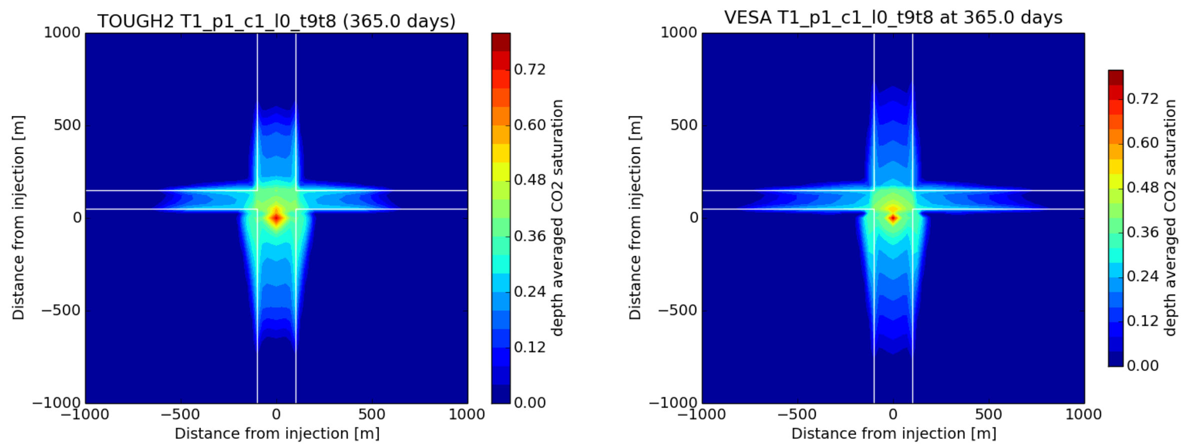
Figure 11: Cross-sections of CO_2 saturation profiles at the injection well after 1 year of injection for a model with a single channel for a clay capillary entry pressure of 200 kPa using a simplified three-dimensional model (a) and a vertical equilibrium model (b).

The next model has two intersecting channels, both of which are 20 m high, but have different widths and span different vertical locations. CO_2 is injected into the wider channel (200 m width) 100 m from the intersection of the center lines of the two channels. The top of the narrower channel (100 m width) is 10 m higher than the top of the wider channel, so that the two channels overlap over a thickness of 10 m. A comparison of the plume extents from the two simulators shows good agreement between the two (Figure 12). In both modeling approaches CO_2 migrates along the wider channel and into the intersecting channel, with high CO_2 saturations at the top of the narrower channel. The narrower channel leads to a jump in the reconstructed saturation profile, because of the jump in available thickness. A comparison of the extent of the CO_2 plumes shows good agreement, with the CO_2 plume extending slightly farther in the vertical equilibrium model (Figure 13).



a) simplified three-dimensional b) vertical equilibrium

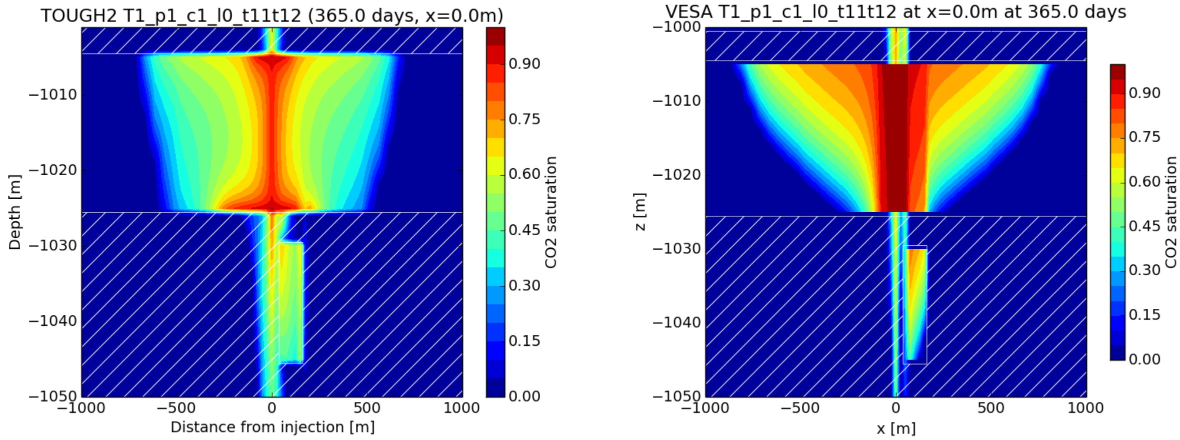
Figure 12: Cross-sections of CO_2 saturation profiles at the injection well after 1 year of injection for a model with two intersecting channels using a simplified three-dimensional model (a) and a vertical equilibrium model (b).



a) simplified three-dimensional b) vertical equilibrium

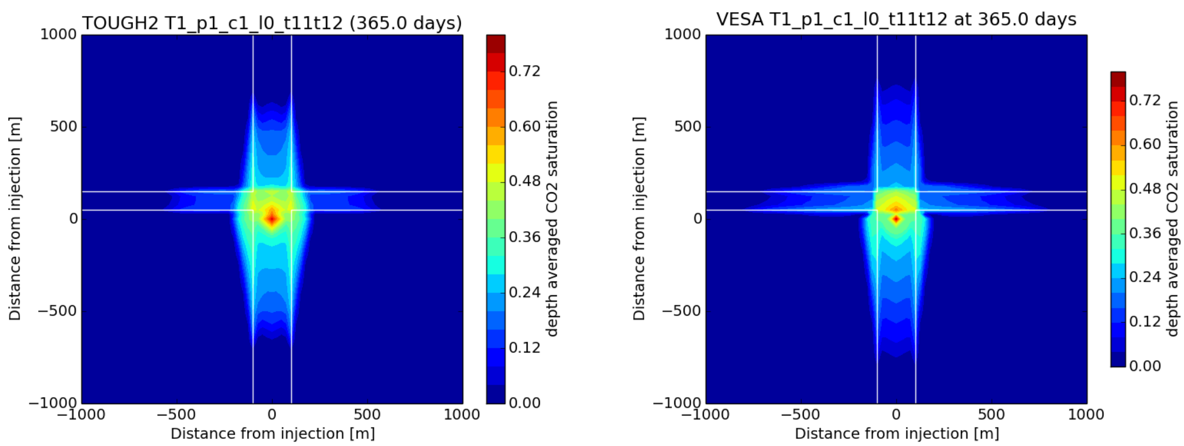
Figure 13: Depth-averaged CO_2 saturations after 1 year of injection for a model with two intersecting channels using a simplified three-dimensional model (a) and a vertical equilibrium model (b).

The next case involves the same two channels, but the vertical location of the channels is adjusted, so that the channels are no longer intersecting (i.e., the wider channel that CO_2 is being injected into passes over the narrower channel). A comparison of the CO_2 saturation profiles shows that the two approaches generally agree, with most of the CO_2 remaining in the injection channel and only low CO_2 saturations in the lower channel (Figure 14). The plume shapes are, however, not as close, with a significant amount of CO_2 collecting at the bottom of the injection channel for the simplified three-dimensional model. This is likely due to downward flow from the injection channel to the lower channel driven by a downward pressure gradient. The vertical flow cannot be captured by the vertical equilibrium model. The difference is less pronounced for the depth-averaged CO_2 plots (Figure 15), although saturations are higher for the vertical equilibrium model in the area where the two channel overlap.



a) simplified three-dimensional b) vertical equilibrium

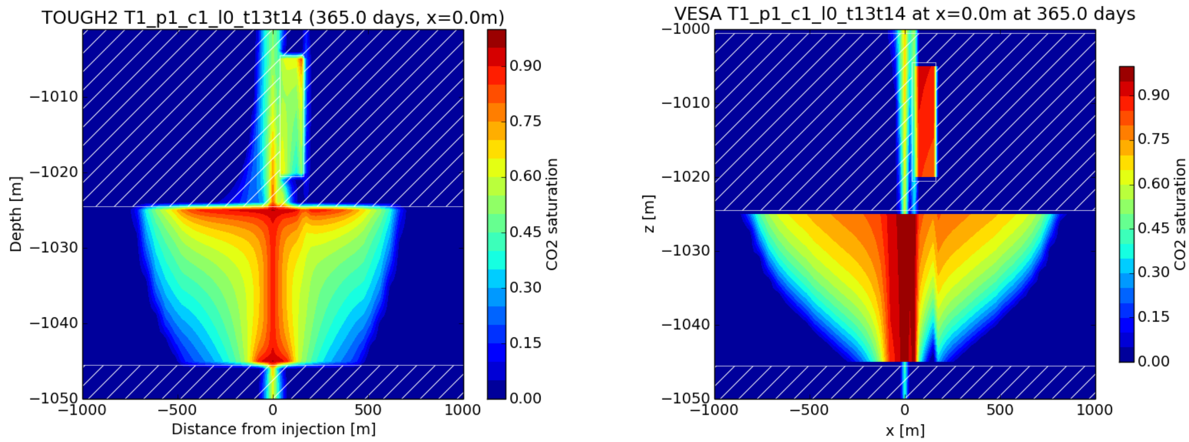
Figure 14: Cross-sections of CO_2 saturation profiles at the injection well after 1 year of injection for a model with two disconnected channels (injection into the upper channel) using a simplified three-dimensional model (a) and a vertical equilibrium model (b).



a) simplified three-dimensional b) vertical equilibrium

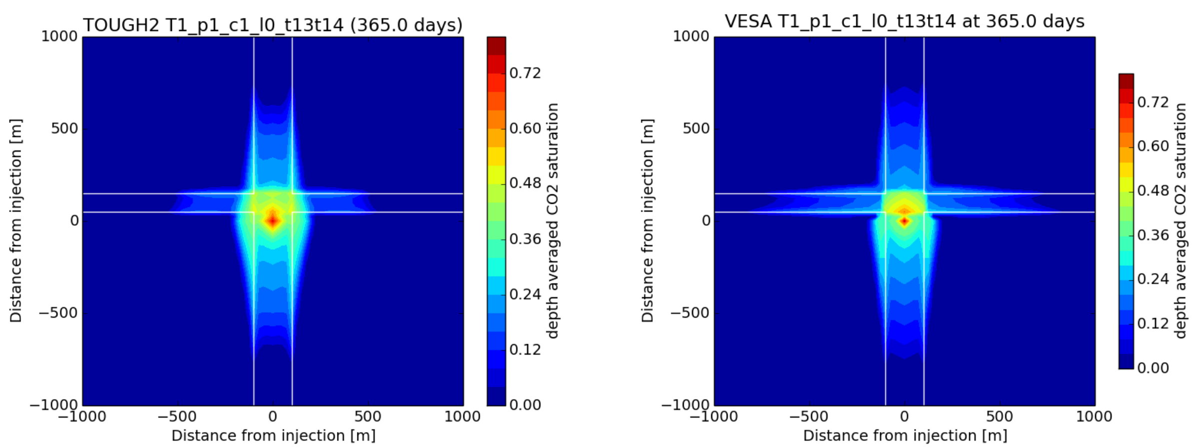
Figure 15: Depth-averaged CO_2 saturations after 1 year of injection for a model with two disconnected channels (injection into the upper channel) using a simplified three-dimensional model (a) and a vertical equilibrium model (b).

In the next modeling run, the vertical locations of the two channels are switched from the previous run: the wider channel with the injection is now below the narrower disconnected channel. While the vertical CO_2 saturation profiles are relatively close in the injection channel, the vertical equilibrium model predicts much higher CO_2 saturations in the upper channel than the simplified three-dimensional model (Figure 16). The higher saturations in the upper channel occur, because vertical permeability is not represented in the vertical equilibrium approach (i.e., there is no barrier for CO_2 to reach the upper channel). In the simplified three-dimensional approach CO_2 saturations in the upper channel are low (similar to the case where injection is in the upper channel (Figure 14)), because CO_2 needs to migrate through the low permeability clay facies. The depth-averaged CO_2 saturations remain relatively similar (Figure 17), even though the profiles are not as close. This can be explained by the high saturation in the upper channel being compensated by lower saturation values in the lower channel right below the upper channel (Figure 16b).



a) simplified three-dimensional b) vertical equilibrium

Figure 16: Cross-sections of CO_2 saturation profiles at the injection well after 1 year of injection for a model with two disconnected channels (injection into the lower channel) using a simplified three-dimensional model (a) and a vertical equilibrium model (b).



a) simplified three-dimensional b) vertical equilibrium

Figure 17: Depth-averaged CO_2 saturations after 1 year of injection for a model with two disconnected channels (injection into the lower channel) using a simplified three-dimensional model (a) and a vertical equilibrium model (b).

In this section we have presented a comparison of a simplified three-dimensional modeling approach and vertical equilibrium modeling approach for CO_2 and brine migration in a heterogeneous domain. Heterogeneity in intrinsic permeability and capillary entry pressure is in the form of sand channels embedded in a clay background. The results show that for the relatively simple channel geometries presented here, the vertical equilibrium model is able to predict the depth-averaged saturations accurately, although the reconstructed saturation profiles are not as close for situations where the two channels are disconnected. Nonetheless, the ability of vertical equilibrium models to accurately predict the CO_2 plume extent is important, as this may be sufficient to answer questions related to CO_2 breakthrough at monitoring wells. It should also be noted, that the vertical equilibrium model used here is computationally much more efficient than the simplified three-dimensional model; simulating one year of CO_2 injection using the vertical equilibrium model takes about 30 minutes on a single processor, while it takes more than 24 hours on a 10 processor cluster for the simplified three-dimensional model using the same horizontal discretization. The computational efficiency becomes important for cases where the exact configuration of channels is not known, so that many realizations may be necessary to investigate uncertainty. It may also be possible to improve the prediction by using vertical dynamic reconstruction models instead of vertical equilibrium models, but that approach was not tested here.

2.4.6 Kimberlina

In this section, we demonstrate the applicability of a vertical equilibrium model and a simplified three-dimensional model for optimization of injection/extraction rates for managing reservoir pressure in GCS. For the demonstration example, we selected the Vedder Formation, at Kimberlina in the Southern San Joaquin Basin in California, USA. Some portion of this section is based on a paper published by Cihan et al. (2015) who used this site to demonstrate an application of the newly developed optimization algorithm, constrained differential evolution (CDE), coupled with a vertical equilibrium model. The details of the vertical equilibrium model used for this section can be found in (Cihan et al., 2015) and the details of the simplified three-dimensional model can be found in González-Nicolás et al. (2016).

Hydrogeological properties of the Vedder Formation are known based on site characterization data available from oil and gas exploration and groundwater development in the area (Scheirer, 2007; Wainwright et al., 2013). The Vedder Formation has sufficient injectivity, and the overlying Temblor-Freeman Shale is considered a suitable caprock for stratigraphic containment of the injected supercritical CO_2. The site has challenging stratigraphic and structural complexity, caused by the existence of numerous faults, and there is concern about reservoir compartmentalization and pressure-induced seismicity. A hypothetical model based on the Vedder Formation has been used in the past to evaluate pressure impacts for a hypothetical storage scenario with injection of 5 Mt CO_2 per year over 50 years (e.g., Birkholzer et al., 2011). The site has also been used for risk assessment, sensitivity and uncertainty quantification studies (e.g., Pawar et al., 2014; Wainwright et al., 2013). One important result from the earlier simulation studies is that the two faults on the east and west of the injection site (Figure 18) will experience significant pressure buildup during and after injection. Concerns about induced seismicity may require pressure management at this site, and pressure management via targeted brine extraction seems suitable because the pressure control needs to be along the faults. Well locations and pumping rates need to be carefully chosen to minimize extraction volumes and to avoid CO_2 breakthrough at the brine production wells or the faults.

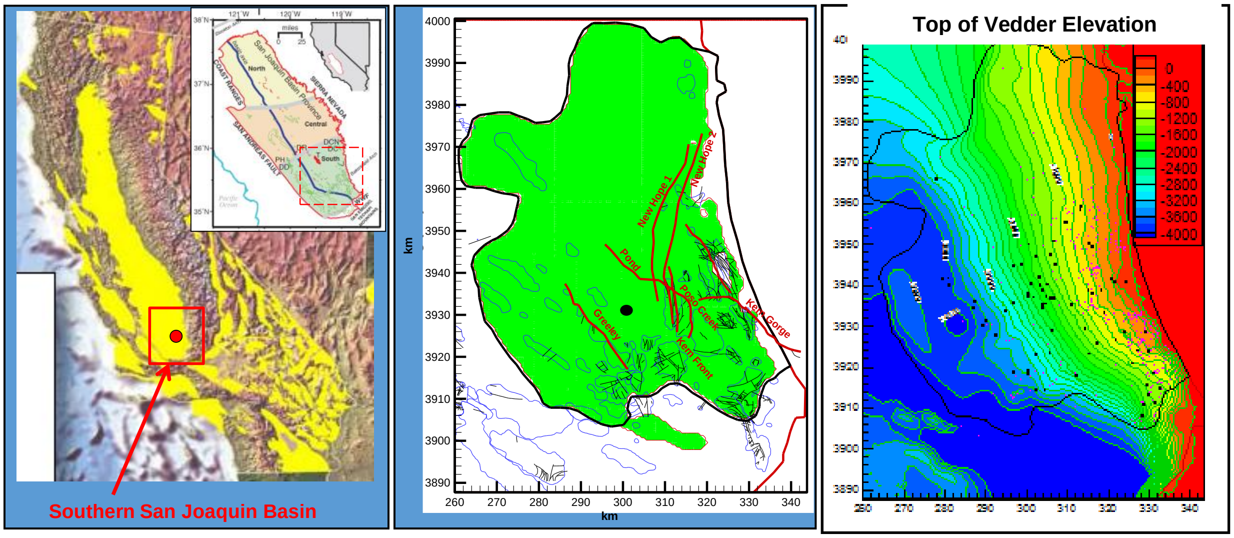


Figure 18: Site map of the Vedder formation in Kimberlina (Southern Joaquin Valley, California), showing multiple faults, injection location and top elevation of the injection formation.

The Vedder Formation involves six alternating sand/shale layers. The thickest sand layer (the first Vedder Sand) with a maximum thickness of 197m is located at the top portion underlying the Temblor-Freeman shale. We considered only the first Vedder Sand to model the hypothetical CO_2 storage and to apply the CDE algorithm for pressure management through brine extraction. Figure 18 shows the injection well location and the contour maps of the first Vedder Sand top elevation (above sea level). As in Wainwright et al. (2013), we considered only the 3 major faults fully penetrating the Vedder Sand. The faults are likely sealing faults and in this study are represented as linear features with two orders of magnitude lower permeability than the Vedder Sand. The Vedder Sand outcrops toward the eastern boundary. Along the northern, western, and southern boundaries, the Vedder Sand pinches out into the shale and becomes thin or absent along these boundaries. Thus, the western, northern and southern boundaries are no-flow boundaries, and the eastern boundary is set to a fixed pressure boundary. For simplicity, the reservoir top and bottom boundaries are also no-flow boundaries. Not allowing pressure diffusion and preventing slow brine flow into the caprock in response to the injection is a conservative assumption in terms of reservoir pressure buildup, and therefore the pressure buildup estimations based on this model are higher than those assuming very low caprock permeability in preceding simulation studies (Birkholzer et al., 2011; Wainwright et al., 2013).

Porosity, permeability, two-phase flow parameters (Table 2) and initial conditions are based on earlier studies on this site (Birkholzer et al., 2011; Wainwright et al., 2013; Zhou & Birkholzer, 2011). Initially hydrostatic conditions (based on pressure, temperature and salinity data) are assumed, and the fluids are also assumed to be incompressible with densities of 989 kg/m^3 for brine and 819 kg/m^3 for scCO_2. Cihan et al. (2015) considered horizontal heterogeneity based on the average horizontal permeability data available from existing wells in the vicinity of the site. However, for the comparison study of the vertical equilibrium and simplified three-dimensional models, we neglected both horizontal and vertical heterogeneity within the formation. For the vertical equilibrium model, the numerical model of the first Vedder Sand was represented by a quasi-two-dimensional mesh (i.e., two-dimensional mesh with varying thickness) using 6290 grid blocks in the x-y plane. For the simplified three-dimensional model, we selected the same resolution in horizontal directions and the vertical resolution is about 5 m, with the average thickness being 100 m.

Table 2: Assumed average values of the two-phase flow properties in the Vedder Sand

Properties	**Local average values**
Porosity	0.264
Permeability (m^2)	2.990×10^{-13}
Pore Compressibility (Pa^{-1})	4.900×10^{-10}
*α (m^{-1})	1.263
*n	1.842
$^+S_{rw}$	0.300
$^+S_{rn}$	0.200

* α, n: van Genuchten model parameters
$^+$ S_{rw}, S_{rn}: Residual saturations for wetting (brine) and nonwetting (CO_2) fluids

Following earlier studies, we assumed a hypothetical storage scenario of 5 Mt CO_2 injected per year at a constant rate for 50 years and a threshold value of 1MPa along the faults as the maximum pressure buildup that could be sustained without re-activating the faults. We first conducted basic optimization studies using the vertical equilibrium and simplified three-dimensional models without brine extraction to calculate the maximum possible constant injection rates for each model that does not violate the 1MPa pressure buildup constraint along the faults. Then, using each modeling approach, we conducted optimization of brine extraction (well locations and rates) for a fixed injection of 5 Mt of CO_2 over 50 years without violating the 1 MPa pressure threshold along the faults, with the additional goals of extracting as little brine as possible and not pulling any CO_2 into the extraction wells.

Both models were coupled to the optimization algorithm and solved for prediction of the optimal injection rate without violation of the pressure buildup constraint along the faults. The injection well location is fixed at 50,239 m East and 34,637 m North of the model origin. The results of the model simulations show that the plume migration appears to be controlled mainly by the slope of the reservoir top elevation, as the buoyancy forces direct the CO_2 plume along the direction of the increasing elevation (Figure 19). The plume extent of the simplified three-dimensional model appears to be slightly greater than that of the vertical equilibrium model

(Figure 19). However, as shown in Table 3, the calculated optimal injection rates without brine extraction are very similar for the two models, which indicates the applicability of the vertical equilibrium model for estimating optimal injection rate under this specific site conditions. Figure 20 shows that the maximum pressure buildup constraint is successfully satisfied using both models, and the optimized pressure changes are similar. However, as demonstrated with the dashed lines for the 5 Mt/yr injection without optimization, the vertical equilibrium model appears to underestimate the pressure changes during the injection and overestimates the pressure changes after the injection, compared to the simplified three-dimensional model.

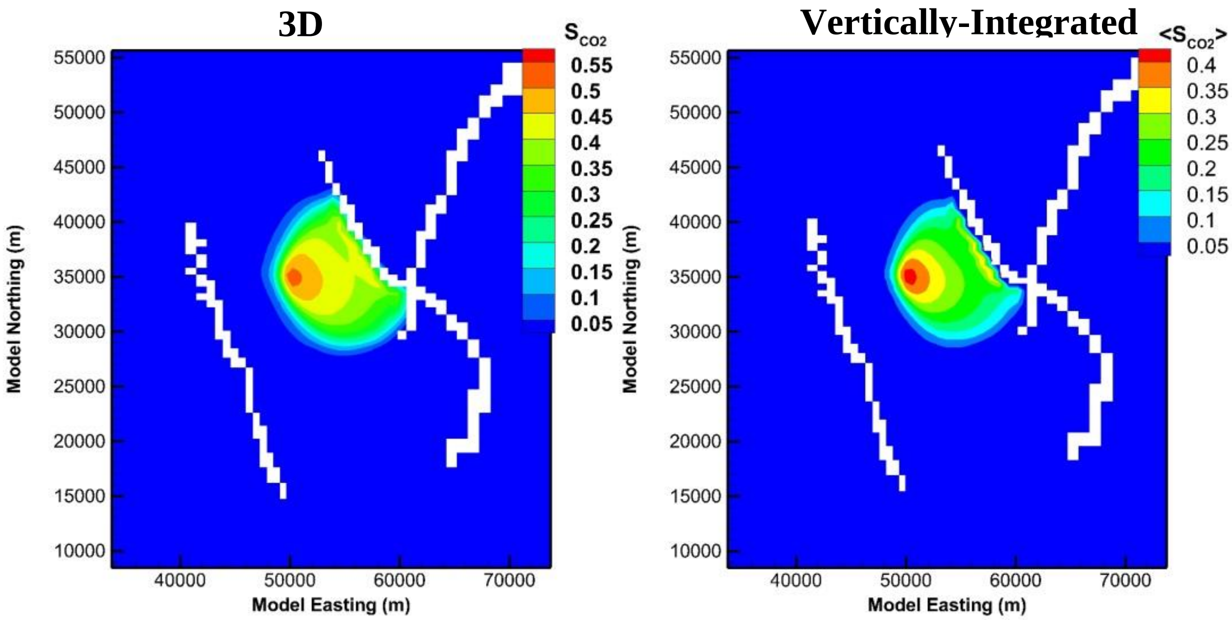


Figure 19: Saturation contour plots of the simplified three-dimensional model (left) and the vertical equilibrium model (right) at the end of injection, using the optimized injection rates.

Table 3: Calculated optimal injection rates without brine extraction for a critical pressure buildup along the faults of 1 MPa

Model Type	Injection rates (Mt/year)
Simplified three-dimensional	0.051
Vertical equilibrium	0.048

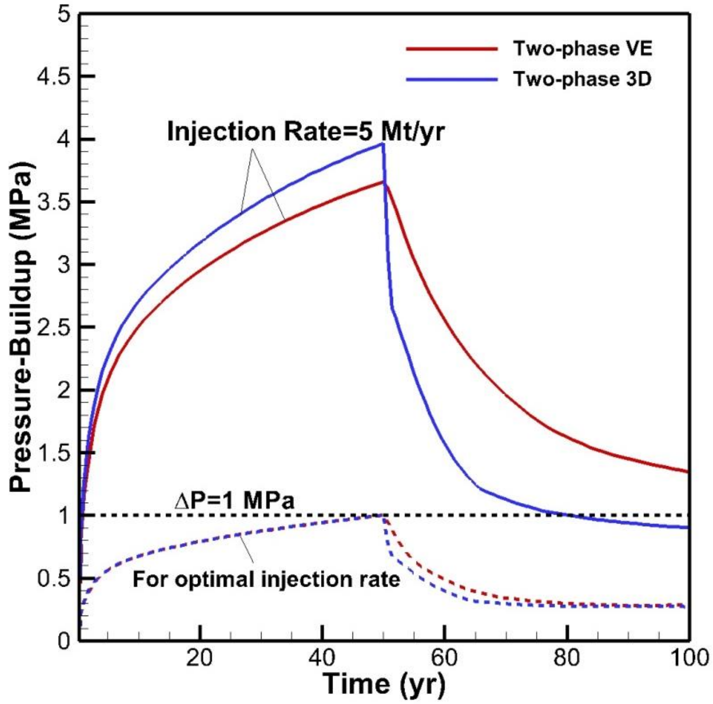
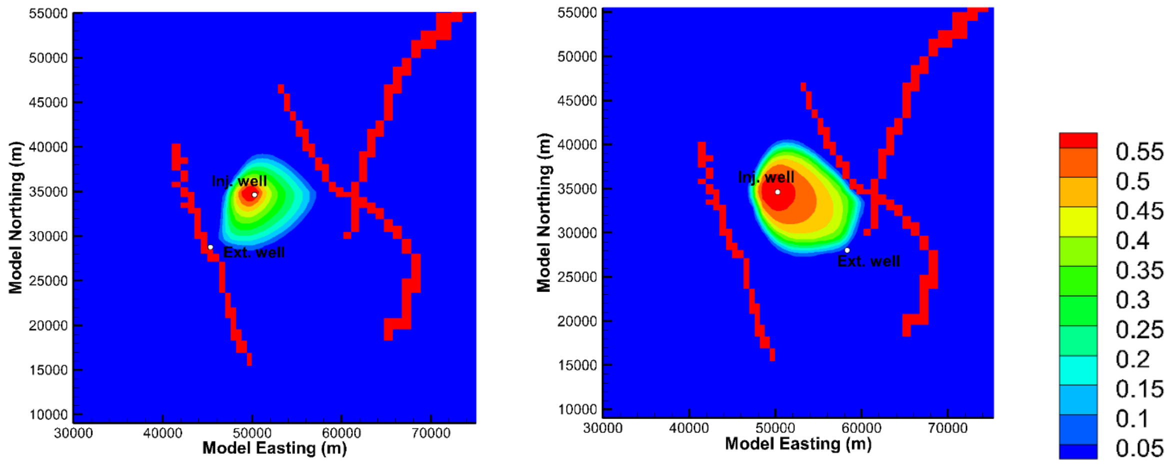


Figure 20: Maximum pressure buildup observed along the faults without applying brine extraction for an injection rate of 5 Mt/year (solid lines) and for optimal injection rates (dashed lines).

The location and flow rate of a single extraction well in both models are optimized for an injection rate equal to 5 Mt/year over the 50-year injection period. As before, the critical pressure buildup that activates the fault is equal to 1 MPa. Optimal position and rate of the extraction well for both models are included in Table 4. The optimal position for the extraction well produced by the simplified three-dimensional model is farther away from the injection well than the position produced by the vertical equilibrium model (Figure 21). This is because the CO_2 plume of the simplified three-dimensional model is larger than the CO_2 plume produced by the vertical equilibrium model and would reach the extraction well if the extraction well is positioned at a radial distance less than about 10 km. The calculated extraction rate is about 5 Mt/year (0.195 m^3/s) for the simplified three-dimensional model with one to one brine extraction ratio versus 4.5 Mt/year (0.174 m^3/s) for the vertical equilibrium model.

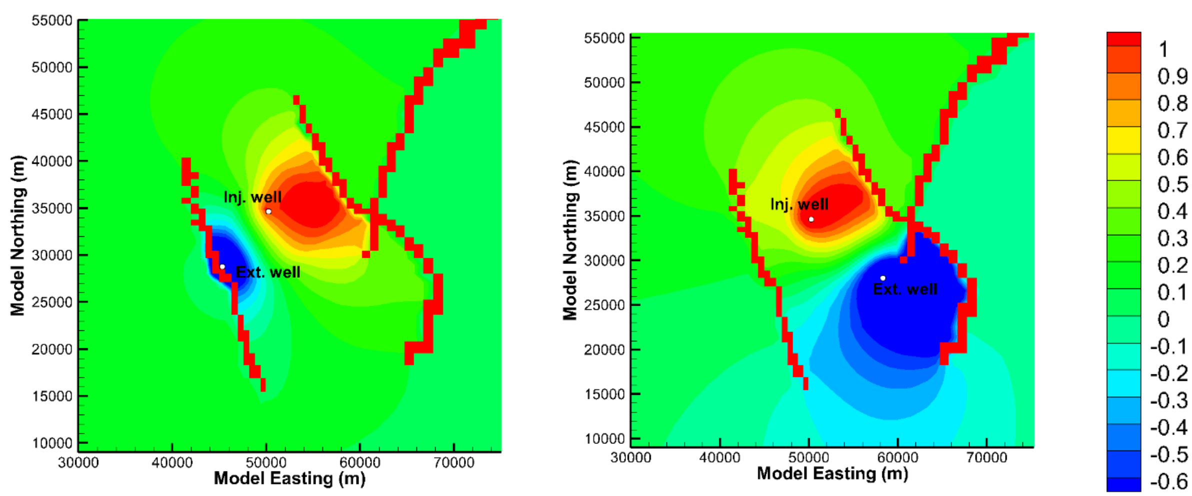
Table 4: Results of the optimization for vertical equilibrium and simplified three-dimensional models.

	Vertically-integrated	**3D model**
Easting extraction well (m)	45,333	58,240
Northing extraction well (m)	28,656	28,205
Distance between injection and extraction well (m)	7,738	10,266
Optimal extraction rate (Mt/year)	4.50	5.03



a) vertical equilibrium b) simplified three-dimensional

Figure 21: Distribution of CO_2 saturation at 50 years (end of injection) for the vertical equilibrium model (a) and the simplified three-dimensional model (b).



a) vertical equilibrium b) simplified three-dimensional

Figure 22: Pressure change in MPa at 50 years (end of injection) for the vertical equilibrium (a) and simplified three-dimensional (b) models.

As appears from Figure 22, the simplified three-dimensional model produces larger pressures at the injection well, and therefore, pressure buildup for the simplified three-dimensional model reaches the faults at an earlier time than the vertical equilibrium model. Figure 23 shows that the critical pressure is not exceeded at any stage of the injection for both models by applying the optimal extraction rates of brine, allowing the injection of 5 Mt/year of CO_2.

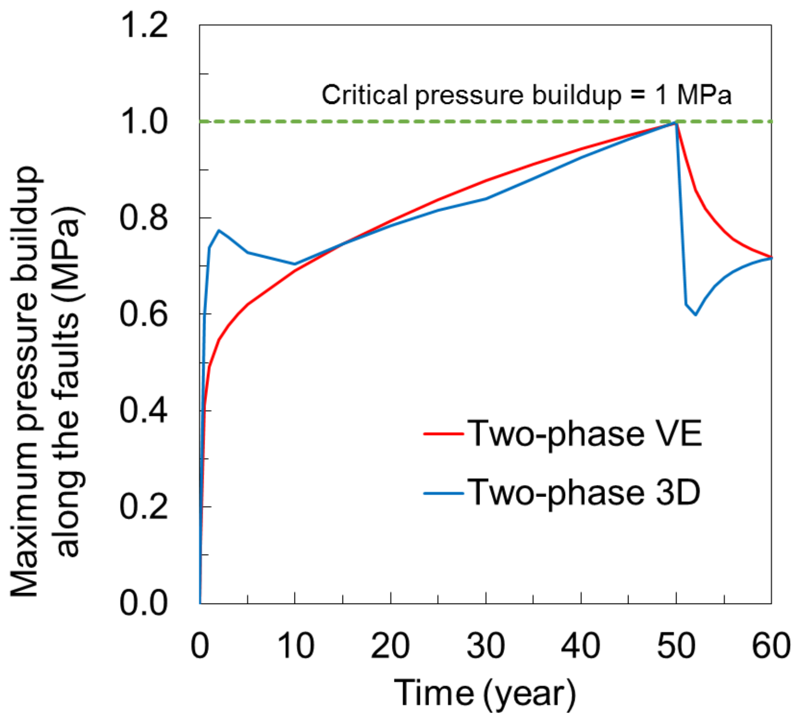


Figure 23: Maximum pressure buildup along the faults for vertical equilibrium (red) and simplified three-dimensional (blue) models applying optimal brine extraction rates and an injection rate of 5 Mt/year.

The estimated well locations are significantly different for the two models. If the optimal solution produced by the vertical equilibrium model is used for the simplified three-dimensional model to simulate the injection of CO_2 and extraction of brine, the constraints of CO_2 breakthrough at the extraction well and 1 MPa pressure increase at the faults will be violated.

Optimization of extraction rate and location of the extraction well allows storage of CO_2 without risking the re-activation of the faults. The location of the faults play an important role for the optimal well placement and extraction rate for both models. The optimal solutions produced by the two models satisfy all the constraints, however the solutions are not similar. The models find the optimal position of the extraction well in different locations. The optimal solution for the simplified three-dimensional model has the extraction well located farther away from the injection well, at a distance equal to 10,266 m, while the vertical equilibrium model produces an optimal location of the extraction well closer to the injection well at a distance of 7,738 m. The distribution of CO_2 within the simplified three-dimensional model is different from that in the vertical equilibrium model, since the plume of CO_2 produced by the simplified three-dimensional model is larger. Therefore, the extraction well will have to be located farther away from the injection well in order not to pump CO_2. This study indicates the importance of the simplified three-dimensional model selection when designing field operations including both injection and extraction activities.

In this project, we have also conducted tests with multiple extraction wells. The primary objectives are to minimize the brine extraction volume and the costs associated with drilling.

Therefore, in most of the optimization cases in Kimberlina for the 50-year injection scenario, our optimization calculations showed that one extraction well would be sufficient under homogeneous reservoir conditions for both the two-phase flow vertically-integrated and simplified three-dimensional models. However, our results indicated that injection duration and heterogeneity could significantly influence the optimal location and number of wells to minimize the extraction volume. The very high injection rate and the 50-year injection period produce large CO_2 plume sizes almost extending toward the fault on the east, limiting choices for extraction well placements. Shorter duration or smaller injection rates decrease the footprint of the CO_2 plume, and thus smaller CO_2 plume extent can give more flexibility to choose extraction well locations. In those cases, more than one extraction wells could be the optimal choice minimizing the cost of extraction and dealing with large volumes of extracted brine. In addition, presence of heterogeneity in the reservoir system significantly influences the optimal well placement and extraction rates. This conclusion is the same for both the two-phase flow vertically-integrated and simplified three-dimensional models. Further discussion on the effects of heterogeneity on the optimal well placements can be found in Cihan et al. (2015), showing reservoir optimizations with more than one extraction well for the storage scenario in the Kimberlina field site.

2.4.7 Publications related to model applications at example sites

Of the thirteen journal articles and one book chapter that were published as part of the project reported on here, eight are related to model applications at the example sites. Bandilla et al. (2015) summarize model applications from the literature for the Sleipner and In Salah sites, among other sites. Bandilla et al. (2014) compare vertically-integrated and simplified three-dimensional models at the Sleipner site, while Huang et al. (2014) compare vertically-integrated multi-phase and single-phase models for the Basal Cambrian Aquifer. The topic of Cihan et al. (2014) and Cihan et al. (2015) is optimization of well location and pumping rates for active pressure management at the Kimberlina site. Guo et al. (2016b) use parameters from the Ketzin, In Salah and Sleipner sites (among others) to investigate the applicability of numerical and semi-analytical solutions. Celia et al. (2015) and Bandilla and Celia (2016) discuss model complexity based on results from the three example sites (Sleipner, In Salah, and Basal Cambrian Aquifer).

2.5 Model choice criteria

In this section lessons learned from the application of the different modeling approaches to a set CO_2 injection sites and other GCS modeling results taken from the literature are distilled into a set of guidelines for choosing an appropriate modeling approach. The guidelines fall into two categories: one based on the type of question asked and the other based on the domain properties. The modeling approaches considered here are fully-coupled three-dimensional models, simplified three-dimensional models, two-dimensional vertically-integrated models with dynamic vertical reconstruction, two-dimensional vertically-integrated vertical equilibrium models, and two-dimensional vertically-integrated single-phase flow models. Macroscopic invasion percolation models are not included here, because they do not seem to apply to GCS modeling. We also do not include models based on analytical or semi-analytical solutions. This section is structured based on the complexity of modeling approach, starting with the simplest approach considered in this project.

2.5.1 Vertically-integrated single-phase models

The simplest modeling approach are two-dimensional vertically-integrated single-phase flow models. The governing equations combines the mass balance equation for water with the Darcy flux equation for water, both of which are integrated and written in the two spatial dimensions parallel to the bedding plane of the formation. These models are simple, because of their reduced dimensionality and because there is no need to solve for the transport of the CO_2 phase, as it is assumed that the presence of CO_2 does not affect significantly the pressure response of the system. Also, the non-linearities due to relative permeability are eliminated, although non-linearities exist for unconfined flow conditions (i.e., the saturated thickness changes over time). However, as the migration of CO_2 is not simulated in this approach, the CO_2 migration cannot be predicted by this approach. Single-phase models have been applied to GCS issues at the basin scale (Huang et al., 2014; Nicot, 2008).

Huang et al. (2014) compared the ability of several modeling approaches to predict the basin-scale pressure response of CO_2 injection into the Canadian part of the Basal Aquifer. For a more detailed description of the comparison study, please refer to section 2.4.2. They compared results based on solutions of two-phase vertically-integrated vertical equilibrium models (both sharp interface and capillary transition zone) and vertically-integrated single-phase models; both numerical and semi-analytical solutions were used. The results showed that the single-phase numerical model was sufficient to simulate the basin-scale pressure response, as it gave very similar results to those given by the more complex vertically-integrated two-phase models, because the areas where CO_2 was present were small compared to overall area of the model. The authors also found that semi-analytical solutions to the single-phase and two-phase models gave significantly different results than the numerical solutions, because the semi-analytic solutions did not properly capture the spatial variations of formation properties.

Based on the results published in Huang et al. (2014), single-phase models should be considered the adequate level of complexity when investigating large-scale pressure response of CO_2 injection, when it can be assumed that the impact of two-phase flow effects within the CO_2 plume(s) can be neglected, due to the plumes' small sizes relative to the areal extent of the pressure perturbations. A second guideline based on the Huang et al. (2014) study is that spatial variations in formation properties are important, so that semi-analytical solutions, which depend on uniform domains, are not applicable for basin-wide pressure response modeling, even when they are superposed using local formation properties.

2.5.2 Vertically-integrated models with vertical equilibrium assumption

Vertically-integrated vertical equilibrium two-phase flow models are the next more complex modeling approach on the model complexity spectrum. These models consist of two mass balance equations (one for water and one for CO_2), two flux equations, and constitutive equations relating capillary pressure, phase saturation and phase relative permeability. The governing equations rely on the vertical equilibrium assumption (i.e., vertical segregation of CO_2 and brine is fast compared to the modeling time scale). This overall approach is considered more complex than single-phase models due to the explicit modeling of both phases, but less complex than vertically-integrated models with dynamic reconstruction and simplified three-dimensional models, because the vertical dynamics of fluid segregation are not taken into account.

Vertical equilibrium models have been used in several GCS studies, ranging from site-scale (several kilometers) to basin-scale (tens to hundreds of kilometers). For instance, Nilsen et al. (2011) and Bandilla et al. (2014) used vertical equilibrium models to simulate CO_2 migration in the 9th layer of Utsira sand at the Sleipner site (domain size 18 km^2), while Person et al. (2010) and Bandilla et al. (2012) used vertical equilibrium models to investigate CO_2 and brine migration in the Illinois Basin (domain size ~300,000 km^2).

Nilsen et al. (2011) and Bandilla et al. (2014) conducted modeling approach comparison studies involving vertical equilibrium and simplified three-dimensional models based on formation data of the 9th layer of the Utsira sand at the Sleipner injection site. Both studies come to the conclusion that the vertical equilibrium assumption is valid at Sleipner, due to a relatively high vertical permeability of about 500 mD. Nilsen et al. (2011) also found that for domains with high vertical permeability vertical equilibrium models often perform better than simplified three-dimensional models, because the fast vertical segregation does not need to be resolved in vertical equilibrium models. Nordbotten and Dahle (2011) give an estimate for the time-scale for the vertical equilibrium assumption to be valid. The estimate depends on formation parameters, such as vertical permeability and formation thickness, and the difference in CO_2 and brine densities. For formation and fluid properties typically found at GCS sites, Court et al. (2012) found that the vertical equilibrium assumption usually is valid for vertical permeabilities above 100 mD, and usually not valid for vertical permeabilities below 10 mD. This threshold was confirmed by simulations in Guo et al. (2014). A thick capillary transition zone enhances the applicability of vertical equilibrium models, because less brine needs to drain out of the CO_2 plume, leading to a faster vertical segregation (Court et al., 2012; Nordbotten & Dahle, 2011).

While the studies of basin-wide industrial-scale CO_2 injection into the Mount Simon Sandstone of Illinois Basin by Zhou et al. (2010), Person et al. (2010) and Bandilla et al. (2012) were not intended as model comparison studies, the three studies used comparable geologic models and injection scenarios with three different simulators; a simplified three-dimensional simulator (Zhou et al., 2010) and two vertical equilibrium simulators (Bandilla et al., 2012; Person et al., 2010). After adjusting the compressibility values in the model by Person et al. (2010) to match those of the other two models, the results from the three simulators agree well with each other, both in terms of CO_2 plume spread and pressure response. These results suggest that vertical equilibrium models are capable of accurately predicting CO_2 and brine migration at the basin scale.

Most applications of vertical equilibrium models assume homogeneous formation properties over the thickness of the formation, although heterogeneities in the lateral directions and interactions with overlying/underlying permeable formations are often included. While the assumption of vertical homogeneity is often valid for large sedimentary basin, other depositional environments, such as fluvial depositions, lead to more complex vertical heterogeneity. Section 2.4.5 describes a comparison of a vertical equilibrium simulator and a simplified three-dimensional simulator for domains where coarse-grained stream channels are embedded in a fine-grained background material. The results show that a difference in vertical permeability of the coarse and fine material is insufficient to keep CO_2 from migrating into overlying fine grained material in the vertical equilibrium model, because vertical permeability is not represented in the vertical equilibrium approach. However, if a difference in capillary entry pressure is included, the two approaches give comparable results for both the extent of the CO_2 plume and vertical CO_2 saturation profiles. Domain geometries containing disconnected coarse grained stream channels can be constructed, where due to the vertical equilibrium assumption CO_2 reaches overlying stream channels that are not connected to the injection location. It may be possible to exclude disconnected stream channels as a pre-processing step, but this approach was not tested here.

Based on results from the study reported here and other studies from the literature, vertical equilibrium models instead of single-phase models should be chosen for basin-wide studies if CO_2 migration is of direct interest, for instance for questions related to leakage risk, storage capacity and active pressure management through brine production. For question that are answered at the site-scale, vertical equilibrium models are appropriate tools, if the vertical permeability is 100 mD or higher and the formation can be assumed to be homogeneous in the vertical direction. Vertical equilibrium models may also be appropriate where significant vertical heterogeneity is introduced by stream channels, if there is a significant difference in capillary entry pressure between the coarse-grained material in the channel and the fine-grained material of the background.

2.5.3 Vertically-integrated models with vertical dynamic reconstruction

A new approach was developed within the project report here, to extend the applicability of vertically-integrated approaches beyond the limitations imposed by the vertical equilibrium assumption. While a vertical permeability of about 100 mD and above is usually sufficient for the vertical equilibrium assumption to be valid for GCS models, many GCS sites have vertical permeabilities below that threshold. In order to model GCS sites where the vertical equilibrium assumption does not apply, Guo et al. (2014) developed the dynamic vertical reconstruction approach, in which the vertical dynamics of segregation of CO_2 and brine are captured by one-dimensional transient flow models; see section 2.3.1 for more details on the dynamic vertical reconstruction approach.

Application of the dynamic reconstruction approach to formations consisting of a single layer (Guo et al., 2014) and multiple layers with different permeabilities in each layer (Guo et al., 2016a) show that results from the newly developed approach compare well to results from a simplified three-dimensional simulator. The vertical dynamic reconstruction approach performs well for formations with permeabilities of 10 mD, partially penetrating injection wells, and multiple layers with a permeability range of 10 – 1000 mD. However, if significant lateral heterogeneity in permeability leads to complex inter-layer vertical flow patterns, the vertical dynamic reconstruction approach may fail.

The vertical dynamic reconstruction approach is the appropriate modeling approach for investigations at the site scale where vertical segregation dynamics are important either due to low vertical permeability (<100 mD) or multiple layers of different vertical permeability. For basin-scale questions the vertical dynamics within the CO_2 plume are expected to be negligible, because the CO_2 plumes are small compared to the entire domain, so that vertical equilibrium models should be chosen, even for formation properties that suggest the use of vertical dynamic reconstruction models. If significant lateral and vertical heterogeneity in permeability leads to complex three-dimensional flow, simplified three-dimensional models should be chosen, instead of vertical dynamic reconstruction models.

2.5.4 Simplified three-dimensional models

Simplified three-dimensional models are the most common models used for GCS modeling. This modeling approach is based on three-dimensional mass balance equations for each phase (CO_2 and brine), along with phase flux equations. This approach may take non-isothermal effects and component transport into account, while feedbacks of geomechanics and geochemistry on flow properties is neglected. As flow is directly modeled in all three spatial dimensions, this modeling approach is considered to be more complex than vertically-integrated approaches (both vertical equilibrium and vertical dynamic reconstruction).

Simplified three-dimensional modeling approaches have been applied at the site scale (e.g., Buscheck et al., 2011; Hosseini et al., 2013; Kempka & Kühn, 2013) to investigate injectivity and to conduct history matching, as well as at the basin scale (e.g., Liu et al., 2014; Zhou et al., 2010) to investigate storage capacity and storage safety, and at the well scale (e.g., Farajzadeh et al., 2007; Pruess, 2008) to investigate gravity enhanced mixing. Considering that simplified three-dimensional modeling approaches are often able to match measured data of plume extent and pressure response at GCS sites and that three-dimensional flow is directly modeled, simplified three-dimensional models are the de facto standard in the GCS modeling community. However, these models often come with high computational costs requiring tens of processors for tens of hours or more of computing time.

Based on modeling studies reported in the literature and conducted as part of this project, simplified three-dimensional models are the appropriate choice of modeling approach at the site scale, if heterogeneities in formation properties lead to complex three-dimensional flow fields, or if non-isothermal effects and/or changes in density and viscosity need to be taken into account. At the basin scale simplified three-dimensional models are likely inappropriate, because vertically-integrated models give comparable results (due to the low aspect ratios of formation thickness to lateral extent) at much lower computational cost, and because reservoir properties are usually not available at a discretization level necessary to justify simplified three-dimensional models.

2.5.5 Fully-coupled three-dimensional models

The most complex models applied to GSC modeling are fully-coupled three-dimensional models, where three-dimensional multi-phase flow is coupled with geomechanics and/or geochemistry, so that changes to porosity and permeability feed back to the flow simulation. They are considered the most complex modeling approach, because all processes that impact CO_2 and brine migration are represented. The interaction of flow, geochemistry and geomechanics are often implemented by coupling flow simulators with geomechanics simulators or geochemistry simulators in a serial way (i.e., coupling occurs in each time step)(e.g., Rinaldi & Rutqvist, 2013). However, directly coupled simulators of flow and geomechanics have also been developed (Preisig & Prevost, 2011).

Fully-coupled three-dimensional models have mainly been applied at the site scale, due to their high computational cost. In several cases fully-coupled models have been used to study the impact of geochemistry and geomechanics on CO_2 and brine migration at specific sites. For instance, Audigane et al. (2007) showed that porosity and permeability alteration due to geochemical reactions are expected to be negligible at the Sleipner injection site, suggesting that there is no need to directly couple flow and geochemistry at that site. Shi et al. (2012) showed that the permeability of an existing fault changed with the injection induced change in ambient pressure, giving a feedback between flow and geomechanics. Also, studies have used fully-coupled models to investigate how CO_2-saturated brine interacts with reservoir material, cap rock, and well cement (e.g., Carey et al., 2007; Huet et al., 2010), however it should be noted that most of these studies only consider single-phase flow (CO_2-saturated brine). Fully-coupled models have also been used to understand the unexpected pattern of surface-uplift at the In-Salah injection site (e.g., Morris et al., 2011; Rinaldi & Rutqvist, 2013).

Fully-coupled three-dimensional modeling approaches have been shown to be appropriate for GCS sites with strong feedback of geomechanics and/or geochemistry on flow. However, for many questions related to GCS operations – such as interpretation of geochemical monitoring or surface-uplift – simplified three-dimensional models in conjunction with decoupled geochemistry or geomechanics simulators are often sufficient. For small-scale studies where significant pore size change may occur (e.g., CO_2 and brine flow through a fracture in well cement or caprock) fully-coupled models are the most appropriate approach, because less complex models, such as simplified three-dimensional models, are not able to capture the feedback between flow and processes that alter the pore size.

2.6 Conclusion

In this project the applicability of a set of modeling approaches to geologic carbon storage (GCS) modeling was investigated. The approaches range in complexity from two-dimensional single-phase models to three-dimensional models that couple multi-phase flow, geochemistry and geomechanics. A literature review of GCS studies identified five relevant modeling approaches. Fully-coupled three-dimensional models include multi-phase flow, geochemistry and/or geomechanics, and are considered the most complex GCS models. Neglecting the feedback of geochemistry and geomechanics on flow leads to the category of simplified three-dimensional models; the most commonly used approach for modeling GCS. Simplified three-dimensional models can be further simplified by integrating the governing equations over the thickness of a formation. The vertical integration is often done in conjunction with the assumption of fast vertical segregation of CO_2 and brine, leading to vertical equilibrium models. For cases where the impact of multi-phase flow effects can be neglected, the CO_2-rich phase can be eliminated in the governing equations, and GCS operations can be simulated using single-phase models. Lastly, macroscopic invasion percolation models neglect the impact of viscosity and simulate the migration of CO_2 as a succession of equilibrium invasion events based on invasion thresholds determined by formation properties. The simplifications used for GCS models fall into two categories: reduction of dimensionality (three-dimensional to two-dimensional) and neglect of processes (geochemistry, geomechanics, viscosity).

Two new modeling approaches were investigated to fill gaps in the model complexity spectrum: vertical dynamic reconstruction (between simplified three-dimensional and vertical equilibrium models) and macroscopic invasion percolation with viscous effects (between simplified three-dimensional and macroscopic invasion percolation models). In the vertical dynamic reconstruction approach the vertical segregation dynamics are incorporated into vertically-integrated equations by representing the dynamics through one-dimensional counter-current flow. The vertical dynamic reconstruction approach has been shown to compare well with simplified three-dimensional models for cases where vertical equilibrium models fail. Also, the vertical dynamic reconstruction approach retains the computational efficiency of other vertically-integrated approaches. The enhanced microscopic invasion percolation approach did not show any significant advantages over simplified three-dimensional models, because a three-dimensional pressure equation needs to be solved, just as for the simplified three-dimensional approach. Further development of this approach was therefore stopped.

The applicability of the modeling approaches described above to GCS modeling was investigated based on five example sites (Sleipner, In Salah, Basal Cambrian Aquifer, Ketzin and Kimberlina) and other GCS modeling studies. The following set of guidelines for modeling approach guidelines was formulated based on this project. Fully-coupled models should only be employed for cases with a significant feedback of geochemistry and geomechanics to the flow system, such as studies of surface uplift and fracture-scale modeling of dissolution processes. Simplified three-dimensional models are the most commonly used approach for GCS modeling. While simplified three-dimensional models give accurate results under many circumstances, their applicability can be limited due to their high computational costs. Therefore, simplified three-dimensional models should only be chosen for cases with significant three-dimensional flow that cannot be accurately be represented by simpler modeling approaches. Vertical dynamic reconstruction models are suitable for cases where vertical flow is mainly due to segregation dynamics and not heterogeneity in formation parameters, such as in layered sedimentary basins. For cases where vertical segregation occurs fast relative to the time scale of horizontal migration, vertical equilibrium models should be chosen. Numerical studies have shown that for vertical permeabilities larger than 100 mD vertical equilibrium is often a valid assumption for typical GCS formations. If the area of CO_2 plumes is small compared to the areal extent of significant pressure perturbations, multi-phase flow effects can be neglected, leading to the choice of single-phase models. Therefore, single-phase models are often appropriate for basin-wide studies of pressure response. Macroscopic invasion percolation models do not seem to be applicable to GCS modeling except under special circumstances.

3 List of Figures

4 List of Tables

5 References

Audigane, P., Gaus, I., Czernichowski-Lauriol, I., Pruess, K., & Xu, T. F. (2007). Two-dimensional reactive transport modeling of CO_2 injection in a saline Aquifer at the Sleipner site, North Sea. *American Journal of Science, 307*(7), 974-1008. doi:10.2475/07.2007.02

Bandilla, K. W., & Celia, M. A. (2016). Geological Sequestration of Carbon Dioxide. In J. H. Cushman & D. M. Tartakowsky (Eds.), *The Handbook of Groundwater Engineering* (3 ed.): Taylor & Francis Group.

Bandilla, K. W., Celia, M. A., Birkholzer, J. T., Cihan, A., & Leister, E. C. (2015). Multiphase Modeling of Geologic Carbon Sequestration in Saline Aquifers. *Groundwater, 53*(3), 362-377. doi:10.1111/gwat.12315

Bandilla, K. W., Celia, M. A., Elliot, T. R., Person, M., Ellett, K. M., Rupp, J. A., . . . Zhang, Y. (2012). Modeling carbon sequestration in the Illinois Basin using a vertically-integrated approach. *Computing and Visualization in Science, 15*(1), 39-51. doi:10.1007/s00791-013-0195-2

Bandilla, K. W., Celia, M. A., & Leister, E. (2014). Impact of Model Complexity on CO_2 plume modeling at Sleipner. *Energy Procedia, 63*, 3405-3415. doi:10.1016/j.egypro.2014.11.369

Bickle, M., Chadwick, A., Huppert, H. E., Hallworth, M., & Lyle, S. (2007). Modelling carbon dioxide accumulation at Sleipner: Implications for underground carbon storage. *Earth and Planetary Science Letters, 255*(1-2), 164-176.

Birkholzer, J. T., Zhou, Q., Cortis, A., & Finsterle, S. (2011). A Sensitivity Study on Regional Pressure Buildup from Large-Scale CO_2 Storage Projects. *Energy Procedia, 4*, 4371-4378. doi:10.1016/j.egypro.2011.02.389

Bourne, S., Crouch, S., & Smith, M. (2014). A risk-based framework for measurement, monitoring and verification of the Quest CCS Project, Alberta, Canada. *International Journal of Greenhouse Gas Control, 26*, 109-126.

Braun, C., Helmig, R., & Manthey, S. (2005). Macro-scale effective constitutive relationships for two-phase flow processes in heterogeneous porous media with emphasis on the relative permeability-saturation relationship. *Journal of Contaminant Hydrology, 76*(1-2), 47-85.

Buscheck, T. A., Sun, Y. W., Hao, Y., Wolery, T. J., Bourcier, W., Tompson, A. F. B., . . . Aines, R. D. (2011). Combining Brine Extraction, Desalination, and Residual-Brine Reinjection with CO2 Storage in Saline Formations: Implications for Pressure Management, Capacity, and Risk Mitigation. *10th International Conference on Greenhouse Gas Control Technologies, 4*, 4283-4290. doi:10.1016/j.egypro.2011.02.378

Carey, J. W., Wigand, M., Chipera, S. J., WoldeGabriel, G., Pawar, R., Lichtner, P. C., . . . Guthrie, G. D. (2007). Analysis and performance of oil well cement with 30 years Of CO_2 exposure from the SACROC Unit, West Texas, USA. *International Journal of Greenhouse Gas Control, 1*(1), 75-85. doi:10.1016/S1750-5836(06)00004-1

Carruthers, D. J. (2003). Modeling of secondary petroleum migration using invasion percolation techniques. *Multidimensional basin modeling: AAPG/Datapages Discovery Series, 7*, 21-37.

Cavanagh, A. (2013). Benchmark calibration and prediction of the Sleipner CO_2 plume from 2006 to 2012. *Energy Procedia, 37*, 3529-3545. doi:10.1016/j.egypro.2013.06.246

Cavanagh, A., & Ringrose, P. (2011). Simulation of CO_2 distribution at the In Salah storage site using high-resolution field-scale models. *Energy Procedia, 4*, 3730-3737. doi:10.1016/j.egypro.2011.02.306

Cavanagh, A. J., & Haszeldine, R. S. (2014). The Sleipner storage site: Capillary flow modeling of a layered CO_2 plume requires fractured shale barriers within the Utsira Formation. *International Journal of Greenhouse Gas Control, 21*, 101-112.

Celia, M. A., Bachu, S., Nordbotten, J. M., & Bandilla, K. W. (2015). Status of CO_2 storage in deep saline aquifers with emphasis on modeling approaches and practical simulations. *Water Resources Research, 51*(9), 6846-6892.

Celia, M. A., Nordbotten, J. M., Court, B., Dobossy, M., & Bachu, S. (2011). Field-scale application of a semi-analytical model for estimation of CO_2 and brine leakage along old wells. *International Journal of Greenhouse Gas Control, 5*(2), 257-269.

Chadwick, R. A., Zweigel, P., Gregersen, U., Kirby, G. A., Holloway, S., & Johannessen, P. N. (2004). Geological reservoir characterization of a CO_2 storage site: The Utsira Sand, Sleipner, Northern North Sea. *Energy, 29*(9-10), 1371-1381.

Cihan, A., Birkholzer, J., & Bianchi, M. (2014). Targeted Pressure Management during CO2 Sequestration: Optimization of Well Placement and Brine Extraction. *Energy Procedia, 63*, 5325-5332. doi:10.1016/j.egypro.2014.11.564

Cihan, A., Birkholzer, J., Trevisan, L., Gonzalez-Nicolas Alvarez, A., & Illangasekare, T. (2016). Investigation of representing hysteresis in macroscopic models of two-phase flow in porous media using intermediate scale experimental data. *Water Resources Research*.

Cihan, A., Birkholzer, J. T., & Bianchi, M. (2015). Optimal well placement and brine extraction for pressure management during CO2 sequestration. *International Journal of Greenhouse Gas Control*, *42*, 175-187.

Court, B., Bandilla, K. W., Celia, M. A., Janzen, A., Dobossy, M., & Nordbotten, J. M. (2012). Applicability of vertical-equilibrium and sharp-interface assumptions in CO_2 sequestration modeling. *International Journal of Greenhouse Gas Control, 10*, 134-147. doi:10.1016/j.ijggc.2012.04.015

Emami-Meybodi, H., Hassanzadeh, H., Green, C. P., & Ennis-King, J. (2015). Convective dissolution of CO_2 in saline aquifers: Progress in modeling and experiments. *International Journal of Greenhouse Gas Control, 40*, 238-266.

Farajzadeh, R., Salimi, H., Zitha, P. L. J., & Bruining, H. (2007). Numerical simulation of density-driven natural convection in porous media with application for CO_2 injection projects. *International Journal of Heat and Mass Transfer, 50*(25-26), 5054-5064.

Gasda, S. E., Nordbotten, J. M., & Celia, M. A. (2009). Vertical equilibrium with sub-scale analytical methods for geological CO_2 sequestration. *Computational Geosciences, 13*(4), 469-481.

Gasda, S. E., Nordbotten, J. M., & Celia, M. A. (2012). Application of simplified models to CO_2 migration and immobilization in large-scale geological systems. *International Journal of Greenhouse Gas Control, 9*, 72-84.

Gaus, I. (2010). Role and impact of CO_2-rock interactions during CO_2 storage in sedimentary rocks. *International Journal of Greenhouse Gas Control, 4*(1), 73-89.

Glass, R. J., Conrad, S. H., & Yarrington, L. (2001). Gravity-destabilized nonwetting phase invasion in macroheterogeneous porous media: Near-pore-scale macro modified invasion percolation simulation of experiments. *Water Resources Research*, *37*(5), 1197-1207.

Glass, R. J., & Yarrington, L. (2003). Mechanistic modeling of fingering, nonmonotonicity, fragmentation, and pulsation within gravity/buoyant destabilized two-phase/unsaturated flow. *Water Resources Research, 39*(3).

González-Nicolás, A., Trevisan, L., Illangasekare, T. H., Cihan, A., & Birkholzer, J. T. (2016). Enhancing capillary trapping effectiveness through proper time scheduling of injection of supercritical CO_2 in heterogeneous formations. *Greenhouse Gases: Science and Technology*.

Guo, B., Bandilla, K. W., Doster, F., Keilegavlen, E., & Celia, M. A. (2014). A vertically integrated model with vertical dynamics for CO_2 storage. *Water Resources Research, 50*(8), 6269-6284.

Guo, B., Bandilla, K. W., Nordbotten, J. M., Celia, M. A., Keilegavlen, E., & Doster, F. (2016a). A multiscale multilayer vertically integrated model with vertical dynamics for CO_2 sequestration in layered geological formations. *Water Resources Research, 52*(8), 6490-6505. doi:10.1002/2016wr018714

Guo, B., Zheng, Z., Bandilla, K. W., Celia, M. A., & Stone, H. A. (2016b). Flow regime analysis for geologic CO_2 sequestration and other subsurface fluid injections. *International Journal of Greenhouse Gas Control, 53*, 284-291.

Hosseini, S. A., Lashgari, H., Choi, J. W., Nicot, J. P., Lu, J. M., & Hovorka, S. D. (2013). Static and dynamic reservoir modeling for geological CO_2 sequestration at Cranfield, Mississippi, USA. *International Journal of Greenhouse Gas Control, 18*, 449-462.

Huang, X. W., Bandilla, K. W., Celia, M. A., & Bachu, S. (2014). Basin-scale modeling of CO_2 storage using models of varying complexity. *International Journal of Greenhouse Gas Control, 20*, 73-86.

Huet, B. M., Prevost, J. H., & Scherer, G. W. (2010). Quantitative reactive transport modeling of Portland cement in CO_2-saturated water. *International Journal of Greenhouse Gas Control, 4*(3), 561-574.

Ioannidis, M. A., Chatzis, I., & Dullien, F. A. L. (1996). Macroscopic percolation model of immiscible displacement: Effects of buoyancy and spatial structure. *Water Resources Research, 32*(11), 3297-3310.

Kempka, T., & Kühn, M. (2013). Numerical simulations of CO_2 arrival times and reservoir pressure coincide with observations from the Ketzin pilot site, Germany. *Environmental Earth Sciences, 70*(8), 3675-3685.

Kueper, B. H., & Mcwhorter, D. B. (1992). The Use of Macroscopic Percolation Theory to Construct Large-Scale Capillary-Pressure Curves. *Water Resources Research, 28*(9), 2425-2436.

Lindeberg, E., Zweigel, P., Bergmo, P., Ghaderi, A., & Lothe, A. (2001). Prediction of CO2 distribution pattern improved by geology and reservoir simulation and verified by time lapse seismic. *Greenhouse Gas Control Technologies*, 372-377.

Liu, G. X., Peck, W. D., Braunberger, J. R., Klenner, R. C., Gorecki, C. D., Steadman, E. N., & Harju, J. A. (2014). Evaluation of large-scale carbon dioxide storage potential in the basal saline system in the Alberta and Williston Basins in North America. *Energy Procedia, 63*, 2911-2920. doi:10.1016/j.egypro.2014.11.314

Martens, S., Kempka, T., Liebscher, A., Luth, S., Moller, F., Myrttinen, A., . . . Grp, K. (2012). Europe's longest-operating on-shore CO_2 storage site at Ketzin, Germany: a progress report after three years of injection. *Environmental Earth Sciences, 67*(2), 323-334.

Metz, B., Davidson, O., De Coninck, H., Loos, M., & Meyer, L. (2005). *International Panel on Climate Change Special Report on Carbon Dioxide Capture and Storage*. Cambridge: Cambridge University Press.

Morris, J. P., Hao, Y., Foxall, W., & Mcnab, W. (2011). A study of injection-induced mechanical deformation at the In Salah CO_2 storage project. *International Journal of Greenhouse Gas Control, 5*(2), 270-280.

Nicot, J. P. (2008). Evaluation of large-scale CO_2 storage on fresh-water sections of aquifers: An example from the Texas Gulf Coast Basin. *International Journal of Greenhouse Gas Control, 2*(4), 582-593.

Nilsen, H. M., Herrera, P. A., Ashraf, M., Ligaarden, I., Iding, M., Hermanrud, C., . . . Keilegavlen, E. (2011). Field-case simulation of CO_2-plume migration using vertical-equilibrium models. *10th International Conference on Greenhouse Gas Control Technologies, 4*, 3801-3808. doi:10.1016/j.egypro.2011.02.315

Nordbotten, J. M., & Celia, M. A. (2012). *Geological storage of CO_2: modeling approaches for large-scale simulation*. Hoboken, NJ: Wiley.

Nordbotten, J. M., & Dahle, H. K. (2011). Impact of the capillary fringe in vertically integrated models for CO_2 storage. *Water Resources Research, 47*, W02537. doi:10.1029/2009wr008958

Norden, B., & Frykman, P. (2013). Geological modelling of the Triassic Stuttgart Formation at the Ketzin CO_2 storage site, Germany. *International Journal of Greenhouse Gas Control, 19*, 756-774.

Oldenburg, C. M., Mukhopadhyay, S., & Cihan, A. (2016). On the use of Darcy's law and invasion-percolation approaches for modeling large-scale geologic carbon sequestration. *Greenhouse Gases-Science and Technology, 6*(1), 19-33.

Pawar, R., Bromhal, G., Carroll, S., Chu, S. P., Dilmore, R., Gastelum, J., . . . Guthrie, G. (2014). Quantification of Key Long-term Risks at CO_2 Sequestration Sites: Latest Results from US DOE's National Risk Assessment Partnership (NRAP) Project. *Energy Procedia, 63*, 4816-4823. doi:10.1016/j.egypro.2014.11.512

Peck, W. D., Bachu, S., Knudsen, D. J., Hauck, T., Crotty, C. M., Gorecki, C. D., . . . Melnik, A. (2013). CO_2 storage resource potential of the Cambro-Ordovician Saline System in the western interior of North America. *Energy Procedia, 37*, 5230-5239. doi:10.1016/j.egypro.2013.06.439

Person, M., Banerjee, A., Rupp, J., Medina, C., Lichtner, P., Gable, C., . . . Bense, V. (2010). Assessment of basin-scale hydrologic impacts of CO_2 sequestration, Illinois basin. *International Journal of Greenhouse Gas Control, 4*(5), 840-854. doi:10.1016/j.ijggc.2010.04.004

Preisig, M., & Prevost, J. H. (2011). Coupled multi-phase thermo-poromechanical effects. Case study: CO_2 injection at In Salah, Algeria. *International Journal of Greenhouse Gas Control, 5*(4), 1055-1064.

Pruess, K. (2008). *Numerical modeling studies of the dissolution-diffusion-convection process during CO_2 storage in saline aquifers*. Retrieved from

Pruess, K., Oldenburg, C. M., & Moridis, G. (1999). *TOUGH2 user's guide.* (LBNL-43134). Retrieved from

Pruess, K., & Spycher, N. (2007). ECO2N - A fluid property module for the TOUGH2 code for studies of CO2 storage in saline aquifers. *Energy Conversion and Management, 48*(6), 1761-1767. doi:10.1016/j.enconman.2007.01.016

Riaz, A., Hesse, M., Tchelepi, H. A., & Orr, F. M. (2006). Onset of convection in a gravitationally unstable diffusive boundary layer in porous media. *Journal of Fluid Mechanics, 548*, 87-111.

Rinaldi, A. P., & Rutqvist, J. (2013). Modeling of deep fracture zone opening and transient ground surface uplift at KB-502 CO_2 injection well, In Salah, Algeria. *International Journal of Greenhouse Gas Control, 12*, 155-167.

Ringrose, P., Atbi, M., Mason, D., Espinassous, M., Myhrer, Ø., Iding, M., . . . Wright, I. (2009). Plume development around well KB-502 at the In Salah CO_2 storage site. *first break, 27*, 85-89.

Rutqvist, J., Vasco, D. W., & Myer, L. (2010). Coupled reservoir-geomechanical analysis of CO_2 injection and ground deformations at In Salah, Algeria. *International Journal of Greenhouse Gas Control, 4*(2), 225-230. doi:10.1016/j.ijggc.2009.10.017

Scheirer, A. H. (2007). *Petroleum systems and geologic assessment of oil and gas in the San Joaquin Basin Province, California* (2330-7102). Retrieved from

Shi, J. Q., Sinayuc, C., Durucan, S., & Korre, A. (2012). Assessment of carbon dioxide plume behaviour within the storage reservoir and the lower caprock around the KB-502 injection well at In Salah. *International Journal of Greenhouse Gas Control, 7*, 115-126.

Singh, V. P., Cavanagh, A., Hansen, H., Nazarian, B., Iding, M., & Ringrose, P. S. (2010). *Reservoir modeling of CO_2 plume behavior calibrated against monitoring data from Sleipner, Norway.* Paper presented at the SPE Annual Technical Conference and Exhibition, Florence, Italy.

Torp, T. A., & Gale, J. (2004). Demonstrating storage of CO_2 in geological reservoirs: The sleipner and SACS projects. *Energy, 29*(9-10), 1361-1369.

Trevisan, L., Pini, R., Cihan, A., Birkholzer, J. T., Zhou, Q. L., & Illangasekare, T. H. (2015). Experimental analysis of spatial correlation effects on capillary trapping of supercritical CO_2 at the intermediate laboratory scale in heterogeneous porous media. *Water Resources Research, 51*(11), 8791-8805.

Vasco, D. W., Rucci, A., Ferretti, A., Novali, F., Bissell, R. C., Ringrose, P. S., . . . Wright, I. W. (2010). Satellite-based measurements of surface deformation reveal fluid flow associated with the geological storage of carbon dioxide. *Geophysical Research Letters, 37*. doi:10.1029/2009GL041544

Wainwright, H. M., Finsterle, S., Zhou, Q. L., & Birkholzer, J. T. (2013). Modeling the performance of large-scale CO_2 storage systems: A comparison of different sensitivity analysis methods. *International Journal of Greenhouse Gas Control, 17*, 189-205.

Wright, I. W. (2007). *The In Salah Gas CO_2 Storage Project*. Paper presented at the International Petroleum Technology Conference, Dubai, U.A.E. .

Yang, Z. B., Tian, L., Niemi, A., & Fagerlund, F. (2013). Upscaling of the constitutive relationships for CO_2 migration in multimodal heterogeneous formations. *International Journal of Greenhouse Gas Control, 19*, 743-755.

Yortsos, Y. C., Satik, C., Bacri, J. C., & Salin, D. (1993). Large-Scale Percolation Theory of Drainage. *Transport in Porous Media, 10*(2), 171-195. doi:Doi 10.1007/Bf00617007

Zhou, Q. L., & Birkholzer, J. T. (2011). On scale and magnitude of pressure build-up induced by large-scale geologic storage of CO_2. *Greenhouse Gases-Science and Technology, 1*(1), 11-20. doi:10.1002/ghg3.001

Zhou, Q. L., Birkholzer, J. T., Mehnert, E., Lin, Y. F., & Zhang, K. (2010). Modeling Basin- and Plume-Scale Processes of CO_2 Storage for Full-Scale Deployment. *Ground Water, 48*(4), 494-514. doi:10.1111/j.1745-6584.2009.00657.x

Zoback, M. D., & Gorelick, S. M. (2012). Earthquake triggering and large-scale geologic storage of carbon dioxide. *Proceedings of the National Academy of Sciences of the United States of America, 109*(26), 10164-10168. doi:10.1073/pnas.1202473109

Appendix A: Journal publications, book chapters and presentations resulting from this project

Journal publications (13)

- Bandilla, K.W., Celia, M.A., Birkholzer, J.T., Cihan, A., Leister, E., 2015. Overview of approaches for modeling of geologic carbon sequestration in saline aquifers. *Groundwater*, 53(3), pp. 362–377.
- Bandilla, K.W., Celia, M.A., Leister, E., 2014. Impact of Model Complexity on CO_2 plume modeling at Sleipner. *Energy Procedia,* 63, pp. 3405-3415.
- Celia, M.A., Bachu, S., Nordbotten, J.M., Bandilla, K.W., 2015. Status of CO_2 Storage in Deep Saline Aquifers with Emphasis on Modeling Approaches and Practical Simulations. *Water Resources Research*, 51(9), pp. 6846–6892.
- Cihan, A., Birkholzer, J.T., Bianchi, M., 2015. Optimal Well Placement and Brine Extraction for Pressure Management during CO_2 Sequestration. *International Journal of Greenhouse Gas Control*, 42, pp. 175–187.
- Cihan, A., Birkholzer, J.T., Bianchi, M., 2014. Targeted pressure management during CO_2 sequestration: Optimization of well placement and brine extraction in a heterogeneous aquifer. *Energy Procedia,* 63, pp. 5325-5332.
- Cihan, A., Birkholzer, J.T., Trevisan, L., Bianchi, M., Zhou, G. Illangasekare, T., 2014. A connectivity-based upscaling-approach for modeling two-phase flow in heterogeneous geological formations. *Energy Procedia,* 63, pp. 3456-3463.
- González-Nicolás, A., Trevisan, L., Illangasekare, T.H., Cihan, A., Birkholzer, J T., 2016. Enhancing Capillary Trapping Effectiveness through Proper Time Scheduling of Injection of Supercritical CO_2 in Heterogeneous Formations. *Greenhouse Gases: Science and Technology*. doi:10.1002/ghg.1646
- Guo, B., Bandilla, K.W., Nordbotten, J.M., Celia, M.A., Keilegavlen, E., Doster, F., 2016. Multiscale multilayer vertically-integrated model with subscale vertical dynamics for CO_2 migration in heterogeneous formations. *Water Resources Research*, 52 (8), pp. 6490–6505.
- Guo, B., Zheng, Z., Bandilla, K.W., Celia, M.A., Stone, H.A., 2016. Flow regime analysis for geologic CO_2 sequestration and other subsurface fluid injections. *International Journal of Greenhouse Gas Control*, 53, pp. 284–291.
- Guo, B., Bandilla, K.W., Keilegavlen, E., Doster, F., Celia, M.A., 2014. Application of a vertically-integrated model with subscale vertical dynamics to field injection sites for CO_2 storage. *Energy Procedia,* 63, pp. 3523-3531.
- Guo, B., Bandilla, K.W., Doster, F., Keilegavlen, E., Celia, M.A., 2014. A Vertically-integrated Model with Vertical Dynamics for CO_2 storage. *Water Resources Research*, 50 (8), pp. 6269–6284.

- Huang, X., Bandilla, K.W., Celia, M.A., Bachu, S., 2014. Basin-scale modeling of CO_2 storage using models of varying complexity. *International Journal of Greenhouse Gas Control*, 20, pp. 73-86.
- Oldenburg, C., Mukhopadhyay, S., Cihan, A., 2015. On The Use of Darcy's Law and Invasion-Percolation Approaches for Modeling Large-Scale Geologic Carbon Sequestration. *Greenhouse Gases: Science and Technology,* 6(1), pp. 19–33.

Books or other non-periodical, one-time publications (1)

- Bandilla, K.W., Celia, M.A., 2016. Geological Sequestration of Carbon Dioxide. In J. H. Cushman & D. M. Tartakowsky (Eds.), *The Handbook of Groundwater Engineering* (3 ed.): Taylor & Francis Group.

Other publications, conference papers and presentations (47)

- Bandilla, K.W., Guo, B., Celia, M.A., 2016. Model Complexity and Choice of Model Approaches for Practical Simulations of CO_2 Injection, Migration, Leakage, and Long-term Fate. Talk presented at the *DOE National Energy Technology Laboratory's Mastering the Subsurface Through Technology, Innovation and Collaboration: Carbon Storage and Oil and Natural Gas Technologies Review Meeting* in Pittsburgh, PA (8/16-8/18/2016).
- Bandilla, K.W., Guo, B., Celia, M.A., 2016. Applicability of vertically integrated models for carbon storage modeling in structured heterogeneous domains. Talk presented at the *XXI International Conference of Computational Methods* in Toronto, Canada (6/20-6/24/2016).
- Bandilla, K.W., Guo, B., Celia, M.A., 2015. Impact of model complexity for carbon dioxide migration in structured heterogeneous domains. Talk presented at the *2015 American Institute of Chemical Engineering Annual Meeting* in Salt Lake City, UT (11/8-11/13/2015).
- Bandilla, K.W., Guo, B., Celia, M.A., 2015. Vertically-integrated Approaches for Carbon Sequestration Modeling. Talk presented at the *American Geophysical Union 2015 Fall Meeting* in San Francisco, CA (12/14-12/18/2015).
- Bandilla, K.W., Celia, M.A., Guo, B., 2015. Model Complexity and Choice of Model Approaches for Practical Simulations of CO_2 Injection, Migration, Leakage, and Long-term Fate. Talk presented at the *Carbon Storage R&D Project Review Meeting* Pittsburgh, PA (8/18-8/20/2015).
- Bandilla, K.W., Celia, M.A., Leister, E., 2014. Impact of Model Complexity on CO_2 plume modeling at Sleipner." Poster presented at the *12th International Conference on Greenhouse Gas Control Technologies (GHGT-12)* in Austin, TX (10/5 – 10/9/2014).
- Bandilla, K.W., Celia, M.A., Leister, E., Guo, B., 2014. Modeling CO_2 migration at Sleipner using models of varying complexity. Talk presented at the *American Geophysical Union Fall Meeting 2014* in San Francisco, CA (12/15 - 12/19/2014).

- Bandilla, K.W., Celia, M.A., Guo, B., 2014. Model Complexity and Choice of Model Approaches for Practical Simulations of CO_2 Injection, Migration, Leakage, and Long-term Fate. Talk presented at the *DOE Carbon Storage R&D Project Review Meeting* in Pittsburgh, PA (8/12-8/14/2014).
- Bandilla, K.W., Birkholzer, J.T., Cihan, A., Celia, M.A., 2014. A multi-tiered approach for carbon sequestration Area of Review delineation. Poster *presented at the American Geophysical Union Science Policy 2014 Conference* in Washington, DC (6/16-6/18/2014).
- Bandilla, K.W., Celia, M.A., Guo, B., 2014. Model Complexity and Choice of Model Approaches for Practical Simulations of CO2 Injection, Migration, Leakage, and Long–term Fate. Talk presented at the *DOE Carbon Storage R&D Review Meeting* in Pittsburgh, PA (8/20–8/22/2013).
- Bandilla, K.W., Celia, M.A., 2013. Active pressure management through brine production for industrial-scale geologic carbon sequestration deployment in the Illinois Basin, USA. Poster presented at the *DOE Carbon Storage R&D Review Meeting* in Pittsburgh, PA (8/20–8/22/2013).
- Bandilla, K.W., Celia, M.A., 2013. Pressure uncertainty and the Implication for Risk. Talk presented at the *IEAGHG Combined Modelling and Risk Management Network Meeting* in Trondheim, Norway, (6/10–6/13/2013).
- Becker, B., Helmig, R., Flemisch, B., Guo, B., Celia, M. A., 2015. Evaluation of the Coupling of a Full-Dimensional Multiphase Model with a Vertical Equilibrium Model for the Simulation of Underground Gas Storage. Poster presented at the *American Geophysical Union 2015 Fall Meeting* in San Francisco, CA (12/14-12/18/2015).
- Birkholzer, J.T., 2014. Studies for Modeling CO_2 Processes, Comparison, and Joint Inversion with Characterization and Monitoring Data. Talk presented at the *DOE Carbon Storage R&D Project Review Meeting* in Pittsburgh, PA (8/12-8/14/2014).
- Birkholzer, J.T., 2013. Studies for Modeling CO_2 Processes: Pressure Management, Basin– Scale Models, Model Comparison, and Joint Inversion. Talk presented at the *DOE Carbon Storage R&D Review Meeting* in Pittsburgh, PA (8/20–8/22/2013).
- Birkholzer, J.T., Cihan, A., Bainchi, M., 2014. Targeted Pressure Management during CO_2 Sequestration: Optimization of Well Placement and Brine Extraction in a Heterogeneous Reservoir. Talk presented at the *12^{th} International Conference on Greenhouse Gas Control Technologies (GHGT-12)* in Austin, TX (10/5 – 10/9/2014).
- Birkholzer, J.T., M. Bainchi, Cihan, A., 2014. Optimization of Well Placement and Brine Extraction for Pressure Control Along Critically Stressed Faults. Talked presented at the 13th Annual Conference on Carbon Capture, Utilization and Sequestration, Pittsburgh, PA, (4/28-5/1/2014).
- Celia, M.A., 2015. CCS: Current Status, Future Prospects, and the Role of NUPUS. Talk presented at the *Non-linearities and Upscaling in Porous Media Conference* in Freudenstadt, Germany (9/8 – 9/12/2015).

- Celia, M.A., 2015. Modeling Approaches for CO_2 Injection in Conventional and Unconventional Reservoirs. Talk presented at the PetroChina Research group in Beijing, China.
- Celia, M.A., 2015. Carbon Dioxide Sequestration in Conventional and Unconventional Reservoirs. Talk presented at the Department of Hydraulic Engineering, Tsinghua University, Beijing, China.
- Celia, M.A., 2015. Leakage along Old Wells with Applications to CO_2 Sequestration and Methane Emissions. Talk at the Division of Earth Sciences, Lawrence Berkeley National Laboratory.
- Celia, M.A., 2015. Carbon Capture and Storage. Talk at the University of Bergen Summer School on Sustainability, Bergen, Norway.
- Celia, M.A., 2015. Model Complexity and Simulation Approaches for Geological Sequestration of Carbon Dioxide. Talk presented at both the City University of Hong Kong (1/23/2015) and at the Polytechnic University of Hong Kong (1/26/2015).
- Celia, M.A., 2015. Leakage along Old Wells with Applications to CO_2 Sequestration and Methane Emissions. Talk presented at the University of Kansas (2/19/2015).
- Celia, M.A., 2013. Can CCS Find Synergies with Geothermal Energy and Shale Gas Production? Talk presented at the *SIAM Conference on Mathematical & Computational Issues in the Geosciences* in Padua, Italy, (6/17–6/20/2013).
- Celia, M.A., Nordbotten, J.M, Bandilla, K.W., Gasda, S., Guo, B., 2012. Multi-scale Modeling and Model Complexity in CO_2 Sequestration Simulations. Talk presented at the *American Geophysical Union 2012 Fall Meeting* in San Francisco, CA (12/3-12/7/2012).
- Cihan, A., Birkholzer, J.T., 2015. Optimization of Fluid Injection and Extraction in Deep Subsurface Reservoirs: Examples from CO_2 Sequestration. Talk presented at the *Technical Workshop on Enhanced Water Recovery*, Livermore, CA (9/14/2015).
- Cihan, A., Birkholzer, J.T., Bianchi, M., 2015. Pressure management during geological CO_2 sequestration: Optimal well placement and brine extraction in a heterogeneous reservoir. TOUGH2 Conference Proceeding Paper, TOUGH2 Symposium 2015, Berkeley, CA (9/28-9/30/2015).
- Cihan, A., Siirila-Woodburn, E.R., Birkholzer, J.T., 2015. Determining the Area of Review (AoR) in Carbon Capture and Storage: A tiered, probabilistic methodology to generate risk map. Talk presented at the *American Geophysical Union 2015 Fall Meeting* in San Francisco, CA (12/14-12/18/2015).
- Cihan, A., Birkholzer, J.T., Bianchi, M., 2014. Targeted pressure management during CO_2 sequestration: Optimization of well placement and brine extraction in a heterogeneous aquifer." Talk presented at the *12th International Conference on Greenhouse Gas Control Technologies (GHGT-12)* in Austin, TX (10/5 – 10/9/2014).
- Cihan, A., Birkholzer, J.T., Trevisan, L., Bianchi, M., Zhou, G. Illangasekare, T., 2014. A connectivity-based upscaling-approach for modeling two-phase flow in heterogeneous

geological formations. Talk presented at the *12th International Conference on Greenhouse Gas Control Technologies (GHGT-12)* in Austin, TX (10/5 – 10/9/2014).

- Cihan, A., Birkholzer, J.T., Bianchi, M.A., 2014. Constrained Differential Evolution algorithm for reservoir management: optimal placement and control of wells for geological carbon storage with uncertainty in reservoir properties. Poster presented at the *American Geophysical Union Fall Meeting 2014* in San Francisco, CA (12/15 - 12/19/2014).
- Guo, B., Bandilla, K.W., Celia, M.A., 2016. Multiscale Vertically-integrated Models with Vertical Dynamics for CO_2 migration in Heterogeneous Geologic Formations. Talk presented at the *XXI International Conference of Computational Methods* in Toronto, Canada (6/20-6/24/2016).
- Guo, B., Bandilla, K.W., Celia, M.A., 2016. Flow regime analysis for geologic CO_2 sequestration and other subsurface fluid injections. Poster presented at the *XXI International Conference of Computational Methods* in Toronto, Canada (6/20-6/24/2016).
- Guo, B., Bandilla, K.W., Celia, M.A., 2015. Flow regime analysis for fluid injection into a confined aquifer: implications for CO_2 sequestration. Talk presented at the *American Geophysical Union 2015 Fall Meeting* in San Francisco, CA (12/14-12/18/2015).
- Guo, B., Zheng, Z., Celia, M.A., Stone, H.A., 2015. Axisymmetric flows from fluid injection into a confined porous medium. Talk presented at the *Non-linearities and Upscaling in Porous Media Conference* in Freudenstadt, Germany (9/8 – 9/12/2015).
- Guo, B., 2015. Flow regimes for fluid injection into a confined aquifer - implications to geological CO_2 sequestration. Talk presented at the School of Environmental Science and Engineering, China Ocean University, Shandong.
- Guo, B., 2015. Multiscale vertically-integrated models for CO_2 sequestration in saline aquifers. Talk presented at the Institute of Mechanics, Chinese Academy of Sciences, Beijing.
- Guo, B., 2015. Multiscale modeling Approaches for CO_2 injection and migration. Talk presented at the *International Congress on Industrial and Applied Mathematics* in Beijing, China and at the Department of Hydraulic Engineering, Tsinghua University, Beijing, China.
- Guo, B., Bandilla, K.W., Keilegavlen, E., Doster, F., Celia, M.A., 2014. Application of a vertically-integrated model with subscale vertical dynamics to field injection sites for CO_2 storage. Talk presented at the *12th International Conference on Greenhouse Gas Control Technologies (GHGT-12)* in Austin, TX (10/5 – 10/9/2014).
- Guo, B., Bandilla, K.W., Keilegavlen, E., Doster, F., Celia, M.A., 2014. A multi-layer vertically integrated model with vertical dynamics and heterogeneity for CO_2 sequestration. Poster presented at the *American Geophysical Union Fall Meeting 2014* in San Francisco, CA (12/15 - 12/19/2014).

- Guo, B., Bandilla, K.W., Doster, F., Keilegavlen, E., Celia, M.A., 2014. Multiscale Model with Vertical Dynamics in a Vertically-integrated Framework for CO_2 Storage. Talk presented at the *XX International Conference on Computational Methods in Water Resources* in Stuttgart, Germany (6/10-6/13/2014).
- Guo, B., Bandilla, K.W., Doster, F., Keilegavlen, E., Celia, M.A., 2013. Inclusion of vertical dynamics in vertically integrated models for CO_2 storage. Talk presented at the *2nd International Conference on Non-Linearities and Upscaling in Porous Media* in Bergen, Norway, (9/30–10/2/2013).
- Guo, B., 2013. A vertically-integrated Model with Vertical Dynamics for CO_2 Storage. Talk presented at the Department of Mathematics at the University of Bergen, Bergen, Norway, September 25, 2013.
- Guo, B., Bandilla, K.W., Celia, M.A., 2012. Inclusion of Vertical Dynamics in Vertically-integrated Models for CO_2 Storage. Poster presented at the *American Geophysical Union 2012 Fall Meeting* in San Francisco, CA (12/3-12/7/2012).
- Huang, X., Bandilla, K.W., Celia, M.A., Bachu, S., 2013. Basin-scale Modeling of Geological Carbon Sequestration: Model Complexity, Injection Scenario and Sensitivity Analysis. Talk presented at the *American Geophysical Union Fall Meeting 2013* in San Francisco, CA (12/9–12/13/ 2013).
- Zhou, Q., Birkholzer, J.T., Bachu, S., Peck, W.D., Braunberger, J., 2014. Assessing the regional-scale dynamic storage capacity of the Northern Plains – Prairie Basal Aquifer. Talk presented at the *12th International Conference on Greenhouse Gas Control Technologies (GHGT-12)* in Austin, TX (10/5 – 10/9/2014).

Appendix B: Data uploaded to EDX

Task 2.1: Review and Analyze Existing Models of Different Complexity

- Bandilla, K.W., Celia, M.A., Birkholzer, J.T., Cihan, A., Leister, E., 2015. Overview of approaches for modeling of geologic carbon sequestration in saline aquifers. *Groundwater*, 53(3), pp. 362–377. (link to the publisher's website)

Task 2.2: Develop Model of Intermediate Complexity that includes Vertical Drainage Dynamics

- Guo, B., Bandilla, K.W., Doster, F., Keilegavlen, E., Celia, M.A., 2014. A Vertically-integrated Model with Vertical Dynamics for CO_2 storage. *Water Resources Research*, 50 (8), pp. 6269–6284. (link to the publisher's website)
- Guo, B., Bandilla, K.W., Nordbotten, J.M., Celia, M.A., Keilegavlen, E., Doster, F., 2016. Multiscale multilayer vertically-integrated model with subscale vertical dynamics for CO_2 migration in heterogeneous formations. *Water Resources Research*, 52 (8), pp. 6490–6505. (link to the publisher's website)
- Executables that run the following test cases:
    - single-layer, fully-penetrating well, 10mD permeability, without capillary pressure
    - single-layer, partially-penetrating well, 10mD permeability, with capillary pressure
    - two-layer, fully-penetrating well, 10mD permeability in the top layer, 100 mD in the bottom layer, with capillary pressure
    - four-layer based on Mt Simon, partially-penetrating well, with capillary pressure

Task 2.3: Develop Generalized Macroscopic Percolation Model

- Executable and input files to run the newly developed macroscopic invasion percolation model for the tank experiment

Task 3: Comparison of Models for Existing Injection Operations

- Basal Aquifer:
    - Huang, X., Bandilla, K.W., Celia, M.A., Bachu, S., 2014. Basin-scale modeling of CO_2 storage using models of varying complexity. *International Journal of Greenhouse Gas Control*, 20, pp. 73-86. (link to the publisher's website)
    - Executable and input files to run vertical equilibrium model for Basal Aquifer with onsite injection

- Sleipner:
    - Bandilla, K.W., Celia, M.A., Leister, E., 2014. Impact of Model Complexity on CO_2 plume modeling at Sleipner. *Energy Procedia*, 63, pp. 3405-3415. (link to the publisher's website)
    - Input files for TOUGH2 simulation of the 9th layer of Sleipner
    - Executable and input files to run vertical equilibrium models of the 9th layer of Sleipner
- Ketzin:
    - Bandilla K.W., Guo B., Celia M.A., 2016. Applicability of vertically integrated models for carbon storage in heterogeneous domains. Talk presented at the *American Geophysical Union Fall 2016 Meeting*, San Francisco, CA (12/12-12/16/2016); slides.
    - Bandilla K.W., Guo B., Celia M.A., 2016. Applicability of Vertically Integrated Models for Carbon Storage Modeling in Structured Heterogeneous Domains. Talk presented at the *13th International Conference on Greenhouse Gas Technologies (GHGT-13)*, Lausanne, Switzerland (11/14-11/18/2016); slides.
    - Bandilla, K.W., Guo, B., Celia, M.A., 2016. Applicability of vertically integrated models for carbon storage modeling in structured heterogeneous domains. Talk presented at the *XXI International Conference of Computational Methods* in Toronto, Canada (6/20-6/24/2016); slides and extended abstract.
    - Bandilla, K.W., Guo, B., Celia, M.A., 2015. Impact of model complexity for carbon dioxide migration in structured heterogeneous domains. Talk presented at the *2015 American Institute of Chemical Engineering Annual Meeting* in Salt Lake City, UT (11/8-11/13/2015); extended abstract and slides.
    - Executable and input files to run vertical equilibrium models for three cases: single channel, two intersecting channels, two intersecting channels at different depths
    - Input files for TOUGH2 simulations of the three test cases above
- In Salah:
    - No data were collected or produced for the In Salah site during this project

Task 4: Identification of Models for Design and Optimization of Injection, Extraction, and Monitoring Wells

- Executables and input files to run the optimized cases of the Kimberlina model using both the simplified three-dimensional approach and the vertical-equilibrium approach

Task 5: Development and Application of Criteria for Appropriate Level of Model Complexity

- No data were collected or produced for the In Salah site during this project