Simulating the Cranfield Geological Carbon Sequestration Project with High-Resolution Static Models and an Accurate Equation of State

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Abstract A field-scale carbon dioxide (CO₂) injection pilot project was conducted as part of the Southeast Regional Sequestration Partnership (SECARB) at Cranfield, Mississippi. We present higher-order finite element simulations of the compositional two-phase CO₂-brine flow and transport during the experiment. High-resolution static models of the formation geology in the Detailed Area Study (DAS) located below the oil-water contact (brine saturated) are used to capture the impact of connected flow paths on breakthrough times in two observation wells. Phase behavior is described by the cubic-plus-association (CPA) equation of state, which takes into account the polar nature of water molecules. Parameter studies are performed to investigate the importance of Fickian diffusion, permeability heterogeneity, relative permeabilities, and capillarity. Simulation results for the pressure response in the injection well and the CO₂ breakthrough times at the observation wells show good agreement with the field data. For the high injection rates and short duration of the experiment, diffusion is relatively unimportant (high Péclet numbers), while relative permeabilities have a profound impact on the pressure response. High-permeability pathways, created by fluvial deposits, strongly affect the CO₂-transport and highlight the importance of properly characterizing the formation heterogeneity in future carbon sequestration projects.

1. Introduction

Geological CO₂ sequestration (GCS) in porous formations is considered as a tool to mitigate greenhouse gas emissions into the atmosphere (e.g., Baines and Worden, 2004; Holloway, 2005; Schrag, 2007). There are different candidate reservoirs for GCS such as saline aquifers, depleted oil and gas reservoirs, and unminable coal seams (Bachu, 2000). CO₂ injection in hydrocarbon reservoirs is also adopted for the purpose of enhanced oil recovery (EOR) (Dai et al., 2014a, 2016; Pan et al., 2016; Ampomah et al., 2016a,b), but saline aquifers offer the largest storage volumes in the context of GCS (DOE-NETL, 2015).

Several field-scale pilot projects have been performed worldwide to 1) test the potential of long-term CO₂ sequestration, 2) monitor the fate and transport of CO₂ using various methods, and 3) evaluate the reservoir response to a large volume of CO₂ injection (e.g., Arts et al., 2004; Emberley et al., 2005; Freifeld et al., 2005; Kharaka et al., 2006; Mito et al., 2008; Vasco et al., 2010; Hovorka et al., 2013; Dai et al., 2014b,c; Bacon et al., 2016). One of these pilot-projects is the large-scale pilot test that was performed near Cranfield, Mississippi, in 2009-2010. The GCS site is a brine-saturated formation down-dip of an oil field where CO₂ was injected for EOR purposes by Denbury Onshore LLC (see Fig. 1). The pilot project was directed by the Southeast Regional Carbon Sequestration Partnership (SECARB), led by the Southern State Energy Board. A Detailed Area of Study (DAS) was defined that includes an injection well (F1) and two nearby observation wells (F2 and F3) in order to collect high-resolution temporal evolution data. A detailed description of the project design and experimental procedures is provided by Hovorka et al. (2011, 2013), describing a collaboration between the University of Texas Bureau of Economic Geology (UTBEG), Sandia Technologies LLC, Oak Ridge National Laboratory (ORNL), Lawrence Berkeley National Laboratory (LBNL), U.S. Geological Survey (USGS), and the Ohio State University (OSU).

Previous studies have modeled the Cranfield pilot-project in order to match various observation datasets. Two important studies were performed by Hosseini et al. (2013) and Delshad et al. (2013). Hosseini et al. (2013) developed static and dynamic reservoir models for the formation that includes both the DAS and a commercial CO₂-EOR project at the Cranfield site. They created hundreds of high-resolution *conditional* realizations of facies-based static models and reduced parameter uncertainties by integrating field data. Then, using dynamic reservoir modeling and history matching, they selected the realizations that best reflected the complex flow pathways arising from subsurface heterogeneity at the site. Delshad et al. (2013) used one of those realizations to study the effect of different trapping mechanisms and hysteresis on pressure responses in the injection well and the CO₂ breakthrough times in the observation wells. The DAS area is a small subsection of the computational domain in the numerical simulations by Hosseini et al. (2013) and Delshad et al. (2013). The full static models developed by Hosseini et al. (2013) contain over 60 million grid blocks and cover the entire Cranfield site, including the oil field. Therefore, to make the computational cost feasible *upscaled* static models were previously adopted to represent the spatial variability in permeability and porosity. The Cranfield pilot test has also been modeled in the Sim-SEQ project using different reservoir simulators (e.g., TOUGH2/EOS7C, STOMP-CO₂e, TOUGH2-MP/ECO2N, VESA, MoReS; see Mukhopadhyay et al., 2012, 2015). In Sim-SEQ, each group developed their own conceptual reservoir characterization, with the DAS represented by a small number of grid cells in an upscaled site-scale static model.

Many candidate reservoirs for GCS and commercial CO₂-EOR have sedimentary architectures reflecting fluvial deposition (McGuire and Stalkup, 1995; McGuire et al., 1995; Gershenzon et al., 2015a; Lu et al., 2012a). The target formation near Cranfield,

located in the lower Tuscaloosa formation, is comprised of fluvial deposits of considerable heterogeneity (Hovorka et al., 2011, 2013). 3D seismic surveys and core samples have revealed this complex heterogeneity with multiple laterally discontinuous 3D sand bodies (facies) (see Figure 3 in Lu et al., 2012a). Hosseini et al. (2013) employed an object-modeling approach by embedding geobodies in order to create high-resolution static models that conform to these observations. The objective of this work is to take advantage of the full detail in these models, i.e. *without upscaling*, to study how the fluvial architecture at the site (e.g., channels and their connectivity) controls fluid flow and CO₂ transport within the DAS during the injection experiment. Developing such predictive models of CO₂ transport is critical for 1) estimating residence time, reservoir storage capacity, and storage mechanisms, 2) testing injection scenarios for process optimization, and 3) assessing potential leakage of CO₂ from the reservoir utilizing long-term monitoring techniques.

Reservoir modeling of CO₂ injection in saline formations relies on the parameterization of certain core-scale processes measured in laboratory experiments. The relative permeabilities of brine and CO₂ are key parameters. We use the measured relative permeabilities reported in Hosseini et al. (2013), and used by Delshad et al. (2013). We also perform parameter studies to determine the sensitivity of CO₂ breakthrough times and pressure responses to different relative permeability parameters such as the residual water saturation, curvature exponents for CO₂ and brine, and CO₂ end-point relative permeability. The influence of capillarity and Fickian diffusion are investigated as well. Without diffusion, injected CO₂ tends to flow primarily through high-permeable pathways, but compositional gradients between different facies with high and low permeability can drive considerable cross-flow behavior (Moortgat and Firoozabadi, 2013, 2016; Moortgat, 2016).

The paper is organized as follows: in Section 2 we briefly describe the Cranfield site with a specific focus on the DAS area. Section 3 presents the governing equations in our simulator, and Section 4 is devoted to a description of the numerical methods used in this study. Section 5 describes the Cranfield static model developed by Hosseini et al. (2013). The set-up of the 3D CO₂ injection simulations is presented in Section 6. Section 7 discusses the results of our numerical simulations with further sensitivity analyses in Sections 8-11. Finally, Section 12 highlights the main conclusions of this work.

Fig.1. Map of the Cranfield site (modified from Hosseini et al., 2013). The DAS area is part of a larger domain called the high volume injection test area (HiVIT), shown by the blue trapezoid. The DAS is shown by the red box with wells F1, F2, and F3 located down-dip of the oil field (locations of other wells in the field are also shown). A major sealing fault (grey line) to the northeast separates the field into east and west sections. The wells in DAS are located below the water-oil contact (WOC) where only injected CO₂ and brine exist.

2. Description of Cranfield site

The Cranfield site is located about 20 km east of Natchez in southwestern Mississippi, U.S.A. (see Fig.1). The oil reservoir in Cranfield was discovered in 1943 and oil production was continued until 1966 (Weaver and Anderson, 1966). An EOR CO₂ injection project began in 2008. The target formation for the pilot project at the DAS area consists of fluvial sandstones of the Cretaceous lower Tuscaloosa Formation at depths of 3,300 m. A more detailed description of the geology can be found in Hovorka et al. (2011, 2013).

The DAS is located in the water leg of the reservoir with close proximity the CO₂-EOR wells (see Fig. 1). The target formation was initially saturated with brine. The DAS has three wells. For the pilot test, CO₂ was injected through an injection well (F1), and was monitored by two observation wells (F2 and F3). Wells F2 and F3 were perforated through the same sand intervals and they are lined up approximately with F1 with distances of about 68 m and 112 m to the east, respectively (more on the well locations below). During the highly integrated pilot project, different types of data were acquired

such as extensive down-hole and surface geophysical and geochemical data. Different monitoring techniques were also evaluated in order to improve understanding of CO₂ behavior (Lu et al., 2012a,b). The CO₂ injection pilot project started on December 1st in 2009 with an initial injection rate of ~175 kg/min. After about 20 days, the rate was increased to ~300 kg/min, and after 156 days the rate was raised again to ~500 kg/min. The focus of this work is on the pressure response and the CO₂ breakthrough times at the observation wells in the first 230 days of CO₂ injection. The field-schedule injection rates and observed pressure responses are taken from Hosseini et al. (2013). The observed breakthrough times of 11 days for F2 and 16 days for F3 are from Hovorka et al. (2013).

3. Governing equations

In this section, we briefly summarize the equations that govern our simulations.

3.1. Species transport equation

The molar balance equations are given by:

$$\phi \frac{\partial c z_i}{\partial t} + \nabla \cdot \vec{U}_i = F_i, \quad i = 1, 2 \quad (1)$$

where f is porosity, c [mol/m³] is the overall molar density; z_i is the overall mole fraction of component i (1 is brine and 2 is CO₂) with $\sum_i z_i = 1$, t [s] is time, $\vec{U}_i$ [mol/m²/sec] is total molar flux of component i , and F_i [mol/m³/s] is a source term of component i . The $\vec{U}_i$ is the sum of diffusive (J_{ai}) and convective phase fluxes:

$$\vec{U}_i = \sum_{\alpha} (c_{\alpha} x_{ai} v_{\alpha} + S_{\alpha} J_{ai}), \quad i = 1, 2, \quad \alpha = w, g \quad (2)$$

$$J_{\alpha 2} = c_{\alpha} \phi D \nabla x_{\alpha 2}, \quad J_{\alpha 1} = -J_{\alpha 2}$$

where the subscript a denotes the brine phase (w) and CO₂ gas phase (g), c_a is phase molar density, x_{ai} is the mole fraction of component i in phase a ($x_{a1} + x_{a2} = 1$), v_a [m/s] is the phase fiducial velocity, S_a is the phase saturation, J_{ai} is the diffusive flux of component i in phase a , and D [m²/sec] is the diffusion coefficient of CO₂ in brine. Note that we neglect water vaporization, so diffusion only occurs within the aqueous phase ($J_{gi} = 0$).

3.2. Darcy's law and pressure equation

In order to find the phase velocity, Darcy's law is invoked as:

$$v_a = - \frac{1}{\alpha} \underline{K} (\nabla p_a - r_a g) \quad (3)$$

where p_a [Pa] is the phase pressure. The phase pressures are related by the capillary pressure between brine and gas ($p_{c,gw} = p_g - p_w$), which is a function of water saturation. g [m/s²] is the gravitational acceleration, $\underline{K}$ [m²] is the permeability tensor, λ_a [m.s/kg] is the phase mobility, calculated from the phase saturation S_a , relative permeability (k_{ra}) and phase viscosity (μ_a [kg/m.s]), as $\lambda_a(S_a) = k_{ra} / \mu_a$. The mass density of phase a , ρ_a [kg/m³], is related to the molar density as:

$$\rho_a = c_a \sum_{i=1}^2 x_{ai} M_i$$

where M_i [g/mol] is the molecular weight of the brine and CO₂ components. Instead of solving for each phase velocity individually, we adopt the fractional flow formulation in terms of a total velocity (Hoteit and Firoozabadi; 2006, Moortgat et al., 2011; Pope, 1980; Binning and Celia, 1999).

We use the concept of volume-balance by Acs et al. (1985), which leads to the following pressure equation:

$$\phi C_f \frac{\partial p}{\partial t} + \sum_{i=1}^2 \bar{v}_i \nabla \cdot \bar{U}_i = \sum_{i=1}^2 \bar{v}_i F_i, \quad i = 1, 2 \quad (4)$$

where C_f [m.s²/kg] is the total compressibility, $\bar{v}_i$ [m³/mol] is the total partial molar volume of component i . The C_f and $\bar{v}_i$ are calculated following Firoozabadi (2015) (see also Moortgat et al., 2011).

3.3. Two-phase relative permeabilities

Relative permeability is a rock-fluid property and represents the fractional reduction in fluid conductivity due to the diversion of fluid flow pathways by the presence of other fluid phases. Relative permeability values are between 0 and 1 and are a strong function of phase saturations (Stone 1970, 1973; Delshad and Pope, 1989; Lake, 2010). The relative permeability model used in this work is a variation of Brooks-Corey type relations (Brooks and Corey, 1964). The brine and gas relative permeabilities (k_{rw}, k_{rg}) are determined by:

$$k_{rg} = k_{rg}^0 \left(\frac{S_g - S_{g,ir}}{1 - S_{g,ir} - S_{w,ir}} \right)^m \quad (5)$$

$$k_{rw} = k_{rw}^0 \left(\frac{S_w - S_{w,ir}}{1 - S_{g,ir} - S_{w,ir}} \right)^n \quad (6)$$

where k_{rg}^0 and k_{rw}^0 are the brine and CO₂ end-point relative permeabilities, $S_{w,ir}$ and $S_{g,ir}$

are the residual or irreducible saturation of brine and CO₂, m and n are the curvature exponents of gaseous CO₂ and brine, respectively.

In Section 8, we perform sensitivity simulations to k_{rg}^0 , $S_{w,ir}$, m , and n . The Cranfield pilot project addressed only the drainage phase (continuous injection of supercritical CO₂ for over 200 days); therefore, k_{rw}^0 and $S_{g,ir}$ are 1 and 0, respectively (as in Hosseini et al., 2013 and Delshad et al., 2013).

4. Description of reservoir simulator

The physical and chemical processes controlling the transport of CO₂ in GCS sites are quite complex, due to, e.g., CO₂ phase behavior and different types of trapping mechanisms (e.g., residual, solubility, structural, and mineral). We utilized numerical methods presented in earlier work (Moortgat and Firoozabadi, 2010, 2013, 2016 a,b; Moortgat et al., 2011, 2012, 2013; Shahraeeni et al., 2015). Specifically, we adopt a second-order discontinuous Galerkin (DG) method for the transport equations, which has low numerical dispersion. A Mixed Hybrid Finite Element (MHFE) method is used to solve the Darcy and pressure equations simultaneously, which provides accurate velocity and pressure fields. These methods were developed specifically to obtain more accurate results in highly heterogeneous media, such as fractured and layered formations (Hoteit and Firoozabadi, 2006). MHFE is useful for the simulations in this work due to sharp contrasts in the heterogeneous permeability fields arising from spatial organization of facies in our static models. The flow and transport problems are coupled by the common IMplicit-Pressure-Explicit-Composition (IMPEC) scheme.

Thermodynamic equilibrium is satisfied by requiring the equality of the fugacities of components in each phase. The calculation of the phase fugacities, phase compositions, molar fractions of each phase, total fluid compressibility, and the total partial molar volume are based on the cubic-plus-association (CPA) equation-of-state (EOS). The CPA-EOS was developed to model the phase behavior of fluids that contain polar molecules, such as water (Firoozabadi, 2015). CPA-EOS takes into account the self-association between water molecules, as well as the (polar-induced) cross-association between water and CO₂ (Li and Firoozabadi, 2009, 2012; Moortgat et al., 2012). Phase split computations based on an EOS are an improvement over empirical correlations, such as Henry's law, and strictly enforce local thermodynamic equilibrium.

5. Description of the Cranfield static model

Reservoir heterogeneity has important effects on fluid flow and mass transport. It can be quite pronounced in formations created by fluvial depositions, which are important target reservoirs for CO₂ sequestration. Well known examples include the lower Mt. Simon Sandstone (Freiburg et al., 2014; Ritzi et al., 2016); the lower Paaratte Formation (Krevor et al., 2012; Dance and Patterson, 2016); the Victor interval of the Ivishak Formation (Tye et al., 2003; Gershenzon et al., 2014, 2015b); the Morrow Sandstone (Dai et al., 2016; Gallagher, 2014); and the lower Tuscaloosa Formation (Krevor et al., 2012; Lu et al., 2012a,b). Fluvial formations exhibit subsurface heterogeneities that are characterized by the spatial organization of multiple facies

types with multiple laterally discontinuous sand facies. This complexity results in variable connectivity and flow pathways arising from the patterns of point-bars and channels (e.g., Sneider et al., 1978; Willis and White, 2000; Snedden et al., 2007; Deveugle et al., 2011; Lu et al., 2012a,b). The nature of fluvial deposits can exert strong control on CO₂ dynamics because of high variability in petrophysical properties (e.g., permeability and porosity; Gershenzon et al., 2015a; Ritzi et al., 2016).

Extensive studies were performed by the UTBEG research team to characterize the nature of the fluvial deposits observed at the Cranfield site and to realistically represent the subsurface heterogeneity. We use the history-matched static petrophysical reservoir models developed by Hosseini et al. (2013). This is the best data available for the Cranfield site. Briefly, the top and bottom of the 3D static models were determined by a 3D seismic survey and are modeled as impermeable layers. *Conditional* realizations of facies types were created by geostatistical simulations using an object-modeling approach (see Fig.10 in Hosseini et al., 2013). There are 8 different operational facies in the model domain: 4 lower permeability facies groups (clay-rich) and 4 higher permeability facies groups (sandstones). Each was given uniform permeability and porosity values. In these static models, sands and channels have sinusoidal shapes with variable wavelength, amplitude, thickness, and width corresponding to the observed fluvial architecture. Subsequently, the partitioning of each facies and the measured facies permeability and porosity values were assigned based on well log locations. Three facies-based static models were created and used to generate hundreds of conditional realizations with different petrophysical properties. History matching was performed using dynamic data (e.g., pressure response, and CO₂ breakthrough times) to pick the best realizations. The resulting static reservoir models have a high-resolution with grid block size of 3.048 m (10 ft) × 3.048 m (10 ft) × by 0.3048 m (1 ft) in the x, y, and z directions, respectively, requiring more than 60 million grid blocks. Therefore, Hosseini et al. (2013) used upscaled static models in a commercial simulator (CMG-GEM) and compared the simulation results with field-measured CO₂ breakthrough times in F2 and F3, along with bottom-hole pressure in F1. Delshad et al. (2013) also used volume-weighted arithmetic averaging and directional arithmetic-harmonic averaging to upscale porosity and permeability, respectively. In these studies the DAS area was represented by a relatively small number of grid blocks in the computational domain.

In this work, we use the high-resolution static models without upscaling. This allows us to more accurately model the effects on pressure response and CO₂ dynamics of small-scale variability in petrophysical properties that arise from the spatial organization of facies. In order to make the numerical simulation computationally feasible we extract only the DAS to reduce the number of grid cells. Our computational domain includes the full 24 m thickness of the target formation and has 257,856 unstructured grid blocks that conform to the formation geometry (see Fig. 2). Fig. 3 and Fig. 4 show the permeability and porosity, respectively, for the best history-matched realization from Hosseini et al.(2013) throughout the grid in both 3D and on a few 2D cross-sections. We refer to this realization of heterogeneity as the Base-Case throughout this article.

6. Modeling approach

We model the transport of brine-CO₂ with our in-house reservoir simulator, Osures, discussed in Section 4. We only consider brine and CO₂ components. The CPA-EOS parameters are tuned to match the fluid properties observed at the Cranfield site (see Table 1). Specifically, the brine density and viscosity are 1,039 kg/m³, and 0.22 cp, respectively. Note that the brine density is higher than that of pure water. The CO₂ density and viscosity are 578 kg/m³, and 0.022 cp, respectively. Our density and viscosity values are close to the calculated values by Delshad et al. (2013). The above values are in line with those in the NIST chemistry webbook (Lemmon et al., 2005) for pure CO₂ and pure water at the aquifer temperature and pressure (given below).

As shown in Fig. 2, we use non-orthogonal hexahedral grid elements to discretize a physical domain of 155 m by 195 m and 24 m in the x, y, and z directions, respectively, to cover the DAS area. The number of grid cells in x, y, and z directions are 64, 51, and 79. The grid includes the perforated injection well (F1) on one boundary and the two non-intrusive/non-interacting observation wells (F2 and F3) inside the computational domain. The initial conditions for CO₂ injection consist of a brine-saturated formation at constant temperature (128 °C) and hydrostatic pressure (initially 32 MPa at the bottom). The initial pressure and temperature are taken from the observed pre-injection values in the injection well (F1) reported in Delshad et al. (2013) and Hosseini et al. (2013). The relative permeability curves for the formation are Brooks-Corey type (Eq.(5) and Eq.(6)) with parameter values listed in Table 2. The boundaries away from the injection well are kept at constant-pressure (open). The top and bottom boundaries are impermeable (no-flow). Sensitivity studies of the effect of capillarity scale the capillary pressure by the Leverett *J*-function (Leverett, 1941) to account for spatial variability in permeability and porosity.

Table 1
EOS parameters.

P= 32 MPa, T= 128 °C	CO ₂	Brine
Critical temperature (°C)	30.85	373.85
Critical pressure (MPa)	7	22
Acentric factor	0.24	0.22
Molecular weight (g/mole)	44	18
Volume-shift parameter	0	0.3
Binary interaction coefficient	0.28	0.28

Table 2

Brooks-Corey type parameters for relative permeability drainage curves (from Delshad et al., 2013) in our Base-Case simulation.

Parameters	Values
$S_{w,ir}$	0.4
$S_{g,ir}$	0.0
k_{rw}^0	1.0
k_{rg}^0	0.8
Gaseous CO ₂ exponent (m)	2.6
Brine exponent (n)	4.2

Fig. 2. Numerical grid for the Cranfield Detailed Area of Study (DAS). The grid is 155 × 195 × 24 m³, with 257,856 hexahedral elements. The injection well F1 and observation wells F2 and F3 are shown by the red straight lines, at 68 m and 112 m from F1, respectively. The domain is inclined in both the x and y directions.

Fig.3. (color online) Formation permeability shown (a) as contours throughout full DAS in 3D, (b) on five 2D horizontal cross-sections (red straight lines showing the location of the injection well, F1, and two observation wells, F2 and F3). The geometry of modeled fluvial channels is clear and it is consistent with the fluvial interpretation of the site (see Hosseini et al., 2013)

Fig. 4. (color online) Formation porosity shown (a) as contours throughout full DAS in 3D, (b) on five 2D horizontal cross-sections (red straight lines showing the location of the injection well, F1, and the two observation wells, F2 and F3).

7. Comparison between observed data and numerical simulations

7.1. Bottom-hole pressure in injection well F1

Fig. 5 shows the field-schedule injection rates provided by UTBEG and published in Hosseini et al. (2013) as well as the injection rate schedule used in our simulations. Fig. 6 compares the bottom-hole pressure (BHP) in the injection well (F1) as measured in the field and for our Base Case simulation.

It is clear from Fig. 6 that we are able to match the BHP in the injection well reasonably well up to 157 days, corresponding to the time that the injection was increased to the highest rate of about 500 kg/min. Overall our simulated pressure evolution in the DAS also agrees well with previous studies that modeled the entire Cranfield site (Delshad et al., 2013; Hosseini et al., 2013; Mukhopadhyay et al., 2012, 2015). After 157 days, the field data indicate that the pressure response was relatively insensitive to a rate increase of ~40%, while simulations show a considerable pressure jump. The discrepancy between measured and simulated pressures for this highest rate is less than in some prior studies, which could be due to 1) the high-resolution (not-upscaled) static model in our simulations, and 2) the use of MHFEM to simultaneously solve for accurate pressures and fluxes in a heterogeneous medium. Delshad et al. (2013) and Hosseini et al. (2013) argued that the formation might have been fractured during this highest CO₂ injection rate and showed that a better match between measured and simulated pressures could be obtained by artificially adding high permeability grid cells (mimicking a fracture) from the injection well to the observation well (and in the opposite direction). While fracture formation is possible, we also believe that this could be a realization-dependent phenomenon. To investigate the sensitivity of the pressure response to the permeability field, we perform high-resolution simulations for two more of the best history-matched static models developed by UTBEG (Static Model 2 and Static Model 3). The main difference between the static models is the spatial distribution of geobodies (facies). The results in Fig. 7 show that 1) the pressure response is quite sensitive to the spatial distribution of facies types, and 2) the Base-Case static model, while not perfect, shows the best match to the field data. The sensitivity of the pressure response to other rock and fluid properties will be investigated below.

Cranfield core samples reveal multiple upward-fining intervals from conglomerate to fine sandstones, dominated by low-angle cross-bedding (see Lu et al., 2012a). This corresponds to conglomerates deposited as lateral migration of channels (see Bridge, 2009). Our simulation results confirm the importance of these channels for CO₂ migration (see Fig. 8 and Supplementary material). Fig. 8 shows a yellow contour of the CO₂ front (a molar fraction of 0.001) with superimposed contours of the permeability field after 10, 15, 20, and 25 days of injection in the Base-Case simulation. The influence of higher permeable channel features (flow channeling) on the evolution of CO₂ is clear. The animations provided in the Supplementary material better show the influence of formation heterogeneity and channeling on the transport of CO₂. The channels have higher permeability and porosity than clay-rich facies and their spatial

Fig.6. (color online) Observed (red dots) and simulated BHP in F1 for the 230 days duration of Cranfield pilot test. Day 0 is on December 1, 2009 and day 230 is July 22, 2010.

Fig.7. (color online) Observed BHP in F1 (red dots) and simulation results for 3 static model realizations, for the 230 days duration of the Cranfield pilot test.

Fig. 8. (color online) Contour of 0.001 CO₂ molar fraction after 10, 15, 20, and 25 days of injection (yellow color). Superimposed contours of the permeability field illustrate the modeled location of depositional channels.

7.2. CO₂ breakthrough times in observation wells F2 and F3

Table 3 lists the observed CO₂ breakthrough times at observation wells F2 and F3 and simulation results from prior studies as well as our Base-Case simulation. The measured CO₂ breakthrough time at the first observation well (F2) occurred at about 11-12 days of injection. This agrees reasonably well with our simulation results, which show an increase in gas saturation at F2 after about 13 days of injection (Fig. 10). The observed CO₂ breakthrough time in the second observation well (F3) was 16 days after injection, which would imply a ~24% increase in average flow rate (68 m in 12 days, versus 112 m in 16 days). In our simulations, breakthrough in F3 occurs after about 26 days (Fig. 10). It seems that our high-resolution static model of the DAS can capture preferential flow paths (channels) between F1 and F2 and F3, while the upscaled static models in the cited studies only have a few grid cells spanning the DAS. The remaining discrepancy suggests that even the best-matched UTBEG permeability realization may

have missed a preferential flow path that intersects F3. Alternatively, as discussed in Section 11, recent studies (Ajo-Franklin et al., 2013; Mukhopadhyay et al., 2015; Sun et al., 2016) suggest bottom-hole locations of F2 and F3 that are separated by only ~60 m and ~98 m, respectively, from F1, rather than 68 m and 112 m in our static model. As shown below, a closer spacing between observation wells leads to better agreement between simulated and observed CO₂ breakthrough times.

Fig.9. (color online) Observed (red dots) and simulated BHP in F1 for the 230 days duration of the Cranfield pilot test. The permeability of facies S (fluvial channel) is 170 md in our Base-Case simulation, and is systematically increased to 340 md, 850 md, and 1700 md.

Table 3 also compares the breakthrough times for simulations that use either a second-order DG or a lowest-order finite volume (FV) for transport update (Eq.(1)). The results are close, which suggests that even FV simulations have converged on the very fine grid used in this study.

Table 4 lists the breakthrough times for the simulations in which the permeability of the facies reflecting the fluvial channels is varied from the Base-Case of 170 md to higher values of 340, 850, and 1,700 md. While a channel permeability of 340 md improves the breakthrough time in F2, there is still a disagreement in F3 (and a poorer match to the pressure data in Fig. 9). The lateral location and connectivity of channel features are clearly a controlling factors on CO₂ migration.

Fig. 10. Simulated gas saturation in observation wells F2 and F3. CO₂ breaks through in the first (F2) and second (F3) observation wells after about 13 and 26 days, respectively. Dashed lines show the gas saturation averaged over the full vertical length of the perforated intervals, while solid lines show the maximum saturations, which occur at the depths within the most permeable conduits for flow.

Table 3

CO₂ breakthrough times at observation wells F2 and F3 for different simulation studies of Cranfield pilot project. The time unit is days.

Observation well	F2	F3
Observed^a	11	16
Delshad et al. (2013)	13	90
Hosseini et al. (2013) ^b	7, 13, 28, 16	21, 28, 33, 46
LBNL model ^c	19	53
PNNL model ^c	8-14	19-53
This study: Base-Case - DG	13.16	26.30
This study: Base-Case - FV	13.21	26.31

^afrom Hovorka et al.(2013)

^bvalues for the best static models chosen by history matching

^cfrom Mukhopadhyay et al. (2015)

Table 4

CO₂ breakthrough times at observation wells F2 and F3 for simulations with different values of fluvial channel permeability. The permeability of facies S (fluvial channel) is increased to 340, 850, and 1700 md compared to 170 md in our Base-Case simulation. The time unit is days.

Observation well	170 md	340 md	850 md	1700 md
F2	13.16	10.8	9.2	8.4
F3	26.3	22.2	21.4	20.5

8. Sensitivity analysis of relative permeability parameter values

Iglauer et al. (2015) provides a comprehensive review of the challenges in contact angle experiments and wettability in GCS. Experimental measurements of end-point relative permeabilities in CO₂ core flood experiments are notoriously difficult (see Levine, 2011 and Levine et al., 2014). Experimental results show low values of end-point CO₂ relative permeability (<0.5) and high values of residual water saturation (>0.4) under drainage conditions (Yoshida et al., 2016). However, reported data for Cranfield have a high value for the end-point CO₂ relative permeability (see Table 2). To investigate the importance of this potential uncertainty, we perform a series of additional simulations to assess the impact of relative permeability parameters on injection BHP and CO₂ breakthrough times. Specifically, we vary the endpoint CO₂ relative permeability (k_{rg}^0), brine residual saturation ($S_{w,ir}$), curvature exponents of gaseous CO₂ (m), and curvature exponents of brine (n). Numerical simulations of the Cranfield pilot project using high-resolution static models provide an opportunity to test the effect of relative permeability parameters and compare the results with field measured data of pressure responses and CO₂ breakthrough times.

Table 5

CO₂ breakthrough times at observation wells F2 and F3 for simulations with different values of brine residual saturation. The bold values correspond to the Base-Case simulation. The time unit is days.

Observation well	0.0	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8
F2	20.5	19.3	17.9	15.1	13.16	10.9	9.3	6.6	4.7
F3	52.2	47.6	31.8	29.2	26.3	23.4	20.8	16.5	11.5

8.1. Sensitivity to brine residual saturation

Fig. 11 shows how the simulated BHP in F1 is affected by varying the brine residual saturation ($S_{w,ir}$) from 0.0 to 0.8. Table 5 lists the corresponding CO₂ breakthrough times at observation wells F2 and F3. We find that higher residual saturations result in a lower BHP at all times, but also that the pressure *jumps* are reduced for $S_{w,ir}$ larger than 0.4. Interestingly, a residual water saturation of 0.6 shows comparable agreement to the measured data at early times, but a much better match after 157 days when CO₂ is injected at the highest rate. In addition, the breakthrough times are also closer to the field data for a $S_{w,ir}$ of 0.6. Both the pressure response and the breakthrough times are sensitive to $S_{w,ir}$.

Fig.11. (color online) Sensitivity to brine residual saturation, with $S_{w,ir} = 0.4$ in the Base-Case.

8.2. Sensitivity to end-point CO_2 relative permeability

We vary the CO_2 (gas) end-point relative permeability (k_{rg}^0) from 0.2 to 1.0. The simulated BPH in F1 is given in Fig. 12 and breakthrough times in Table 6. As in Yoshida et al. (2016), we find that the results are sensitive to the CO_2 end-point relative permeability. Small values of $k_{r,g}^0$ dramatically increase the BHP in the injection well due to low gas mobility, which also delays the breakthrough times. The values chosen in Delshad et al. (2013) and Hosseini et al. (2013) also provide the best agreement between observations and our simulations.

Table 6

CO_2 breakthrough times at observation wells F2 and F3 for simulations with different values of end-point CO_2 relative permeability. The bold values correspond to the Base-Case simulation. The time unit is days.

Observation well	0.06	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1.0
F2	25.1	23.0	20.0	18.1	16.3	15.4	14.5	13.7	13.16	12.7	12.3
F3	52.9	48.9	41.1	35.8	32.7	30.6	28.8	27.4	26.3	25.3	24.6

Fig.12. (color online) Sensitivity to end-point CO₂ relative permeability, with $k_{rg}^0 = 0.8$ in the Base-Case.

8.3. Sensitivity to CO₂ and brine curvature exponents

We change the CO₂ and brine curvature exponents (m and n) from linear relationships ($m = n = 1$) to high values of 6 to study their effect on the pressure response and the CO₂ breakthrough times at observation wells F2 and F3. Fig. 13a and Fig. 13b show how increasing curvature exponents influence the simulated BHP in the injection well. Table 7a and Table 7b list the CO₂ breakthrough times at observation wells F2 and F3 for CO₂ and brine curvature exponents, respectively. Increasing CO₂ and brine exponents result in higher BHP in the injection well. The simulations are more sensitive to the CO₂ exponent. As seen in Fig. 13 linear curvature exponents for CO₂ and brine under-predict the BHP in the injection well. Importantly, increasing the CO₂ curvature exponent results in later breakthrough times.

Table 7a

CO₂ breakthrough times at observation wells F2 and F3 for simulations with different values of the CO₂ curvature exponent. The bold values correspond to the Base-Case simulation. The time unit is days.

Observation well	$m=n=1$	$m=1.2$	$m=2.6$	$m=4.2$	$m=6$
F2	3	4.2	13.16	19.4	23.1
F3	5.2	11.3	26.3	35.5	47

Fig.13a. (color online) Pressure response for different CO_2 curvature exponents, with $m = 2.6$ kept as in the Base-Case, except for the simulation with $m = n = 1$.

Fig.13b. (color online) Pressure response for different brine curvature exponents, with $n = 4.2$ kept as in the Base Case, except for the simulation with $m = n = 1$.

Table 7b

CO₂ breakthrough times at observation wells F2 and F3 for simulations with different values of the brine curvature exponent. The bold values correspond to the Base-Case simulation. The time unit is days.

Observation well	$m=n=1$	$n=1.2$	$n=2.6$	$n=4.2$	$n=6$
F2	3	15.7	13.3	13.16	12.7
F3	5.2	25.5	25.4	26.3	26.6

9. Effect of Fickian diffusion

To investigate the importance of Fickian diffusion, we performed simulations with both $D = 1.33 \text{ m}^2/\text{sec}$, and with $D = 0$. We find that the pressure response and the breakthrough times are nearly identical for both simulations. This is due to the high injection rates (high Péclet numbers for advection dominated flow) and short duration of the pilot test. Fickian diffusion is expected to be important for the longer-term evolution of the CO₂ plume post injection. Steep compositional gradients between the CO₂-filled preferential flow paths will slowly diffuse into the mostly water-saturated lower permeability clay-rich facies. This cross-flow effect delays the spreading of the plume over larger time-scales.

10. Effect of capillarity

Capillary pressures are scaled by the Leverett J -function ($J = \sqrt{f/K}$) to account for variations in permeability and porosity. As a reference curve, we use the capillary pressure function in Hosseini et al. (2013) and Delshad et al. (2013). Fig. 14 shows the simulated BHP in F1 with and without considering capillary effects. Unlike the findings in Delshad et al. (2013) we do not find a significant impact of capillarity on the pressure response during the injection period. This is because injection rates are high, while the reported capillary pressures are only of the order of KPa. When we increase the capillary pressures by a factor of 10 and 20, we do see an increased pressure response at later times because CO₂ has a harder time invading the low permeability facies.

Fig. 14. Observed and simulated injection BHP with and without considering capillary effects. The 10x, 20x, cases correspond to increasing capillary pressures by a factor of 10 and 20, respectively

11. Location of observation wells

In the simulation results presented in previous sections we used the observation wells (F2 and F3) separated by distance of 44 m which are located 68 m and 112 m away from the injection well (F1). These locations are based on the static models developed by Hosseini et al. (2013), and used by Delshad et al. (2013). However, Ajo-Franklin et al. (2013) used high-resolution characterization of a CO₂ plume using cross-well seismic tomography, and they reported 30 m distances between F2 and F3. Similar distances were also used in the Sim-SEQ project (Mukhopadhyay et al., 2015). Sun et al. (2016) reported the bottom-hole distance between F1 and F2 as 60 m and between F1 and F3 as 93 m with F2 and F3 separated by 33.5 m. The discrepancy in well locations reported in the literature motivates us to do another sensitivity study (see Fig. 15). We find that simulated breakthrough times agree better with field data for the aforementioned closer distance between F2 and F3. By placing F3 at 98 m the CO₂ breakthrough time is 21.8 days as compared to the value of 26.3 days when F3 is located in 112 m away from the injector. Breakthrough at 60 m occurs at 10.5 days, very close to the observed breakthrough time of 11 days in F2.

In section 8.1 we showed that a residual water saturation of 0.6 shows good agreement with the BHP in the injection well for the full duration of the pilot project. Placing F3 at 98 m and assuming a residual water saturation of 0.6 results in CO₂

breakthrough time of 16 days, which is in perfect agreement with the field observation. Note that irreducible water saturations were carefully measured for well cores, but residual saturations and relative permeabilities can vary for different facies throughout a formation. It is not inconceivable that a different average, or effective, relative permeability relation (including residual saturations) is more appropriate to describe the global flow paths.

Fig. 15. Location of the CO₂ front at different times, with $S_{w,ir} = 0.4$ in the Base-Case shown in the left panel and $S_{w,ir} = 0.6$ in the right panel.

12. Conclusions

The Cranfield pilot project provides one of the richest data sets to study geological carbon dioxide sequestration in large-scale brine aquifers. Yet, measurements of subsurface processes are inherently limited and numerical simulations of carbon dioxide sequestration are invaluable to further constrain uncertainties. Multiple simulation studies have been published in recent years that model the flow and transport of CO₂ throughout the entire Cranfield site (Hosseini et al., 2013; Delshad et al., 2013;

Mukhopadhyay et al., 2012, 2015) using upscaled static models for the permeability and porosity fields. In this work, we focus on a Detailed Area of Study (DAS) that includes the injection well and two nearby observation wells. Due to the smaller size of the DAS we are able to use the most detailed history-matched static models for the formation characterization. These petrophysical models have a vertical resolution of only 1 foot. In addition, we use advanced reservoir simulation tools, such as higher-order finite elements and accurate EOS-based modeling of phase behavior and thermodynamic phase-split computations. On one hand, we are reassured to find good qualitative agreement with prior studies that used a range of well-established reservoir simulators. On the other hand, by using the highest-resolution static model in combination with advanced numerical methods and robust physical models our simulation results are quantitatively the closest yet to the measured field data. This is important because in future work, we plan to also model the perfluorocarbon (and other) tracers that were injected in different pulses as part of the Cranfield pilot project (Hovorka, 2011).

Extensive sensitivity studies further help to identify potential causes of earlier discrepancies between measured and simulated results. Relative permeabilities, for instance, may vary for different rock types (facies). Measurements for cores from a limited number of wells may not necessarily represent the effective relative permeability throughout a formation. We find that simulations with an irreducible water saturation of 60% agree much better with the observed pressure response and CO₂ breakthrough times than the 40% used in previous studies. A different porosity distribution could have a similar effect (immobile brine acts as an effective porosity reduction). There is also some disagreement in the literature regarding the bottom-hole location of the monitoring wells F2 and F3. We find the best agreement with CO₂ breakthrough times when F2 is located ~60-68 m from F1, and F3 at 98 m from F1 (as in Ajo-Franklin et al., 2013; Mukhopadhyay et al., 2015; Sun et al., 2016).

General conclusions from the sensitivity analyses are as follows:

- (1) The most critical uncertainties relate to heterogeneous permeability and porosity fields. Cranfield, like many candidate GCS and CO₂-EOR sites, consists of fluvial deposits that exhibit channelized conduits of high permeability flow pathways, interspersed with tighter facies. 3D seismic data and core samples from a small number of exploration wells provide only limited information on the volume fractions and connectivity of different facies throughout the aquifer. The facies architecture, though, is the primary factor that determines the flow and transport of CO₂. For example, the arrival time (breakthrough) of the CO₂ displacement front at any particular location (e.g., an observation well) is largely determined by whether or not it happens to be intersected by (or lies close to) one or more of the fluvial channels. Our simulations for three of the best history-matched realizations of high-resolution petrophysical models still show quite a wide spread in breakthrough times and pressure responses. Similarly, we show that the results are sensitive to the mean permeability in the fluvial channels.
- (2) The flow rates of injected CO₂ are directly proportional to its relative permeability, which is therefore an important parameter. Low gas relative

permeabilities result in a slower spreading of the CO₂ plume and more pressure build-up, while a high relative permeability contrast with respect to brine can result in a viscously unstable displacement front. The latter can result in viscous fingering (in addition to permeability channeling), which makes predicting the location of the CO₂ front more challenging. Relative permeabilities are non-trivial to measure and depend strongly on the rock types. Even accurate measurements on one core sample may not represent the relative permeability in different facies types throughout the formation. To complicate matters further, CO₂ is known to alter the wettability of rock under certain conditions. Our parameter studies for different residual water saturations, gas end-point relative permeabilities, and curvature exponents demonstrate how sensitive simulation results are to accurate measurements of appropriate relative permeabilities.

- (3) Fickian diffusion and capillarity are shown to be less important for the early time evolution of the CO₂ plume, because injection rates are high and flow is dominated by advection. Both of these processes are expected to be more important for the post-injection long-term migration of CO₂, by driving cross-flow between more gas-saturated high permeability facies and more brine-saturated facies like clay-rich. These processes enhance the mixing of CO₂ and brine and delay the spreading of CO₂.

Constraining the uncertainties in spatially variable permeabilities and porosities of fluvial depositional facies (and their associated relative permeabilities) is clearly paramount for accurate predictions of the fate of CO₂ in GCS applications. This requires new observables in addition to pressure data and CO₂ arrival times in observation wells. Natural (e.g., isotopes) and introduced (e.g., perfluorocarbons, SF₆, and noble gases) tracers can provide such additional information. For instance, by measuring the arrival times of small amounts of tracers that are co-injected with CO₂ at a particular time, one can determine flow rates at different times (e.g., for different injection rates), while the arrival of the CO₂ displacement front itself can only be measured once. These additional degrees of freedom can be used to characterize a GCS target formation's geology in even more detail than in this study. Incorporating such tracer measurements at the Cranfield site into reservoir modeling is the subject of ongoing work as part of the project referenced in the acknowledgements.

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