Benchmark modeling of the Sleipner CO₂ plume: Calibration to seismic data for the uppermost layer and model sensitivity analysis

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ABSTRACT

An important question for the Carbon Capture, Storage, and Utility program is “can we adequately predict the CO₂ plume migration?” The Sleipner project in the Norwegian North Sea provides more time-lapse seismic monitoring data than any other sites for tracking CO₂ plume development, but significant uncertainties still exist for some reservoir parameters. In order to simulate CO₂ plume migration and assess model uncertainties, we applied two multi-phase compositional simulators to the Sleipner Benchmark model for the uppermost layer (Layer 9) of the Utsira Sand and calibrated our model against the time-lapsed seismic monitoring data at the site from 1999 to 2010. Approximate match with the observed plume was achieved by introducing lateral permeability anisotropy, CH₄ in the CO₂ stream, and adjusting reservoir temperatures. Model-predicted gas saturation, thickness of the CO₂ accumulation, and CO₂ solubility in brine—none of them used as calibration metrics—were all comparable with interpretations of the seismic data in the literature.

Hundreds of simulations of parameter sensitivity (pressure, temperature, feeders, spill rates, relative permeability curves, and CH₄) showed that simulated plume extents are sensitive to permeability anisotropy, temperature, and CH₄ but not sensitive to the other analyzed parameters. However, adjusting a single parameter within the reported range of values would not reproduce the north-south trending CO₂ plume. It took a combination of permeability, CH₄, and temperature adjustments to match simulated CO₂ plume with seismic monitoring data. On the other hand, even with a range of uncertain modeling parameters, the predicted fate of CO₂ fell within a narrow band, $\sim 93 \pm 2\%$ structural/hydrodynamic trapping and $\sim 7 \pm 2\%$ solubility trapping. The calibrated model is not unique. Other possibilities for reproducing the elongated plume such

as a slight tilting of the caprock surface to the south and subtle geological features in the Layer 9 were not experimented with in this study, but are worthy of exploration for future studies. While it appears that we were able to reproduce the north-south elongated CO₂ plume, which is a modest improvement over previous models, the adjustments of parameters need to be verified with new observations.

Keywords: Sleipner, multiphase flow, CO₂ plume, CO₂, CCUS, Utsira, Sequestration, compositional reservoir simulation

1. Introduction

The predictive modeling of CO₂ plume is indispensable for Carbon Capture, Utility, and Storage (CCUS) projects. Numerical models are used by applicants and regulators to make decisions at all phases of a project ranging from site selection, characterization, and injection to post-injection monitoring. A mathematical model is also a management tool; models are updated and refined as data from characterization, injection, and monitoring become available. However, the accuracy of modeling results and information concerning the uncertainties of a model must be taken into account. The complexity of multiphase flow and the complexity of geological systems both pose challenges to modeling adequately and predicting CO₂ plumes. The Sleipner project provides an opportunity to explore some of these issues addressed above.

The Sleipner project, situated in the Norwegian North Sea, is the world's first industrial-scale geological carbon storage project. Beginning in 1996, CO₂ separated from natural gas has been injected into the Utsira Sand at the rate of approximately one million metric tons of CO₂ per

year (NRC, 2013). By the middle of 2012, a total of ~13.5 Mt of CO₂ had been injected (NRC, 2013). Seismic surveys of the site were conducted prior to injection in 1994, and then repeated in 1999, 2001, 2002, 2004, 2006, 2008, and 2010 (Chadwick et al., 2009; Chadwick et al., 2010; Boait et al., 2012; Hagen, 2012). These surveys have produced 4D seismic data that have delineated a CO₂ plume migration along a north-south trending topographic ridge in the Utsira Sand. The Utsira Sand has a storage potential of 2-15.7 billion tons of CO₂, and could become a major reservoir for neighboring countries for years to come (NRC, 2013).

Because of these circumstances, the Sleipner project provides an opportunity to answer several important questions: (1) Can we adequately predict CO₂ plume sizes and flow directions? (2) What does it take to match observed CO₂ plume migration data? (3) Are widely available reservoir simulation tools adequate to simulate multiphase flow?

CO₂ migration in the subsurface is a complex process, and numerous “conceptual models” have been developed and published (Doughty and Pruess, 2004; Johnson et al., 2004; Kumar et al., 2004; Audigane et al., 2007; Xu et al., 2007; Cameron and Durlofsky, 2012; Cheng et al., 2012; Court et al., 2012; Nilsen et al., 2012; Zhang and Sahinidis, 2013). In these models, idealized geometry, homogeneous and isotropic permeability, and isothermal aquifers are typically assumed. While these models have helped to elucidate the many processes and the complex interplay between processes that ultimately determine CO₂ migration, these models do not provide an insight into how CO₂ migrates in real geological systems. Applying mathematical models to real geological systems helps to illustrate the complexity of the geological systems, such as reservoir geometry, spatial heterogeneities, and uncertain boundary conditions. Therefore, although various models in the literature, which explored different aspects of the complex

processes, have served to identify the critical processes and parameters that determine CO₂ migration and fate, these models must be tested in geological systems with calibration data.

In this study, we first applied two advanced compositional simulators, GEM® and TOUGH2, to the Sleipner Benchmark model released by Statoil, and calibrated the model to match approximately with CO₂-brine contact development (1999-2008) by introducing permeability anisotropy and a combination of reservoir temperature and CH₄ composition adjustments. Secondly, we conducted sensitivity analysis for CO₂ plume migration and fate at Sleipner Project in order to identify the critical factors controlling CO₂ sequestration. Finally, based on the analysis results, we discussed model uncertainties in order to guide future data collection and observation.

2. Geological Settings and Field Data

Starting in 1996, CO₂ separated from the natural gas at Sleipner Field has been injected into the Utsira Sand. The Utsira Sand extends along the Viking Graben near the UK/Norwegian median line for more than 450 km south-north between 58 °N and 61°40N, and 75~130 km east-west between 1°E and 3°50E (**Fig 1**). The Utsira Sand has an average porosity of 36% and a permeability range from 1 to 5 Darcy. Its thickness ranges between 200 and 300 m with the top of the formation at about 800-1000 m below sea level at the injection point (Baklid et al., 1996; Zweigel et al., 2004; Singh et al., 2010). The injection point is located 1012 m below the mean sea level (Chadwick et al., 2005).

Baseline time-lapse 3D seismic data were acquired in 1994, prior to the injection. Repeat surveys were conducted from 1999 to 2010, the latter two augmented by a high resolution 2D seismic and seabed imaging survey (Chadwick et al., 2009). Nine CO₂ accumulation layers have been identified through seismic data (**Fig 2**). The topography (lateral extent, continuity, etc.) of

each layer is markedly different. However, only the uppermost CO₂ plume in the “Sand Wedge” unit (Layer 9), which is separated by a 5 m shale unit as its lower boundary, is clearly resolved based on the shallowest bright reflection in the seismic data. CO₂ accumulation through time has also been quantified in this layer (Chadwick and Noy, 2010; Boait et al., 2012). On the other hand, the interpretation of lower CO₂ plume layers is affected by the overlying bright seismic reflections (Lumley, 2009). Therefore, this study focuses on only the uppermost CO₂ storage in the Layer 9 where topography is well defined. Layer 9 is in immediate contact with the overlying sealing caprock. Therefore, CO₂ behavior and fate in this layer is determinative to the long-term effectiveness and security of the containment.

Although the availability of time-lapsed seismic data makes Sleipner an ideal site for comparing simulated and observed CO₂ plume, the lack of well data near the injection site has resulted in uncertainties of reservoir temperature and pressure as well as in brine chemistry (Singh et al., 2010). Therefore, sensitivity analysis to evaluate the effects of uncertainties of these parameters on CO₂ plume migration is valuable for assessing model uncertainties.

3. Model Construction and Calibration

History-matching the development of CO₂ plume is essentially an inverse problem. Considerable progress has been made with respect to solutions to inverse problems in geophysics and hydrogeology during the last two decades (Box et al., 1994; Parker, 1994; Law and Kelton, 2000; Aster et al., 2005; Hill and Tiedeman, 2007). These procedures, nevertheless, are difficult to apply to the Sleipner field-scale reservoir model. Therefore, we relied on the conditional trial-and-error method.

Based on the principles of inverse problem solving theories, a workflow was developed (**Fig 3**). First, we translated the Sleipner Benchmark model into GEM® and TOUGH2. The

Sleipner Benchmark is a modeling benchmark, released by Statoil and managed by the IEAGHG R&D program. The model comprises a numerical mesh with a cell resolution of $50 \times 50 \text{ m}^2$ and related data package that is designed for comparative high resolution simulations (Singh et al., 2010). Second, we calibrated the model against the boundaries of the imaged CO_2 plume as the only history match metrics. The horizontal permeability anisotropy, reservoir temperature, and CH_4 % in CO_2 streams were adjusted as model input until reasonable matches were obtained. Third, a range of parameters, such as temperature, pressure, relative permeability curves, number and locations of feeders, and CH_4 content, still remain uncertain (Singh et al., 2010). The potential impacts from the uncertainties of these parameters were evaluated and the model uncertainty is discussed in detail below.

3.1. Model Parameterization

The grid mesh from the Benchmark model was translated into GEM® and TOUGH2. GEM® is an adaptive-implicit multiphase multi-component flow simulator with phase equilibrium and mineral dissolution/precipitation that uses the fully-coupled approach (Nghiem et al., 2004; CMG, 2009). The modeled area is approximately $3 \times 6 \text{ km}$. The grid dimensions are $x = 65$, $y = 119$, $z = 43$ with a total of 332,605 blocks. Modeling parameters are shown in **Table 1**. GEM® uses a Peng-Robinson equation of state (Harvey, 1996) for calculating CO_2 density and solubility. CO_2 viscosity was calculated based on the HZYT method (Herning and Zipperer, 1936; Jossi et al., 1962; Yoon and Thodos, 1970). The viscosity of brine was calculated using the equation from Whitson and Michael (2000) and data from Kestin et al. (1981).

TOUGH2 is developed by the Lawrence Berkeley National Laboratory and is a simulator for modeling non-isothermal multiphase flow in the system $\text{H}_2\text{O}-\text{NaCl}-\text{CO}_2$ (Pruess, 2005). In

TOUGH2, density and viscosity of CO₂-rich phase, approximated as pure CO₂, are obtained from correlation developed by Altunin (1975). Brine density for binary system water-salt is calculated first from the correlations of Haas (1976) and Andersen et al. (1992). The density of aqueous phase with dissolved CO₂ is calculated assuming additivity of the volumes of brine and dissolved CO₂ (Pruess, 2005). Brine viscosity is obtained from the correlation presented by Phillips (1981), but no allowance is made for dependence of brine viscosity on the concentration of dissolved CO₂. In this study, Cartesian grid is employed in TOUGH2 model for spatial discretization.

The reservoir was initially saturated with water ($S_w = 0.9999$). The method of gravity initialization for a reservoir was used in GEM. When this initialization is performed, a table is constructed, which give water pressure and several other properties as functions of depth. This table is constructed by Runge-Kutta integration of the differential equation determining the hydrostatic pressure. The initial pressure of each cell is then assigned based on the values in the table.

The boundary condition applied to our simulations for solving the mass transport equations was a Dirichlet condition boundary. This Dirichlet boundary was implemented by assigning a large (infinite) volume to the boundary grid block (Pruess et al., 2012). Consequently, any influence from the influx became negligible compared to the large volume of the formation brine. The aqueous chemical composition of the boundary element, as well as its thermodynamic conditions, such as temperature and pressure, was therefore kept essentially unchanged from the original formation brine (Pruess et al., 2012). In this study, background Darcy velocity of groundwater was considered to be zero.

In many cases, we used both GEM® and TOUGH2 for inter-simulator comparison. For simplicity, all discussions below use the results from GEM® unless otherwise indicated.

3.2 Model Calibration

The starting point of our calibration was permeability values and distribution in the original Benchmark model: k value near 2 Darcy, no horizontal permeability anisotropy, and vertical permeability of $\sim 1/10$ of the horizontal permeability. However, geological studies of the Utsira Sand at Sleipner have suggested that the system has deep channel/canyon-like feature at the northeast margin of the Utsira Sand (Gregersen, 1998; Eidvin and Rundberg, 2001). Similar incised channel-like features have also been identified at the western or eastern base of the formation that are suspected to be entry for some of the sand transport into the basin (Gregersen, 1998). The channel features suggested that the system was formed with a north-south trend, indicating preferential north-south permeability anisotropy (Gregersen, 1998; Gregersen and Johannessen, 2007). This is also consistent with the observation from the seismic data that revealed an elongated north-trending CO₂ plume after the injection.

We adopted $k = 2$ Darcy east-west and 10 Darcy north-south and compared with the scenario of $k = 2$ Darcy isotropic in all horizontal directions (**Fig 4a**). The results were comparable with the TOUGH2 simulations from Chadwick and Noy (2010). We reached similar conclusions as Chadwick and Noy (2010) that anisotropic permeability improved the match somewhat, but it is not possible to match the observed spreading of the topmost layer by adjusting permeability alone.

Next, we calibrated our model against the CWC development by adjusting temperature and CH₄ and found plume migration is highly sensitive to both parameters. However, adjusting T or CH₄ alone would not result in a match with the observed plumes unless the T or CH₄ was

outside of realistic ranges. Nevertheless, a combination of temperature and CH₄ values that are within the ranges of reported values in the literature could generate approximate matches. We settled on a combination of 33.5 °C and 2.4% CH₄. Detailed discussion of the literature temperature and CH₄ values will be presented below.

The simulated CWC matched approximately with the observed areal extent of the CO₂ plume in 1999, 2001, 2002, 2004, 2006, and 2008 and showed improvements over previous models (**Fig 5**), in replicating the elongated, northward extension of the observed plume. In order to compare different model runs, we used image analysis software to calculate the percentages of areas within the CO₂ plume outline that the models failed to fill with CO₂ (gap areas) (**Fig 6**). It should be noted, however, that the image analysis was two-dimensional while CO₂ distribution was three-dimensional, and hence the comparison does not always paint a whole picture.

3.3 The Calibrated Model

For our calibrated model, the only calibration targets were the CO₂-water contacts (CWC) because the lateral spread of the CO₂ plume can be tracked in detail by seismic data (Chadwick and Noy, 2010). The only adjusted parameters were permeability anisotropy, reservoir temperature, and CH₄ in CO₂ streams. Other physical attributes of the model discussed below are forward predictions or inferences. These predictions are compared to the interpretations of seismic data below. We need to emphasize here that the interpretations are not observations but estimates with widely ranging uncertainties (Chadwick and Noy, 2010).

In our model, Layer 9 was divided into 34 vertical sub-layers (~ 0.35 m per sub-layer). The sizes and saturation of CO₂ distribution in each sub-layer decreased significantly from top to

bottom. The area of CO₂ distribution in the topmost sub-layer delineated the maximum extent of the CO₂ plume migration.

The distribution of gas saturation simulated by our calibrated model is comparable to gas saturation maps from Chadwick and Noy (2010). As mentioned earlier, the gas saturation maps from seismic data interpretations are less accurate than the CO₂ plume outlines, and our simulated gas saturation distributions were results of “forward modeling.” This means that the seismic data-based gas saturation maps were not used as calibration targets. Seismic data alone do not quantify the maximum CO₂ saturation (S_{CO_2}) in the field, and the relative permeability curve that we used in our model limited S_{CO_2} to 0.89. The average gas saturation maps from Chadwick and Noy (2010) were constructed from the relationship between gas saturation and capillary pressure, which was determined by centrifuging experiments on cores from the Utsira Sand (Singh et al., 2010). Although the high gas saturation areas from the multiphase flow simulations and seismic interpretations are similar, the simulation results show that much more dispersive gas saturation along the plume fringes, particularly in the west.

The thicknesses of the CO₂ plume inferred from the model are also comparable to the estimates reported in Chadwick and Noy (2010). For 2001, the thickness is 4.1 m for the thickest area and 0.3 m for the thinnest area; for 2004, 6.2 m for the thickest area and 0.3 m for the thinnest area; and for 2006, 7.4 m for the thickest area and 0.35 m for the thinnest area. These values compared well with CO₂ plume thickness reported in the literature. Note that Chadwick et al. (2005) obtained the CO₂ layer thickness both from reflection amplitudes and structural analysis.

Our model calculated a CO₂ gas solubility of ~ 1.134 mol/kgw, which is similar to the CO₂ solubility calculated following Duan et al. (2006) (1.135 mol/kg at 33 °C, 83 bars, and 0.57

m NaCl). Considering the relatively short time (several years) after the initial injection, the injected CO₂ is mainly in a supercritical state as expected. Dissolved CO₂ is the dominant phase in the first several days as CO₂ encounters fresh brine that was undersaturated with respect to CO₂, but free phase supercritical CO₂ took over after several days because the solubility limit of CO₂ was reached and supercritical CO₂ displaced CO₂ saturated brine afterwards. With time, the fraction of dissolved CO₂ approaches 7%. The previous estimates of dissolved CO₂ based on seismic data are in the range of 5-10% total CO₂ injected (Chadwick and Noy, 2010).

4. Sensitivity Analysis

The primary model output considered in the sensitivity analysis for this paper was the CWC in Layer 9. The justification for choosing CWC was that other plume attributes reported in the literature, such as the distribution of CO₂ saturation within the plume, plume thickness, and the amount of CO₂ trapped, are more subject to interpretations and are generally of lower accuracy (Chadwick and Noy, 2010). In addition, CWC is often related to the area of review (AoR) in regulatory decisions.

For Sleipner, Chadwick and Noy (2010) investigated the effects of temperature and topography gradient error on the CWC development. The effects of different simulators (such as black-oil simulator, invasion percolation simulator, and compositional simulator) on CO₂ sequestration modeling were investigated by Singh et al. (2010) and Cavanagh (2011). Cavanagh (2013) has employed a black-oil simulator with power-law and straight line respectively for relative permeability curves, and found that the general trend of CWC for these two scenarios is similar. However, the effect of impurities in the injected CO₂ stream on CO₂ plume, and the combined effects of temperature, pressure, and CH₄ have never been investigated. As shown below, it turned out that these combinations are important to generate an approximate match with

the observations. Here, we focus on the factors of temperature, pressure, CO₂ spill rate, and impurities in injected CO₂ stream. We also found that relative permeability curves had small effects and the details are omitted from further discussion here. The issues of local topography error and geochemical process will be analyzed in our discussion on model uncertainty.

4.1 Reservoir temperature

No direct measurement of reservoir temperature in Layer 9 is available. Chadwick and Noy (2010) used a temperature of 31.5 °C in their base case for a pure CO₂ stream, which is equivalent to density of a CO₂-methane (2% CH₄) mixture at 29 °C. They also tested a case with a temperature of 36 °C for sensitivity analysis. Bickle et al. (2007) calculated the temperature at Layer 9 to be 35 °C based on the following factors: the temperature of 41 °C at the injection depth 1012 m, the temperature of 7 °C at the depth 80 m, and the variable thermal conductivity that accompanies depth. We calculated the temperature at Layer 9 based on the temperature being 41 °C at the injection depth and a geothermal gradient of 35.6 degree/km in Sleipner Benchmark. A temperature of 33.2 °C was thereby calculated and used as a basis for sensitivity analysis.

In order to evaluate the effect of reservoir temperature on migration and fate of the injected CO₂, we used a range of temperatures in our model (29-37 °C). **Figure 7a** presents a case with an extreme value of 37 °C and the results are compared with that in the Base Case. Simulated CWC do not show much change in south, east, or west, but CWC extend further north with increased reservoir temperature. Supercritical CO₂ under Sleipner *P*, *T* conditions has gas-like properties, and CO₂ density and viscosity decrease drastically with temperature (**Fig 8**). Lower CO₂ density and viscosity helped CO₂ to spread along the topographic ridge from south to

north (**Fig 7a**), and also helped increase the spreading speed of CO₂ (**Fig 9**). Therefore, the simulated CWC is quite sensitive to the reservoir temperature at Sleipner.

4.2. Reservoir pressure

There are no direct measurements of reservoir pressure for Layer 9. In previous studies, the pressures in Layer 9 were calculated based on the hydrostatic gradient, assuming that pressures are hydrostatic (Bickle et al., 2007). The pressure calculated by Cavanagh based on the hydrostatic gradient (personal communication) is 8.0 MPa at the reservoir top and 8.6 MPa at the reservoir bottom. We adopted the value of 8.3 MPa at 820 m as a reference for our Base Case. To analyze the effects of pressure on the simulation results, we used a range of pressures in our model (8.0-8.6 Mpa, **Table 2**). **Fig 7b** compared the Base Case and the Test Case-Pressure by using a pressure of 8.0 MPa at 820 m.

The results show that the simulated CWC do not change much in the west, east, or south (**Fig 7b**). Within the range of pressures reported in the literature (e.g., the box in **Fig 8b**), small changes of pressure can drastically alter the density of CO₂, again, because CO₂ at the P-T condition of Sleipner has gas like properties. This is further complicated with CH₄ contents (**Fig 8b**). Combinations of P-T-CH₄, all within reported ranges, can have much lower density and CO₂ migrates further north. From that point of view, plume migration is also very sensitive to pressure although its effect is much smaller than that of temperature (within the reported range) when considered independently.

4.3. CO₂ spill rate and total mass into Layer 9

Our Base Case used the volume and rate of CO₂ spill into Layer 9 that were provided by Statoil. For sensitivity analysis, we increased the CO₂ spill rate 20% from that in the Base Case

to evaluate its effect on CO₂ migration and fate. While simulation results show slightly increased areal expansion of the plume (**Fig 7c**), the plume thickness increased by 15%. Therefore the simulated plume thickness is more sensitive to a CO₂ spill rate than CWC and verifying the model only through comparing CWC on the plane view could result in large estimation errors for CO₂ accumulation at Sleipner.

4.4. Composition of injected CO₂ Stream

The CO₂ at Sleipner contains about 1.5-2.5% methane and also unspecified amounts of butanes, toluenes, and xylenes (BTX) (Zweigle and Heill, 2003; Zweigle et al., 2004; Arts et al., 2008; Chadwick and Noy, 2010). In order to evaluate the effects of the composition of injected CO₂ on the simulation results, we used a range of CH₄ (0-4%) in our model and evaluated the modeling results. GEM® uses the Peng-Robinson equation for describing the mixing properties of CO₂ and CH₄. Significant different density values could be predicted using different models. **Figure 8b** shows predicted densities of CO₂-CH₄ mixture calculated using the SAFT2 approach.

Figure 7d,e,f show the simulation results using CH₄ of 1.8%, 2.7%, and 4% in the CO₂ stream in our model. **Figure 5b** shows the case of 2.4% CH₄. These CH₄ values are paired with respective temperatures, and with the exception of the 4% CH₄ case, the CH₄-*T* pairs produced similar matches with observed plumes. For the extreme case of 4% CH₄, the difference in densities between brine and gas phase increased from 384 kg/m³ for cases with no CH₄ to 619 kg/m³, and the viscosity of the gas phase decreased from $\sim 5 \times 10^{-2}$ to 3×10^{-2} cp (**Fig 8**). The velocity of the CO₂ flow is much higher than that in the Base Case (**Fig 9**). As a result, the test case simulated a plume that migrated beyond the north narrow ridge in all years (**Fig 7d**). The plume, however, spreads over to both the west and east flank of the main plume body. The

addition of CH₄ also produced a thicker CO₂ plume on the vertical profiles (not shown).
Therefore, the simulated plume is quite sensitive to the CO₂ stream compositions at Sleipner.

4.5. Sensitivity for CO₂ fate

The fate of CO₂ can be expressed as trapping mechanisms: structural (hydrodynamic), solubility, residual (capillary), and mineral trapping (IPCC, 2005). **Figure 10** shows the maximum ranges of hydrodynamic and solubility trapping in terms of total injected CO₂ when a range of modeling parameters was used. Here, we only analyzed the effects on structural trapping and solubility trapping. Residual trapping is small at Sleipner because it is still in the injection phase. Residual trapping will become more important when CO₂ injection stops and formation water flows back into the reservoir again (Liu et al., 2011). Mineral trapping is a slow process (IEA, 2008) and here at Sleipner it is negligible (see below).

Figure 10 shows that the largest uncertainties in simulated trapping mechanisms are from the CH₄ content and temperature. Adding CH₄ content to 4% can increase CO₂ solubility trapping by ~1.8%, while, with the temperature increased to 37 °C, CO₂ solubility trapping can be raised by ~1.4%.

In Test Case-CH₄ with 4% CH₄, CO₂ plume volume increased due to both increased areal extent and thickness of the CO₂ plume compared with Base Case. Water saturation did not change and CO₂ solubility was reduced slightly to 1.09 Molal from 1.13 Molal in Base Case. The cumulative effects are that solubility trapping increased ~1.8% as shown in **Fig 10**. Therefore, solubility trapping is much sensitive to CH₄ content due to the increased CO₂ plume volume.

In Test Case-Temperature with 37 °C, CO₂ plume had behavior similar to that in Test Case-CH₄. CO₂ plume volume increased due to both increased areal extent and thickness of the CO₂ plume when compared with Base Case. Water saturation changed little and CO₂ solubility

was reduced slightly to 1.08 Molal. As a result, solubility trapping increased ~1.4% (**Fig 10**).

Thus, temperature has an effect on solubility trapping due to the increased CO₂ plume volume, which is caused by lower CO₂ density because of higher temperature.

In summary, even with a wide range of parameter uncertainties (even with extreme values outside of known ranges), the resultant simulated trapping mechanisms only differ by $\pm 2\%$. However, the above analysis can be undermined by the mass balance error in numerical models. We computed mass errors and the CO₂ mass balance accounting error is ~-0.13% for the Base Case and they vary slightly in different test cases. Therefore, the major part of the uncertainties is not related to software artifacts.

5. Discussion on model uncertainty issues

5.1. Number of Feeders

Most of the previous modeling work (Bickle et al., 2007; Chadwick and Noy, 2010; Singh et al., 2010; Cavanagh, 2013) pointed out the need and justifications for more feeders even though both Chadwick and Noy (2010) and Singh et al. (2010) used a single feeder in their models.

We experimented with the scenario of two feeders in this study. The main feeder is above the injection point in Layer 9. A second, smaller feeder was added at the coordinates $x = 438,925$ and $y = 6,472,250$, which is beneath one of the thickest areas of the CO₂ plume in the north ridge. This thick area appears in the 2004 and 2006 seismic survey maps, but not in the 2001 map. For the purpose of numerical experiments, we assumed that the second feeder started to contribute from January 1, 2002. 100% mass of CO₂ was distributed to the main feeder during

1999-2001; starting from 2002, 85% mass was assigned to the main feeder and 15% mass was assigned to the second feeder. The reservoir temperature used was 33.2 °C and no CH₄ was included in the model.

Figure 4b shows that using two feeders improved CO₂ migration to the north ridge. **Figure 5c, d** show simulated plume developments using GEM® and TOUGH2, respectively. Although there is marked improvement for match with plume migration, there is no sufficient seismic evidence to support for a second feeder and its spill rate, with the exception of the CO₂ plume thickness information interpreted from seismic data (Chadwick and Noy, 2010). Therefore, the model with two feeders is a forced model to favor the history match and a numerical experiment used to test the idea suggested by previous modeling work.

5.2. Topography uncertainty and its effect on the CO₂ plume

The simulated CO₂ for this study is always outside of the east or west boundary interpreted from seismic data (**Fig 11**). Varying temperature, pressure, CO₂ spill rate, and CH₄ content did not remediate the mismatches. Chadwick and Noy (2010), Singh et al. (2010), Cavanagh (2013), and Haukaas et al. (2013) obtained similar results although they employed different simulators and model settings in comparison with ours. Therefore, we inferred that the mismatch in east or west boundary resulted from topographic interpretation errors and they cannot be eliminated by adjusting modeling parameters.

At Sleipner, the depths of Layer 9 top were calculated using a laterally uniform “layer-cake” overburden velocity model based on average velocities from a number of wells in the vicinity, but these wells are too spatially scattered (typically more than 2 km apart) and the velocities of the wells in the vicinity are different (Chadwick and Noy, 2010). Chadwick and Noy (2010) analyzed the velocity difference between pairs of wells, which indicates significant

velocity variation, with differences up to more than 50 ms^{-1} . Therefore, the topography of Layer 9, which was interpreted from average velocities of the adjacent wells, can carry significant uncertainties. These uncertainties could contribute to the apparent mismatches between simulated and seismic CWC outlines.

In order to further explore possible local topographic errors in the east and west boundary, we analyzed our simulated CO_2 plume in Layer 9 in detail. In **Fig 11 (a)-(b)**, two vertical profiles are described along grid cell J51 and J62, respectively. The positions of these profiles are shown in **Fig 11 (c)**. In the profiles, the red solid lines represent the simulated CO_2 plume bottoms and the black vertical dashed lines indicate the locations of seismic CWC from the areal maps.

In the profile along J51 (**Fig 11a**), the main CO_2 plume body, with a thickness of 5~6 m, filled in the structure trap that manifested by the topographic ridge of the top of Utsira surface. However, both sides of the simulated plume extend outside of the CWC of ~150 m. Nevertheless, the CO_2 layer outside the CWC is thin (Note that the vertical scale is greatly exaggerated in **Fig 11**). Along J62, we see a similar pattern. The simulated main CO_2 plume body was within the topographic ridge. However, the simulated CO_2 plume matched with the observation on the west side, but extended too far east to the right. Again, the CO_2 layer outside the CWC is thin. One could speculate that topography errors of approximately $\sim \pm 1 \text{ m}$ would not affect the boundaries of the main CO_2 plume body. Therefore, the simulated thick CO_2 plume body matched with seismic CWC well, as we showed in this study. On the other hand, the same topography errors of approximately $\sim \pm 1 \text{ m}$ on the fringes of the CO_2 plume would have resulted in large relative errors in topography, which would in turn lead to apparent mismatches between simulated and observed CWC. However, these overspill areas are characterized by a thin layer of CO_2 . As a

result, the matches between simulated and observed CWC are better than it appears to be on a plane view.

From these analyses, we can conclude that (1) we need to be careful in judging what constitutes a good match between simulated and observed plumes. On a plane view, simulated CO₂ plume spilled over outside of CWC on the west and east, which obscures the excellent match for the main CO₂ plume body. The case study at Sleipner is therefore useful in developing regulatory criteria for quality modeling work. (2) These local mismatches of plume boundaries cannot be eliminated by adjusting parameters other than local topography. Resources should not be directed to such efforts.

5.3. Geochemical process

Most previous modeling studies incorporating geochemistry have used idealized aquifers. Can models with realistic and complex topography have locations of enhanced geochemical reactions? Can this feedback to CO₂ plume migration? To explore these questions we constructed a test case with geochemistry. There is no formation water composition available at the Sleipner site and previous studies used Oseberg formation water as a substitute for the Sleipner site (Audigane et al., 2007; Gaus et al., 2005). Johnson et al. (2004b) slightly modified the chemical composition of Oseberg formation water in order in better accordance with the mineralogy of Utsira formation. In this study, we adopted the formation water composition from Johnson et al. (2004b) (**Table 3**). Because the simulation time from 1999-2010 is short and the reaction rate of calcite is much higher than silicate minerals, the only active mineral considered in the current study is calcite. The volume fraction of calcite (6%) is based on Chadwick et al. (2004). The kinetic parameters for calcite dissolution are rate constant of $10^{-5.81}$ mol/m²/s at 25

°C, activation energy of 23.5 kJ/mol (Palandri and Kharaka, 2004) and reactive surface area of 88 m²/m³ (Nghiem et al., 2009).

Figure 12 (middle and lower panel) indicates that calcite reaction favors the topographic high in Layer 9. The percentage of calcite dissolution can be up to ~1% which is comparable with the value ~1.9% derived from Audigane et al. (2007)'s simulation for Sleipner with TOUGHREACT. After CO₂ injection, a certain amount of CO₂(g) will dissolve into the brine, and will make the brine acidic and corrosive to all minerals in the formation resulting in the calcite dissolution. The solute (such as Ca⁺², HCO₃⁻) in the brine is transported by advection, diffusion, and dispersion processes, which cause the calcite dissolution region to be larger than the CWC (**Fig 12 upper panel**). Calcite can achieve equilibrium quickly and the dissolved quantity is only of ~1% and porosity only increases by ~0.0004. Hence we can ignore the geochemical process in short time simulation.

5.4. Prediction uncertainty

To test the forecasting ability of our calibrated model, we made model prediction to 2018. When the model was calibrated, the 2010 seismic data were not available, and hence the 2010 data were not part of the calibration and can be good criteria to assess the model. In 2010 (**Fig 13**), the simulated CWC approximately matches with the observed plume outline in south and north.

We also made predictions of CO₂ plumes to 2018 using the two-feeder test case. The predicted plumes from this test case are much smaller than those from the model with CH₄ described above. The calibrated model comparing to the two-feeder test case has a slightly higher temperature (33.5 °C versus 33.2 °C) and CH₄ (2.4 % versus 0% CH₄). With time, CO₂

plumes predicted from these two models diverge in sizes and distributions. This shows promises that non-unique models can be verified and discriminated with new observations.

6. Conclusions and Remarks

In order to simulate CO₂ plume migration in the uppermost layer (Layer 9) of the Utsira Sand in the Norwegian North Sea, we applied two multi-phase compositional simulators to the Sleipner Benchmark model and calibrated the model against the time-lapsed seismic monitoring data from 1999, 2001, 2002, 2004, 2006, 2008, and 2010. Calibration against plume outlines, specifically the CO₂-water contacts, which are based on the geophysical monitoring data, was accomplished by introducing permeability anisotropy, adjusting reservoir temperature, and taking into account the CH₄ impurity in the CO₂ stream at Sleipner.

Our modeling results show:

(1) The simulated CO₂-water contacts approximately matched with the observed areal extent of the CO₂ plume in 1999, 2001, 2002, 2004, 2006, and 2008 and showed improvements over previous models. To quote Cavanagh (2013): “These (previous) models have failed to quantitatively or qualitatively reproduce the plume morphology to date.” Here, our model was generally able to match the elongated, northward extension of the observed plume.

(2) The approximate history match at Sleipner was achieved by calibrating the model against CO₂-water contacts delineated by seismic data with adjustments of permeability (k), reservoir temperature (T), and CH₄ composition in the CO₂ streams. An increase of N-S permeability is justified by the sedimentary geology of the site and the presence of an N-S trending CO₂ plume. Reservoir temperature and CH₄% used in the model are within the ranges of reported values in the literature. However, the model is not unique. Many combinations of k , T , and CH₄ would produce similar matches, and other possibilities that would have improved the

development of an N-S elongated CO₂ plume, such as a slight tilting of the surface of Utsira top to the south, were not considered.

In general, because the CO₂ stream at Sleipner has gas like properties, subtle adjustments of parameters that facilitate CO₂ migration to the north would result in better history matches. However, adjusting only one parameter at a time, as those in previous modeling efforts, would not lead to an N-S elongated CO₂ plume when the adjustment is within the reported ranges. This study shows that it must be a combination of several sensitive parameters, adjusted within reported ranges, to produce an N-S elongated CO₂ plume.

(3) Although many parameters are uncertain, which leads to uncertainty of the simulated plume extent, the predicted fate of CO₂ at Sleipner nevertheless fell within a narrow band, $\sim 93 \pm 2\%$ structural/hydrodynamic trapping and $\sim 7 \pm 2\%$ solubility trapping.

(4) The model-predicted gas saturation, thickness of the CO₂ accumulations in Layer 9 through time, and the overall dissolved CO₂ in brine (solubility trapping) versus supercritical CO₂ (hydrodynamic trapping), none of them are calibration targets, all matched well with estimates from geophysical data interpretation reported in the literature (e.g., Chadwick and Noy, 2010). In particular, approximate estimates of the percentage of CO₂ which is dissolved into brine (5-10%) have been made based on seismic data interpretation (Chadwick and Noy, 2010). These solubility estimates are comparable to the about 7% in the simulation model. Caution must be exercised for these comparisons, however. These estimates in the literature (Chadwick and Noy, 2010) are not direct observations but interpretations with a widely ranging uncertainties, and the agreements could be fortuitous.

(5) Detailed analysis of the topography in the Benchmark Model and positions and extents of the simulated CO₂ plume show much better match between CWC and boundaries of

the main CO₂ plume than what appears on the plane view (**Fig 5b**). The overspill outside of the CWC on the east and west fringes of the plume constitute a thin CO₂ layer, which could result from errors of seismic interpretation of the topography. On one hand, this shows that the criterion of a good match cannot be simply a comparison between observed and simulated plume outlines. On the other hand, it would be a futile effort to attempt to achieve a perfect match. Our study shows that adjusting other parameters other than topography would not reduce the overspill areas.

(6) Model simulations show the feedback between topography and geochemical reactions. While calcite dissolution reactions concentrated in the topographic highs, only up to ~1% calcite was dissolved and porosity only increased by ~0.0004. Therefore, we can safely ignore the geochemical reactions in model structure for short time simulation.

In conclusion, it appears that we were able to use widely available reservoir simulation tools to simulate multiphase flow at Sleipner and reproduce an N-S elongated CO₂ plume. However, our model is at best a modest improvement over the previous models and a work in progress. The adjustments of parameters need to be verified with new observations. With more observations, this model will certainly be superseded.

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Table 1: Parameters Used in This Study

Parameters	Base Case	Range	References and comments
Reservoir geometry (depth to the reservoir top and reservoir thickness)	Statoil Benchmark model		Sleipner Benchmark
Porosity for Utsira and Shale units	~34-36%	~34-36%	Geophysical logs from 300+ wells (gamma-ray, sonic, density, resistivity and neutron logs); Sleipner Benchmark
Caprock permeability k_i	~0.001 Millidarcy	~0.001 Millidarcy	Sleipner Benchmark
Utsira permeability k_i	~2 Darcy	~2 Darcy	Sleipner Benchmark
Shale permeability k_i	~0.001 Millidarcy	~0.001 Millidarcy	Sleipner Benchmark
Vertical permeability anisotropy $k_v:k_h$	0.1		Sleipner Benchmark
Horizontal permeability anisotropy $k_j:k_i$	5	1~10	(Chadwick and Noy, 2010)
L9 model area	18 km ²		Sleipner Benchmark
Top L9 depth	817.3	802.2-840.5	Sleipner Benchmark
L9 thickness	11.3 m	3.5-26.3	Sleipner Benchmark
Critical gas saturation	0.02		Sleipner Benchmark
Connate water saturation	0.89		Sleipner Benchmark
Residual gas saturation	0.21		Sleipner Benchmark
Reservoir temperature	33.5 °C	29 °C ~ 37 °C	(Boait et al., 2011; Cavanagh and Haszeldine, 2014)
Reservoir pressure	8.3 MPa at 820 m as reference	8.0~8.6 MPa	(Chadwick et al., 2005; Boait et al., 2011)
Hydrostatic gradient	Assumed hydrostatic equilibrium		Sleipner Benchmark
CO ₂ injection rate into the Layer 9			Based on seismic data and injection rate to the whole reservoir by Statoil
Main feeder Layer 9	x = 438,516; y = 6,471,210		Sleipner Benchmark (Singh et al., 2010)
Boundary conditions	Dirichlet boundary conditions (infinite large volume for the boundary grid cells)		(Pruess, 2004)
CO ₂ density	479 kg/m ³ at reservoir temperature, pressure, and 2.4% CH ₄		Calculated with GEM ®
Pore Water Salinity	33500 ppm		Sleipner Benchmark
Water density	1021 kg/m ³		Calculated based on salinity

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Table 2. Layer 9 temperature and pressure ranges reported in literatures and used in our analysis

References	Temperature (°C)	Pressure (MPa)
(Aines et al., 2011)	29.4	8.5
(Bickle et al., 2007)	35	8.0
(Chadwick et al., 2005)	29	8.6
Boait et al. (2011)	29	8.0
Cavanagh and Haszeldine (2014)	31-37	8.1

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Table 3: Aqueous Concentrations (in Molality) for Utsira Formation Water

Component	Adopted value ^a
Na	0.4520
K	0.0053
Ca	0.00742
Al	1.3×10^{-8}
Si	1.66×10^{-4}
Cl	0.5213
C	0.00232
pH	6.5
Temp (°C)	33 ^b

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^aJohnson et al. (2004). ^bAssumed values.

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Figure 1. Left panel: Location of the Sleipner fields (after Holloway et al., 2005). Dots with names other than Sleipner refer to other oil and gas fields nearby. Right panel: Isopach map (100 m contour interval) of Neogene sandy units and sediment input directions (Gregersen and Johannessen, 2007).

Figure 2. Time-lapse seismic images of the CO₂ plume at Sleipner. Seismic reflection profiles through time with the nine CO₂ accumulation horizons numbered in the 2002 profile. The pre-injection profile shows the base and top of the Utsira Sand but little detail within the reservoir. The subsequent post-injection profiles show bright reflections where CO₂ is ponding under thin mudstones. Note the pushdown of the basal Utsira Sand reflection resulting from low velocity of CO₂ in the reservoir and development of a low amplitude vertical ‘chimney’ just to left (south) of the injection point (IP) presumed to be the main vertical conduit of CO₂ in the plume. Vertical scale is in two-way travel time (Bickle et al., 2007).

Figure 3. Workflow for CO₂ sequestration modeling and analysis of sensitivity and uncertainty at Sleipner.

Figure 4. The extents of CO₂ plume in 2006. Black outlines represent the observations (Chadwick and Noy, 2010b). (a) results of simulation in this study with $k = 2$ Darcy east-west, 10 Darcy north-south, and one feeder for Layer 9; (b) simulation in this study with 100% CO₂ mass into the main feeder (circle) during 1999-2001, 85% CO₂ volume injected into the main feeder and 15% into the second feeder (the triangle) starting from 2002, $k = 2$ Darcy east-west and 10 Darcy north-south.

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(e) Cavanagh (2013) Invasion percolation migration model

(f) Singh et al. (2010) CO₂ Black Oil Simulator using up-scaled relative permeability curves

(g) Singh et al. (2010) CO₂ Black Oil Simulator using the Vertical Equilibrium option

Haukaas et al. (2013)

Figure 5. Comparison of simulated time-series CO₂ plume extent with observed plumes from seismic amplitude data (Boait et al., 2012).

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Figure 6. Percentages of areas within the CO₂ plume outline (delineated by seismic data) that were not filled by CO₂ in model runs in 2006. The bars (left to right) are from (1) Base Case in this study; (2) test case with 2 feeders in this study, simulated with GEM; (3) from Cavanagh (2013), employing a black oil simulator to the Benchmark model with upscaled Corey curves; (4) from Cavanagh (2013), with a compensation period of several decades until the overpressure has dissipated; (5) from Chadwick and Noy (2010), with TOUGH2; and (6) Singh et al. (2010), with Eclipse 300 with Corey exponents of 1.0.

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(a) Test Case-Temperature

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1999 2001 2002 2004 2006 2008

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(b) Test Case-Pressure

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(c) Test Case-20% more CO₂ spill into Layer 9

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(d) Test Case-4% CH₄

(e) Test Case-1 Feeder, T=35 °C, CH₄=1.8%

(f) Test Case-1 Feeder, T=34 °C, CH₄=2.7%

Figure 7. Results of sensitivity and uncertainty analyses. The black outlines represents CWC observed from 4D seismic (Boait et al., 2012). Red lines represent the Base Case. Blue lines in (a)-(f) represent simulated results of test cases.

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(b)

Figure 8. Variations of CO₂ density (a,b) and viscosity (c) with temperature, pressure, and CH₄ content. All density and viscosity values were computed with GEM® except the density values in (b). In (b), density values of the CO₂-CH₄ mixture (lines without notation of “WINPROP”) were predicted with SAFT2, using parameters of CO₂ and CH₄ from previous work (Tan et al., 2006; Ji and Adidharma, 2010). To predict the effect of CH₄ on the density of CO₂, the mixing rules without any adjustable parameters were used in SAFT2. The box is the range of pressure in Layer 9 reported in literature.

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Figure 9. Comparison of CO₂ fluid velocities in various test cases. Flow velocity along the south-north direction at the position shown in plume diagram.

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Figure 10. Sensitivity of model parameters on simulated trapping mechanisms. Upper panel: tornado diagram for supercritical CO₂ (structural or hydrodynamic trapping); lower panel: tornado diagram for dissolved CO₂ (solubility trapping). The lines represent the simulation results for the Base Case (~93.5% of total injected CO₂ for structural trapping and ~6.5% for solubility trapping); green color denotes parameter values higher than those in the Base Case and blue color lower than those for the Base Case. Parameters used in the Base Case are listed in Table 1.

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Figure 11. Vertical profiles of the CO₂ plume in Layer 9 in 2006. The red solid lines represent the simulated bottom of the CO₂ plume in the Base Case; the black solid lines are the topography of the caprock bottom in the model. The vertical black dash lines represent the boundary of CO₂ plume. (c) locations of the profiles. The black outlines denoted CWC interpreted from seismic data (Boait et al., 2012).

Figure 12. Upper panel: The concentration (molality) distribution of HCO_3^- at the crossing section I=33 in 2006. The blank area in the sandstone indicates the initial HCO_3^- concentration in 1999. The top 2 sub-layer and bottom 7 sub-layer of block grid are shale layers; other sub-layers are the sandstone. The bold black line represents CWC boundary derived in the Base Case. Middle panel: The percentage of calcite dissolution at the top sub-layer of Layer 9 in 3D in 2006. Lower panel: Porosity change distribution at the top sub-layer of Layer 9 in 2006. Negative value represents the increase of porosity due to mineral dissolution.

Figure 13. Simulated time-series of CO₂ plume in the top sub-layer of Layer 9 from 2010 to 2018 with Base Case- 33.5 °C, 2.4% CH₄ (upper panel) and Test Case- 2 two feeders, 33.2 °C, 0% CH₄ (lower panel). The black line in 2010 is the CWC interpreted from the seismic data of Statoil; the blue background color indicates the horizontal range of the mesh grid of the Sleipner Benchmark.

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