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Impact of Model Complexity on CO_2 plume modeling at Sleipner

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Abstract

The goal of geologic carbon sequestration (GCS) is to store carbon dioxide (CO_2) in the subsurface for time periods on the order of thousands of years. Mathematical modeling is an important tool to predict the migration of both CO_2 and brine to ensure safe and permanent storage. Many modeling approaches with different levels of complexity have been applied to the problem of GCS ranging from simple analytic solutions to fully-coupled three-dimensional reservoir simulators. The choice of modeling approach is often a function of the spatial and temporal scales of the problem, reservoir properties, data availability, available computational resources, and the familiarity of the modeler with a specific modeling approach. In this study we apply a series of models with different levels of model complexity to the 9th layer of the Utsira Formation. The list of modeling approaches includes (from least complex to most complex): numerical vertical-equilibrium model with sharp-interface, numerical vertical-equilibrium model with capillary transition zone, vertically-integrated model with dynamic vertical pressure and saturation reconstruction, and fully-coupled three-dimensional model. The model domain consists of a 3 x 6 km section of the 9th layer, as described in the IEAGHG benchmark dataset. The layer thickness varies in space, ranging from 5 to 30 m, while porosity and permeability are close to constant at 0.36 and 1.8 Darcy, respectively. The models are all based on the same input data, and initial and boundary conditions are chosen in a way that ensures the different models are comparable. In addition, a simple box model is used for preliminary simulations. The models are compared based on the predicted CO_2 plume footprints and saturation cross-sections. The predicted CO_2 plumes are also compared to the actual CO_2 plume footprint from seismic surveys to determine the ability of the different models to predict the actual CO_2 plume footprint. The results show that vertical-equilibrium models are sufficient to model CO_2 migration in the 9th layer of Sleipner, due to the formation's higher permeability and relatively thin capillary transition zone. None of the models used in this study was able to accurately predict the actual plume footprint; this suggests the modeling approaches used here are missing essential physics or that some parameters in the site model (e.g., topography of the caprock) are inaccurate.

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1. Introduction

Geologic carbon sequestration (GCS) is seen as a possible climate change mitigation approach [1,2]. Carbon dioxide (CO_2) is captured from large stationary sources, such coal-fired power plants, and is injected deep underground for long-term storage. Saline aquifers and depleted oil and gas fields are considered the most viable injection targets. Computer modeling is routinely used to assess long-term storage safety and operational parameters. Currently, there are several pilot-scale and industrial-scale injection operations such as the ADM-Decatur site in the USA and the Sleipner site in Norway. The Sleipner site in Norway commenced injection operations in 1996 and has injected about 1 million tonnes (Mt) of CO_2 per year into the Utsira sand formation. The Utsira sand is a thick formation with high permeability that has interbedded thin shale layers that act as baffles for the vertical migration of CO_2. While the shale layers are difficult to detect from seismic surveys, the CO_2 pooling underneath the baffles can be detected through repeat seismic surveys. As a result of the repeat seismic surveys, the CO_2 plume in the uppermost sand layer is well delineated. The plume is non-radial with a distinct finger developing in a northerly direction, suggesting a strong impact of the caprock topography on CO_2 migration. In 2010 IEAGHG published a dataset describing the uppermost sand layer of the Utsira Formation, to allow the carbon sequestration modeling community to study CO_2 migration based on a consistent dataset [3].

In this study, we used the IEAGHG benchmark dataset to compare the impact of model complexity on CO_2 migration predictions in the uppermost sand layer of the Utsira formation. We compare results from a fully three-dimensional approach to results from vertically-integrated approaches. First, we present the modeling approaches used in this study, followed by a description of the IEAGHG benchmark dataset and how it is used with the numerical models of this study. Then, we discuss the modeling results and finish with a set of conclusions.

2. Modeling approaches

Geologic carbon sequestration leads to migration of both the injected CO_2 and resident brine. Mathematical models are commonly used to predict the fluid movement in the subsurface. The mathematical models are usually based on mass balance equations for each of the phases α (α=*c:* supercritical CO_2; α=*b:* resident brine):

$$\frac{\partial}{\partial t}\left(\rho_\alpha \phi s_\alpha\right)+\nabla\cdot\left(\rho_\alpha \mathbf{u}_\alpha\right)=\psi_\alpha \tag{1}$$

where ρ_α is the density of phase α, ϕ is the porosity, s_α is the saturation of phase α, and ψ_α is the source/sink term. The volumetric phase flux $\mathbf{u}_\alpha$ is defined by the multi-phase form of the Darcy equation:

$$\mathbf{u}_\alpha=-\frac{k_{r,\alpha}\mathbf{k}}{\mu_\alpha}\left(\nabla p_\alpha-\rho_\alpha \mathbf{g}\right) \tag{2}$$

where $\mathbf{k}$ is the intrinsic permeability, $k_{r,\alpha}$ is the relative permeability of phase α, μ_α is the viscosity of phase α, p_α is the phase pressure, and $\mathbf{g}$ is the gravity acceleration vector. Both the relative permeability and the difference between the phase pressures (capillary pressure p^{cap}) are usually assumed to be empirical functions of saturation:

$$k_{r,\alpha}=k_{r,\alpha}\left(s_\alpha\right) \quad \text{and} \quad p_c-p_b=p^{cap}\left(s_\alpha\right) \tag{3}$$

The constraint that the two phase saturations sum to unity closes the system of equations:

$$s_c+s_b=1 \tag{4}$$

Other processes that may impact the migration of CO_2 and brine include geomechanics and geochemistry. Injection-induced pressure changes will change the stress field, and thus may create and/or reactivate fractures in the host rock, increasing the permeability. Due to the relatively low injection-induced pressure increase observed at the Sleipner site, geomechanical effects are not expected to have a significant impact on the CO_2 migration, and therefore geomechanical effects on permeability are neglected here. CO_2 injection may lead to conditions that either dissolve the host rock or precipitate minerals in the pore space. Therefore, geochemistry can either increase or decrease permeability. A study by [4] showed geochemistry had an insignificant impact on permeability at the Sleipner site,

and therefore geochemistry is neglected in this study. Dissolution of CO_2 into brine has a significant impact on the migration of CO_2, because brine containing dissolved CO_2 is denser than pure brine, and thus dissolved CO_2 is considered to be stably stored. While [5] found that significant amounts of CO_2 would dissolve into brine at Sleipner, the dissolved CO_2 is not expected to impact the results from this study, because dissolved CO_2 does not change the fluid mobilities, and leakage rate estimates are based on the mass of CO_2 detected by seismic surveys and thus do not include the dissolved CO_2. Therefore, dissolution of CO_2 into brine (and vice-versa) is neglected here.

The system of equations given by equations 1 - 4 needs to be solved to predict the migration of CO_2 and brine. The primary unknowns are the two phase pressures and the two phase saturations. The solution of this system of equations is complicated by the dependence of relative permeability ($k_{r,\alpha}$) and capillary pressure (p^{cap}) on saturation, leading to a non-linear system of equations. To deal with these non-linearities, the system is usually solved using a nonlinear solver, with a simple example being the Implicit Pressure – Explicit Saturation (IMPES) approach. While the system may be solved analytically for some simple problem geometries, for most cases the domain is discretized and the system is solved using finite differences or finite elements. Many simulators, such as TOUGH2 [6,7], Eclipse [8] and DuMuX [9], which are based on such numerical solutions of equations 1 – 4, are routinely used to model the migration of CO_2 and brine.

The density difference between CO_2 and brine leads to vertical segregation of the two fluids, with CO_2 rising up above the denser brine. For cases where the vertical segregation is fast relative to the simulation time, it can be assumed that the two fluids are at vertical pressure equilibrium (i.e., there is no vertical flow). This assumption is termed *vertical equilibrium* assumption. This assumption allows for integration of the three-dimensional governing equations (i.e., equations 1 - 4) in the vertical direction. The integration leads to the following set of two-dimensional equations

$$\frac{\partial\left(\Phi S_\alpha\right)}{\partial t} + c_\alpha \Phi S_\alpha \frac{\partial P_\alpha}{\partial t} + \nabla \cdot \mathbf{U}_{\alpha,\|} = \Psi_\alpha \tag{5}$$

The vertically-averaged saturation S_α is defined as

$$S_\alpha = \frac{1}{\Phi}\int_{\xi_B}^{\xi_T} \phi s_\alpha dx_3 \tag{6}$$

where the x_3-direction is perpendicular to the main bedding plane of the reservoir (i.e., the vertical direction) and is positive upwards, and Φ is the vertically integrated porosity. ξ_B and ξ_T give the bottom and top elevation of the reservoir, respectively. As vertically integrated pressure is not a very useful measure, P_α is taken to be a representative pressure; chosen here to be the phase pressure at the bottom of the reservoir. The vertically-integrated Darcy fluxes, $\mathbf{U}_{\alpha,\|}$, are given by

$$\mathbf{U}_{\alpha,\|} = -\mathbf{K}\Lambda_\alpha \cdot \left(\nabla_\| P_\alpha - \rho_\alpha \mathbf{G}\right) \tag{7}$$

The vertically-integrated permeability, $\mathbf{K}$, the vertically-averaged phase mobility, Λ_α, the vertically-integrated porosity, Φ, and the vertically-integrated phase sources/sinks, Ψ_α, are defined as

$$\mathbf{K} = \int_{\xi_B}^{\xi_T} \mathbf{k}_\| dx_3 \qquad \Lambda_\alpha = \mathbf{K}^{-1}\int_{\xi_B}^{\xi_T} \mathbf{k}_\| \frac{k_{r,\alpha}}{\mu_\alpha} dx_3 \qquad \Phi = \int_{\xi_B}^{\xi_T} \phi dx_3 \qquad \Psi_\alpha = \frac{1}{\rho_\alpha}\int_{\xi_B}^{\xi_T} \psi_\alpha dx_3 \tag{8}$$

where $\|$ indicates the (two-dimensional) direction of the bedding plane (x_1, x_2) and $\mathbf{G} = \mathbf{e}_\| \cdot \mathbf{g} + \left(\mathbf{g}\cdot\mathbf{e}_3\right)\nabla_\| \xi_B$, with $\mathbf{e}_\| = \left(\mathbf{e}_1, \mathbf{e}_2\right)$. Just as for the three-dimensional set of equations, the saturations sum to unity, so that

$$S_c + S_b = 1 \tag{9}$$

This set of equations (equations 5 – 9) can then be solved using simple algebraic expressions to reconstruct the vertical pressure and saturation profiles. While reconstruction of the phase pressures is straight forward, the reconstruction of the saturation profiles is more involved, due to the non-linear shape of the capillary transition zone. For cases where the capillary transition zone is small compared to the thickness of the reservoir, the fluids can be assumed to be separated by a macroscopic sharp interface with full CO_2 saturation above and full brine saturation below the interface. Incorporating this so called sharp-interface assumption simplifies the governing equations to a point where they can be solved semi-analytically for homogeneous reservoirs. For a more complete derivation of vertical equilibrium models, please refer to [10].

In a study on the applicability of vertical equilibrium approaches for geologic carbon sequestration modeling, [11] found that the vertical-equilibrium assumption is sometimes not valid for models representing realistic reservoir conditions; especially close to the outer edge of CO_2 plumes. [12] developed a vertically-integrated method that does not rely on the vertical equilibrium assumption. This new method retains the computational efficiency of solving a two-dimensional instead of three-dimensional system, while accurately predicting CO_2 and brine migration for a broad range of realistic reservoir conditions. The main difference compared to the vertical-equilibrium approach is that the vertical redistribution of CO_2 and brine is modeled explicitly in time instead of assuming that the two phases segregate instantaneously. The new approach is termed *dynamic reconstruction* approach, where the vertical saturation profiles are reconstructed based on the numerical solution of the vertical fractional flow equation. It should be noted, that in this approach, unlike for the vertical-equilibrium approaches, there is no a priori assumption of the cross-sectional plume shape. For a detailed description of the dynamic reconstruction approach the reader is referred to [12].

The list of approaches described above ranges from three-dimensional multi-phase models to simplified vertical equilibrium models. In general, models with higher complexity require more input parameters, many of which may be associated with significant uncertainty, and are computationally more expensive. This article investigates the impact of model selection choice on CO_2 migration in the 9th layer at Sleipner. In this study TOUGH2/ECO2N was used for the three-dimensional models, while in-house codes were used for the vertically-integrated models.

3. Model description

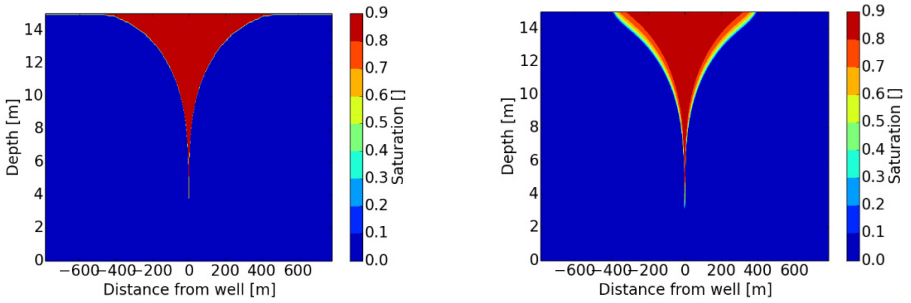
In order to compare the modeling approaches described in the previous section, a model of the 9th layer of the Sleipner site was constructed based on the IEAGHG benchmark dataset [3]. The dataset consists of a three-dimensional grid with a horizontal extent of 3 x 6 km and varying thickness between 5 and 30 m. The model includes the upper-most sand layer and the low-permeability layers above and below the sand. The horizontal resolution is approximately 50 x 50 m, leading to a grid of 65 x 119 cells. In the vertical direction the model is discretized into 43 cells of equal thickness. The top two and bottom seven cells represent the low-permeability layers, while the remaining 34 cells represent the sand. Porosity and permeability are given for each cell. Overall, the domain is relatively homogeneous with a clearly layered structure. The horizontal permeability and porosity of the sand layer vary between 1700 and 2000 mD (millidarcy) and 0.355 and 0.36, respectively. The permeability and porosity of the confining layers are 0.001 mD and 0.34. The permeability anisotropy ratio in the sand layer is 0.28 and it is 0.17 in the confining layers. The permeability and porosity in the sand layer are directly correlated with depth, so that there is no heterogeneity in the horizontal direction. Other parameters such as the relative permeability relationship, capillary pressure, reservoir temperature and leakage point location are also given. The leakage rate of CO_2 into the domain is highly uncertain as the CO_2 takes an unknown path from the injection point to the bottom of the 9th layer. The leakage rate is estimate based on mass estimates from seismic surveys. The leakage rate increases from 0.0018 Mt in 1999 to 1.56 Mt in 2009.

Three models were developed for this study: a three-dimensional model and two two-dimensional models (a vertical equilibrium model and a dynamic reconstruction model). The low-permeability layers above and below the sand layer are neglected for both models, as a sensitivity analysis (not shown here) showed that they essentially act as no-flow boundaries. The lateral boundaries are set to constant pressure boundaries. The original grid structure from the IEAGHG benchmark dataset was retained for both models, but permeability and porosity were set to constant values of 2000 mD and 0.35, respectively. The cell thicknesses in the three-dimensional model are the same as in the original grid, while the thicknesses of the 34 layers representing the sand layer are summed up to give the thickness for the cells in the two-dimensional models. A constant CO_2 leakage rate of 0.1418 Mt/year was chosen for both models. Density and viscosity were calculated internally in TOUGH2/ECO2N based on pressure and temperature. Average values from TOUGH2/ECO2N were used as constant values in the two-dimensional models (CO_2 density: 688 kg/m^3; CO_2 viscosity: 5.45 x 10^{-5} Pa s; brine density: 1020 kg/m^3; CO_2 viscosity: 6.9 x 10^{-4} Pa s). The saturation - relative permeability relationships and saturation – capillary pressure relationship are defined by Brooks-Corey curves with a capillary entry pressure of 2.5 kPa and a Brooks-Corey parameter of 2.8. These values were chosen based on [13].

In addition to the two models based on the IEAGHG benchmark dataset, a simplified two-dimensional box model was constructed to investigate the applicability of the different vertically-integrated approaches. The domain is 1600 x 1600 m in the horizontal and has a thickness of 15 m. CO_2 enters the domain at the center of the domain. The formation properties and CO_2 leakage rate are the same as in the two-dimensional Sleipner model.

4. Results

In this section we present modeling results based on both the full 9th layer model and the simplified box model using the modeling approaches described above. Results are compared using CO_2 plume footprint and vertical CO_2 saturation profiles as comparison metrics. First, we compare three vertically-integrated approaches (vertical equilibrium with sharp-interface, vertical equilibrium with finite capillary transition zone, and dynamic reconstruction) to determine the impact of buoyancy driven vertical flow. This is followed by a comparison of the three-dimensional approach to results using the vertical-equilibrium approaches to find the level of model complexity necessary for GCS modeling of the 9th layer. Finally, we compare results from the different approaches to the CO_2 plume footprint determined from the seismic data, to investigate the ability of the simulators to predict the plume migration.



a) sharp-interface b) finite capillary transition zone

Figure 1: CO_2 saturation profiles for the box model after 1 year of injection: a) sharp-interface; b) capillary transition zone

The comparison of the two vertical equilibrium approaches – sharp-interface and finite capillary transition zone – shows that capillary forces have little impact on the plume development. CO_2 saturation profiles for the two simulations after 1 year of injection (Figure 1) are very similar, with a capillary transition zone thickness of only about 1 m for the model including capillary forces. Plots of the CO_2 plume thickness after 1 year (Figure 2) also show very good agreement. The relatively small impact of capillary forces on the modeling results, shows that capillary forces may be neglected when using vertically-integrated modeling of the Sleipner site.

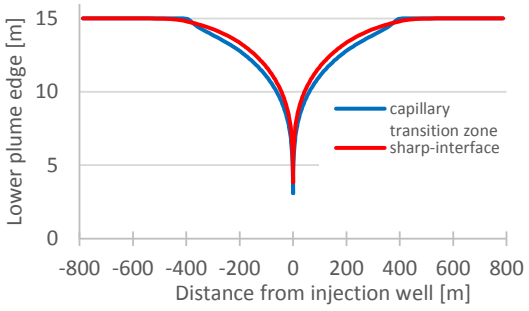
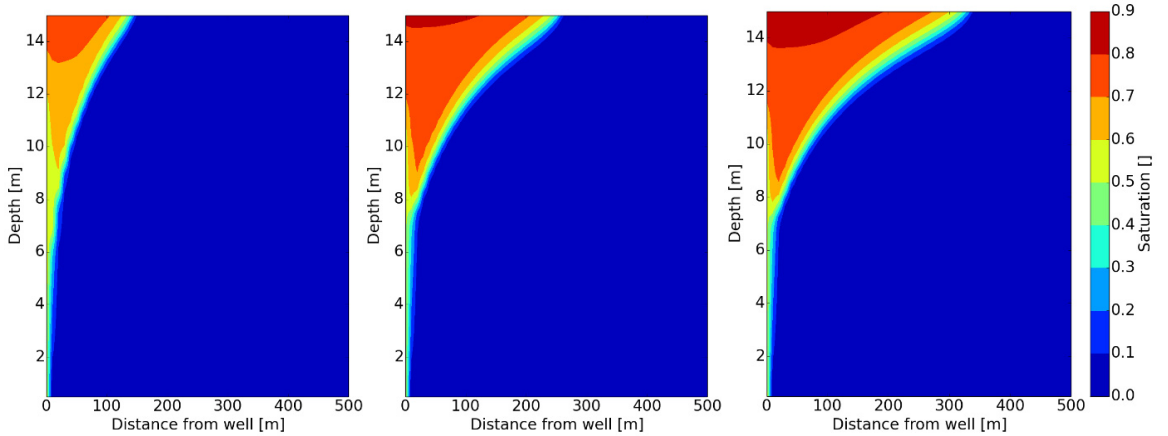


Figure 2: Lower plume edge for the box model after 1 year of injection based on the two vertical equilibrium models (sharp-interface and capillary transition zone)

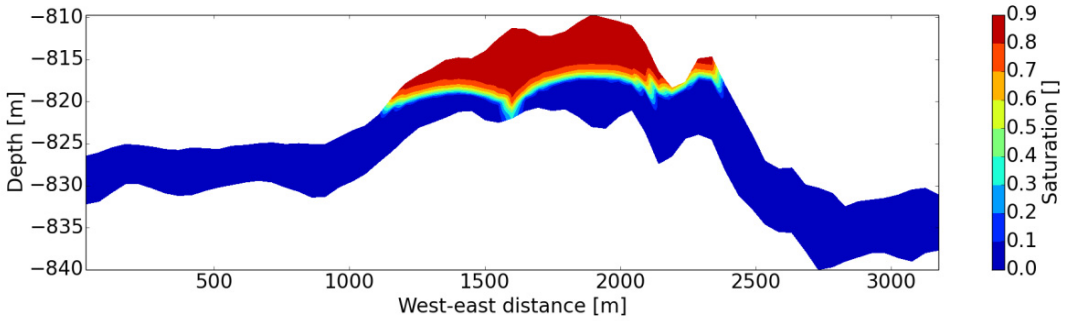


a) 73 days b) 219 days c) 365 days

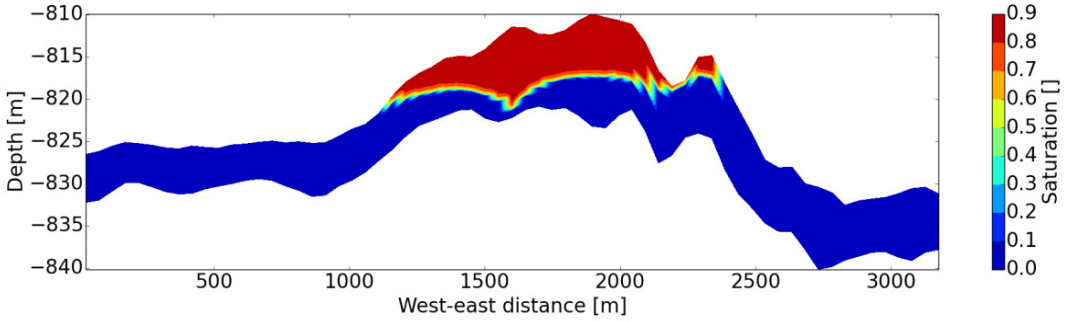
Figure 3: CO_2 saturation profiles for the box model using the vertically-integrated approach with dynamic reconstruction after: a) 73 days; b) 219 days; c) 365 days

Figure 3 shows CO_2 saturation profiles for the box model using the vertically-integrated approach with dynamic reconstruction. The vertical segregation for the parameter set representative of the 9th layer occurs on the time scale of tens of days. After 73 days CO_2 and brine have clearly segregated in the vertical, with CO_2 on top of brine. While most of the vertical redistribution occurs quickly, the results also show that it may take considerable time for all of the brine to drain vertically. For instance, after 365 days only the topmost region has saturation values approaching residual brine saturation. While this looks like a wide capillary transition zone, it is actually due to close-to-zero relative permeability values for brine at low brine saturations. It should be noted that in order to capture the fast vertical dynamics of this problem, very fine vertical and temporal resolutions are necessary, making this approach impractical for the full Sleipner model.

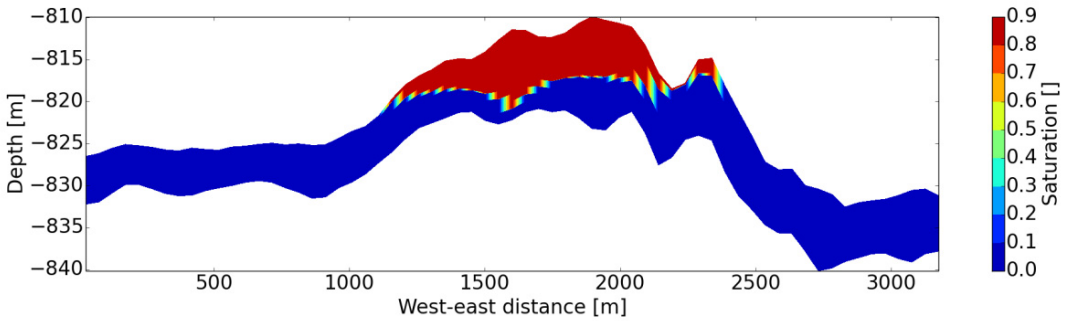
The Sleipner model was run using the three-dimensional simulator TOUGH2/ECO2N as well as an in-house vertical-equilibrium simulator, both with a sharp-interface and a capillary transition zone. Figure 4 shows a cross-section of CO_2 saturation through the domain, going from west to east through the leakage point, after 10 years of CO_2 migration into the 9th layer. The three simulations are in good agreement for the CO_2 distribution. In the sharp-interface simulation, the CO_2 plume directly above leakage point appears wider than in the other two simulations, but this is an artifact of the coarse grid resolution in combination with the interpolation scheme used for plotting. These simulations suggest that a vertical-equilibrium sharp-interface approach may be sufficient for CO_2 migration predictions in the 9th layer of Sleipner, especially considering the low computational cost of vertical-equilibrium simulations; the vertical-equilibrium simulation took several minutes on a single core, while the three-dimensional simulations took several hours on 100 cores. The three-dimensional results do not show the same slow final drainage as the dynamic reconstruction simulations of the box model, because the relative permeability implementations are slightly different for the two models, and because the Sleipner simulation is run for a longer time. However, these results confirm that vertical-segregation occurs relatively quickly, as the three-dimensional simulations include vertical dynamics while the vertical-equilibrium models do not.



a) three-dimensional simulation

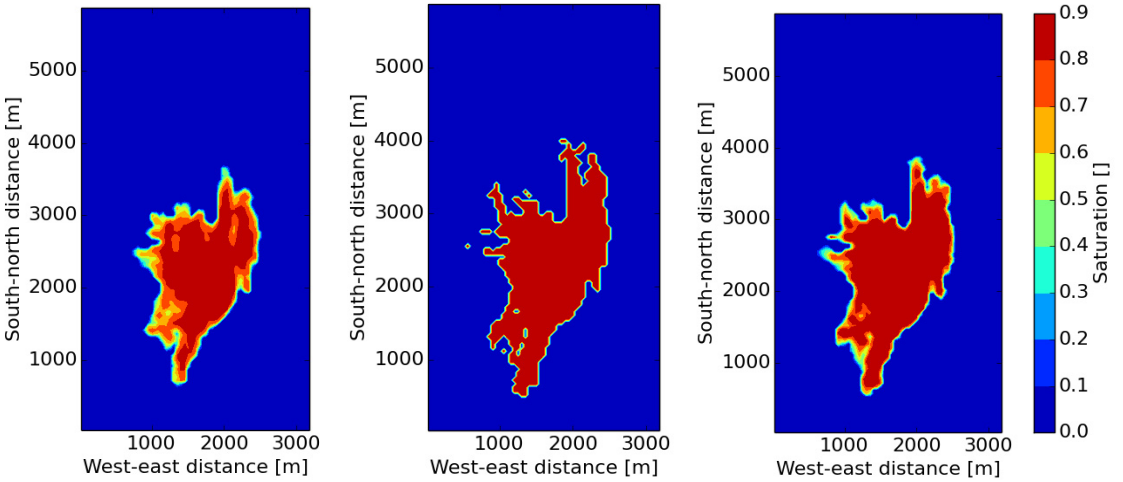


b) vertical-equilibrium with capillary transition zone simulation



c) vertical-equilibrium with sharp-interface simulation

Figure 4: CO_2 saturation cross-sections from west to east through the leakage point after 10 years of CO_2 migration: a) three-dimensional simulator; b) vertical-equilibrium simulator with capillary transition zone; c) vertical-equilibrium simulator with sharp-interface



a) three-dimensional b) sharp-interface c) capillary transition zone

Figure 5: CO_2 saturation at the top of the 9th layer after 10 years of CO_2 migration: a) three-dimensional simulator; b) vertical-equilibrium simulator with sharp-interface; c) vertical-equilibrium simulator with capillary transition zone

Figure 5 shows the CO_2 plume footprint at the top of the 9th layer after 10 years of CO_2 migration. The three approaches show good agreement in the extent of the plume, with the vertical-equilibrium approaches predicting a slightly larger plume extent in the South-north direction. It should be noted, that the saturation value from the three-dimensional simulator represents the CO_2 saturation in the uppermost cell, while the saturations from the vertical-equilibrium simulators represent point values at a specific relative distance from the top of the formation. The difference between cell-averaged and point values may explain the difference between the South-north extents.

Figure 6: CO_2 plume in the 9th layer in 2008 based on seismic data (modified from [3])

A comparison of the plume footprint predictions (Figure 5) to the plume footprint based on seismic data (Figure 6) shows that the simulators are not able to predict the plume finger that reaches far to the north or the separate plume to the south. This discrepancy may be due to physical processes not being adequately represented in the simulators, and/or due to the model of the 9th layer not correctly describing the real formation. For instance [13] argues that simulators based on Darcy-flow over-emphasize viscous forces relative to gravitational forces, while [14] discuss how changes to the caprock topography impact the migration of CO_2.

5. Conclusions

In this study four different numerical approaches were used to model CO_2 migration in the 9th layer of the Sleipner site. A three-dimensional multi-phase flow model was the most complex model. The other three approaches were vertically-integrated approaches where the integrated governing equations are solved in two dimensions (horizontal) and the vertical distribution of phase saturations and phase pressures is reconstructed based on the solution of the two-dimensional domain. The most complex reconstruction is to allow for dynamic vertical redistribution of CO_2 and brine. In this case the reconstruction is based one-dimensional vertical flow models. The two simpler approaches assume that vertical segregation occurs instantaneously (vertical-equilibrium), allowing for analytic expressions for the vertical reconstruction. The more complex vertical-equilibrium model has a capillary transition zone, where saturation changes gradually, while the simpler approach assumes a macroscopic sharp-interface between CO_2 and brine.

The modeling approaches were applied to models of the 9th layer of the Sleipner site as well as a simple box model. Modeling results based on the box model using the vertically-integrated approach with dynamic reconstruction showed that the bulk of vertical segregation occurred on a time-scale of tens of days, suggesting that vertical-equilibrium approaches are applicable to CO_2 migration modeling at the Sleipner site. A comparison of the two vertical-equilibrium approaches applied to the box model showed that the capillary transition zone was relatively thin and had little impact on the migration of CO_2 at this site. The three-dimensional approach and the two vertical-equilibrium approaches were applied to the full 9th layer model and the results for both the CO_2 saturations cross-sections and plume outlines compared well to each other. Considering the much lower computational cost of the vertical-equilibrium models compared to the three-dimensional model (several minutes on a single core compared to several hours on 100 cores), the results of this study suggest that vertical-equilibrium approaches are the more appropriate choice for migration modeling in the 9th layer of Sleipner. However, none of the models was able to accurately predict the plume outline as established by seismic surveys. This discrepancy will need to be addressed in future studies.

Acknowledgments

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