Impact of 3D capillary heterogeneity and bedform architecture at the sub-meter scale on CO₂ saturation for buoyant flow in clastic aquifers

L. Trevisan¹, P. G. Krishnamurthy², T. A. Meckel¹

¹Gulf Coast Carbon Center, Bureau of Economic Geology, Jackson School of Geosciences, The University of Texas at Austin, Austin, TX, USA

²Petroleum and Geosystems Engineering Department, The University of Texas at Austin, Austin, TX, USA

Corresponding author: Luca Trevisan (luca.trevisan@gmail.com)

Abstract

During the post-injection and stabilization period of geological carbon sequestration, the primary forces governing CO₂ migration and entrapment are capillarity and buoyancy, delineating a specific field of application for numerical flow models. In contrast with conventional modeling approaches that assume laminar viscous flow regime, a modified invasion percolation simulator is used to mimic the physics of fluid flow for vanishing pressure gradients. The current investigation extends a previous study simulating 2D CO₂ invasion through stochastic and natural geologic models. Research presented here expands methods for addressing role of heterogeneity on fluid migration by quantifying the influence of 3D variability in threshold capillary pressure and bedform architecture on CO₂ saturation. The goal is to develop a predictive method for volumetric storage capacity for buoyant flow conditions. Realistic sedimentary models are generated for eight common clastic facies with accurately represented bedform morphology. Resulting 3D models consist of matrix and lamina cells that are populated independently with probability density functions representative of sandstone lithologies with different grain sizes and sorting. Results from thousands of MIP simulations reveal saturation in the eight models to be a non-linear function that is primarily influenced by the contrast in threshold capillary pressures between matrix and lamina (observable lithologic heterogeneity), suggesting some predictive ability is achievable from common sedimentologic descriptors, although quantifying the independent effect of depositional architecture remains more difficult.

Keywords: 3D bedforms; local capillary trapping; textural contrast, buoyant migration; invasion percolation, capacity estimation; capillary heterogeneity; sedimentary structures

1. Introduction

Injection and long-term storage of carbon dioxide (CO₂) in deep sedimentary basins is widely considered to be a critical technology for reducing anthropogenic greenhouse gas emissions. Far from injection wells, and after injection ceases, buoyancy of CO₂ dominates flow forces and small scale heterogeneities strongly influence saturation distributions [Cavanagh and Haszeldine, 2014]. In order to predict subsurface plume behavior and to assess storage capacity, continuum-based multiphase flow models are conventionally applied at the reservoir scale. Typically, these models utilize coarse grids (10's to 100's m edge length) with upscaled properties (e.g. permeability, residual gas saturation) in order to be computationally efficient. Inaccurately representing geological heterogeneity at large scales can result in overestimation of the migration speed [Li and Benson, 2015], mismatch of breakthrough times [Green and Ennis-King, 2010; 2013], and underestimation of final trapped saturation [Saadatpoor *et al.*, 2010] and lateral extent of CO₂ [Hesse and Woods, 2010].

An alternative to developing upscaled properties for reservoir scale simulations [Pickup *et al.*, 1994; Pickup and Hern, 2002; Ringrose *et al.*, 2008; Mouche *et al.*, 2010; Toussaint *et al.*, 2012; Gasda *et al.*, 2013; Rabinovich *et al.*, 2015] is to simulate flow for smaller, highly resolved domains that represent the heterogeneity at the scales previously established as critical for understanding flow and saturation [Hartkamp-Bakker, 1991; Graue, 1994; Ringrose and Corbett, 1994; Li and Benson, 2015]. Ideally, characteristic saturations for a range of geologic facies at small scales could be constrained and then reconciled with upscaling methods to correctly account for expected saturations at reservoir scales [Green and Ennis-King, 2013].

Different flow simulators have advantages and drawbacks for modeling a range of flow physics at various scales [Welte *et al.*, 2000], but should converge when applied appropriately. In a recent review by Oldenburg *et al.* [2015] the ranges of applicability of Darcy's law and invasion percolation (IP) method are evaluated for the modeling of CO₂ migration. Despite the criticism drawn by the IP method due to its lack of time-dependence, advantages such as low computational demand and the ability to honor fine-scale heterogeneity are unquestioned. The modified invasion percolation (MIP) approach [Wilkinson and Willemsen, 1983; Frette *et al.*, 1992; Glass and Yarrington, 1996; Meakin *et al.*, 2000; Carruthers, 2003] is considered here for two fundamental reasons: 1) buoyancy-dominated flow conditions are relevant for the key

problem of long term CO₂ migration, plume stabilization, and resulting saturation, similar to oil losses during migration [Catalan *et al.*, 1992; Carruthers and Ringrose, 1998; Sylta *et al.*, 1998; Luo *et al.*, 2004; Luo *et al.*, 2007; Vasseur *et al.*, 2013; Luo *et al.*, 2015]; and 2) MIP methods allow a wide range of models to be considered efficiently in order to generate sufficient data for revealing fundamental characteristic trends and quantifying influencing factors [Meckel *et al.*, 2015].

The published literature documents an evolution of methods for addressing role of heterogeneity on fluid migration. Critical aspects of geological heterogeneity have been recognized using different approaches: theoretical/analytical [Siddiqui and Lake, 1992; Neufeld and Huppert, 2009; Kuo and Benson, 2015], numerical [Sylta, 1993; Meakin *et al.*, 2000; Corradi *et al.*, 2009; Green and Ennis-King, 2015;], experimental [Thomas and Clouse, 1995; Choi *et al.*, 2011; Yan *et al.*, 2012; Polak *et al.*, 2015], and field studies [Wilson *et al.*, 2011; Jung *et al.*, 2014]. A common outcome from these studies is that geometry and distribution of bedding and facies represent critical aspects of small-scale heterogeneity (lamina to bed-set) in the context of slow migration of hydrocarbons as well as CO₂ in brine formations [van Lingen *et al.*, 1996; Mikes and Bruining, 2006].

For the purposes of this research, heterogeneity is considered to be composed of 1) a lithological component and 2) a fabric component. The lithological component relates to grain sizes, and specifically to contrasts in grain size between depositional laminae (typically finer-grained; baffles) and the matrix. These grain sizes and contrasts are controlled by the average energy (magnitude) of flow velocity (average grain size in transport) and fluctuations in energy of deposition, with more consistent energy producing more homogenous materials (less overall grain size contrast). The fabric component relates to the depositional organization of the laminae, typically described as ripples, etc., and depends on the flow regime of deposition. It is well known in sedimentology that different bedforms are formed in different flow velocities with different grain-sized material [Boggs, 2012], and that some bedforms are physically impossible in some conditions (combinations of flow and grain sizes). Our goal is to consider a wide range of lithological contrasts and fabrics representative of typical geologic depositional settings to understand the primary factors influencing buoyant fluid saturation in realistic materials.

In the present study, we expand on the methods above and build upon previous work by *Meckel* [2013] and *Meckel et al.* [2015] to address the influence of stratigraphic heterogeneity at the sub-meter scale on the containment of CO₂ for different types of sedimentary architectures. To adequately represent 3D heterogeneity, we present numerical models that combine a deterministic bedform architecture component mimicking realistic crossbedding geometries with stochastic variability of petrophysical properties. One advantage of this approach is that it allows consideration of domain sizes larger than whole core and core plugs typically used for laboratory flow experiments, where small sizes may not fully capture depositional architecture. A similar approach has been described for different purposes in previous studies [*Cox et al.*, 1994; *Kjongsvik et al.*, 1994; *Nordahl et al.*, 2005; *Nordahl and Ringrose*, 2008; *Behzadi et al.*, 2012], which shared the influential work of *Rubin* [1987] on computer modeling of crossbedding. Conclusions reported by *Meckel et al.* [2015] for 2D simulations suggest that basic geological features such as grain size distribution and sedimentary bedform architecture can be used to predict the fraction of rock invaded by CO₂ during capillary/buoyancy-dominated flow conditions. In the present work, we aim at improving capacity estimations by accounting for the third dimension, as well as through a more realistic representation of the sub-meter scale heterogeneity.

Our approach for efficiently including capillary heterogeneity trapping in storage capacity estimations consists in developing a predictive method that involves systematic IP simulations applied to a large range of geological models characterized by different bedform architectures and threshold capillary pressure (P_{th}) fields with increasing contrast between matrix and laminae facies. Our conceptual model relies on the assumption that for post-injection, far-field scenarios, the multiphase system can be considered at capillary equilibrium, reducing the problem to a static balance between capillary and buoyancy forces. The main contribution of this study consists in developing a predictive model for CO₂ capacity estimation based on a comprehensive, yet simplified, set of geological models resembling a range of fluvial facies. These models are unique in regard to their geological realism and permit evaluation of the impact of sub-meter scale capillary heterogeneity on buoyant fluid flow scenarios that are relevant to the long term behavior of CO₂ through saline formations.

1.1. Invasion percolation approach

During injection and post-injection stages, buoyant CO₂ plume will be subject to a range of flow regimes, depending on the interplay of forces governing the multiphase flow. These flow regimes are characterized by specific displacement patterns that are described by dimensionless groups, like Bond number, capillary number, and viscosity ratio, constraining a parameter space such as the one introduced by *Lenormand et al.* [1988]. When large pressure gradients are present, e.g. in the near-wellbore zone, viscous-dominated displacements are likely to occur, while capillary and buoyancy-dominated flow regimes become more prevalent in far-field areas, where the injection-induced pressure gradient has already dissipated (see conceptual Figure 1 of *Meckel et al.* [2015]). As a result of this dualism, a number of studies have proposed the separation of flow regimes as an approach to reduce problem complexity in this type of subsurface operations [*Celia and Nordbotten*, 2009; *Altman et al.*, 2014]. This approach is supported by the assumption that the performance of trapping mechanisms occurring across different timescales can be evaluated individually. In the context of this study only CO₂ trapping due to capillary forces is taken into account, specifically we focus on the capillary barrier phenomenon, disregarding immobilization caused by hysteresis, dissolution, or mineralization. As a matter of fact, the type of dominant flow regime has a direct impact on the suitability of numerical models used to describe the displacement process [*Riaz and Cinar*, 2014; *Oldenburg et al.*, 2015]. However, no numerical or analytical solution has been proved capable of simulating the whole range of flow physics without compromises on the spatial and temporal resolution.

Based upon laboratory observations through synthetic [*Dembicki and Anderson*, 1989; *Catalan et al.*, 1992; *Frette et al.*, 1992] and natural systems [*Rasmussen*, 1997] on capillary-dominated immiscible fluid displacement, *Chandler et al.* [1982] and *Wilkinson and Willemsen* [1983] proposed invasion percolation, as opposed to the continuum approach based on Darcy's law, to better honor the mechanics of migration processes occurring under capillary equilibrium conditions. These authors observed that displacements such as secondary oil migration were controlled by the balance between forces exerted by buoyancy and capillarity, which is described by the Young-Laplace equation, relating the capillary pressure, P_c , to the interfacial tension

between fluids, γ , the contact angle, θ , and the meniscus curvature, R , which is proportional to the pore size:

$$P_c = P_{nw} - P_w = 2\gamma\cos\theta/R \quad (1)$$

For practical applications this balance implies that, when the column height of buoyant fluid exceeds the capillary force, fluid will migrate upwards until the next sufficient capillary barrier is encountered. This condition can be described by rearranging equation (1) to estimate a critical column height, h_c :

$$h_c = 2\gamma\cos\theta/\Delta\rho gR \quad (2)$$

Where $\Delta\rho$ is the density difference between the fluids and g is the gravitational constant.

As long as the capillary force is not overcome, fluid will accumulate to build higher buoyant column heights. Eventually, the invading cluster will grow by occupying the neighboring sites with lower capillary resistance until it will span the entire region between the injection face and the outlet face. In the context of this work, the defending fluid, in this case brine, wets the grains surface, while CO_2 , which is the invading fluid, represents the non-wetting phase. The invasion progression is therefore represented by a stepwise drainage cycle occurring along the largest pore throats, due to their least resistance to displacement [Berkowitz and Ewing, 1998; Knackstedt and Paterson, 2009].

If we consider the low migration rates involved with the long-term behavior of CO_2 plume, the application of invasion percolation to geological carbon sequestration is justifiable by the similarity in flow phenomena with secondary oil migration. As a matter of fact, not only these two processes share the dominance of capillary forces, described by low capillary numbers [England *et al.*, 1987; Cavanagh and Haszeldine, 2014], but also a considerable density difference between the invading and defending phases, leading to significant buoyancy forces [Frette *et al.*, 1992; Bryant *et al.*, 2008].

One of the main benefits of IP simulation with respect to Darcy-based solvers is the capability to represent geological heterogeneity with a higher degree of resolution, without compromising on computational time. We take advantage of this by carrying out stochastic simulations through a large number of realizations of the P_{th} field. This approach allows us to

account for the high uncertainty of natural geological heterogeneity by correlating grain size distribution with standard deviation of the P_{th} probability distribution function (PDF). For this purpose, batch simulations including 200 equiprobable realizations of the P_{th} field were carried out to represent the variability of solutions for each scenario considered in this study.

2. Geologic 3D models

The influence of geological heterogeneity on capillary entrapment of non-aqueous non-wetting phases has been widely studied, both numerically and experimentally, in the context of enhanced oil recovery, or EOR [Kortekaas, 1985; Ringrose *et al.*, 1993], contaminant hydrology [Glass *et al.*, 2000; Barth *et al.*, 2003], and geological carbon sequestration, or GCS [Saadatpour *et al.*, 2010; Krevor *et al.*, 2011; Trevisan *et al.*, 2015]. In contrast with the former two fields, which aim at reducing the amount of non-wetting phase in place, the goal of GCS lies in maximizing it, hence the need for understanding the impact of sub-meter scale heterogeneity on long-term storage capacity. Moreover, as opposed to EOR, where flow conditions are often controlled by viscous forces between relatively closely-spaced wells, post-injection stage of GCS is characterized by predominance of capillary forces, which manifest themselves particularly at the boundaries between zones with contrasts in capillary pressure. Consequently, substantial amounts of CO₂ are expected to be trapped by capillary forces in the coarser regions of crossbedded sedimentary structures.

We undertake a numerical investigation on the impact of bedform architecture and capillary pressure heterogeneity on CO₂ trapping by considering sedimentary heterogeneity involving cross stratification at the sub-meter scale. Three type of methods are commonly applied to represent lithological variations in reservoir modeling: structure-imitating, process-imitating, and descriptive [Koltermann and Gorelick, 1996]. The approach adopted in this study falls into the second category; by means of forward modeling sedimentary processes [Rubin and Carter, 2005] we attempt to mimic depositional architectures, focusing on unconsolidated clastic deposits of fluvial origin. Due to the strong influence of small-scale heterogeneity attributable to this type of stratigraphic architecture on capillary trapping of CO₂, these type of reservoirs are often considered valuable when screening for candidates [Gershenzon *et al.*, 2015].

The approach to consider a large spectrum of possible geological models embraces three concepts: (1) different sedimentary processes lead to a variety of *bedform architecture models (BAM)*, (2) each depositional environment can be defined by a unique *facies* with characteristic grain size distribution, (3) the impact of crossbedded stratification on capillary heterogeneity can be inferred by pairing facies with variable *textural contrast* in a series of *matrix-laminae cases*.

2.1. Bedform architecture models (BAM)

With the goal of reproducing various types of bedforms with cross stratification produced by a range of depositional processes, *Rubin* [1987] developed a computer model that generates images of sedimentary structures resembling several types of bedform and provided reference cases in the form of scaled photographs of outcrops. More recently, *Rubin and Carter* [2005] have converted the existing program into an open-source Matlab™ package that simplifies the generation of physically-rational bedforms. Even though the main purpose is to visually interpret sedimentary deposits and depositional environments, Rubin's code has been adopted by a number of authors to investigate the effect of cross-laminated sediments on hydrocarbon recovery [*Cox et al.*, 1994; *Kjongsvik et al.*, 1994; *Ringrose et al.*, 2003; *Nordahl et al.*, 2005; *Ma et al.*, 2008]. For the specific application of this study, which involves three-dimensional IP simulations, *Meckel et al.* [in preparation] implemented the original script from *Rubin and Carter* [2005] with a routine that converts the workspace variables associated with the computer-graphics output into three-dimensional binary volumes (matrix = 0; laminae = 1) that can be used to populate numerical grids.

Among the 62 bedforms illustrated in *Rubin* [1987], we take into account those related to fluvial depositional environments and characterized by sub-meter scale heterogeneity (**Fig. 1**). Also, in order to represent each of the main bedform subsets described by *Rubin and Carter* [2005], we select eight models characterized by different classification criteria, such as dimensionality, variability, and orientation relative to transport (**Table 1**). The first model (# 3 in *Rubin* [1987]) is a structure formed by two-dimensional bedforms climbing vertically. The second model (# 5) represents a structure qualitatively described by tabular sets and 'deposited by two-dimensional bedforms climbing at a stoss-erosional, lee-depositional, net-positive angle of climb'. The third model (# 13) represents a structure formed by 'bedforms climbing at an angle that is fluctuating but always positive'. The fourth model (# 19) represents a structure

qualitatively described by zig-zag bedding features and ‘produced by symmetrical bedforms that migrate back and forth a fraction of the distance of the bedform spacing with no net displacement’. The fifth model (# 27) represents a structure formed by ‘bedforms with superimposed bedforms migrating in the opposite direction’. The sixth model (# 36) represents a structure formed by ‘bedforms with pseudorandom plan-form geometry’. The seventh model (# 42a) represents a structure qualitatively described by trough sets and ‘formed by bedforms with along-crest-migrating in-phase sinuositities’. The eighth model (# 63) represents a structure qualitatively described by rippleform features and ‘formed by reversing, three-dimensional bedforms’. While these descriptors are rigorous, they are observational and process-based, making them entirely suitable for systematic descriptions of geologic materials (e.g. subsurface cores).

Table 1 Bedform classification criteria used in *Rubin and Carter* [2005].

	Planform Shape			Shape and Behavior Through Time		Crest Orientation		
	2D	3D		variable	invariable	transverse	oblique	longitudinal
		sinuous	superimposed					
# 3	X				X			X
# 5	X				X	X	X	
# 13	X			X		X	X	X
# 19	X			X				X
# 27	X			X		X	X	X
# 36		X			X	X		
# 42a		X			X		X	
# 63			X	X		X		

To summarize, the sedimentary models presented in this study allow for representation of different depositional environments by generating patterns of grain size heterogeneity emphasized by finer-grained laminae in a more prevalent coarser-grained matrix. Although grain size variability in natural sedimentary deposits can exhibit a continuum of values [Meckel, 2013], the primary assumption made in this study is that each BAM can be described by the spatial arrangement of two depositional and rigorously descriptive features: matrix and laminae facies. These finer-grained (lower-permeability, higher threshold pressure) laminae are known to influence fluid flow and accumulation arrangements at variable scales [Corbett *et al.*, 1992; Mikes and Bruining, 2006; Gershenzon *et al.*, 2015; Luo *et al.*, 2015]. Models developed here

specifically emphasize these two components, and explore the degree of contrast that could occur between them. A major advantage of these models is their geological realism, making them recognizable and correlated to depositional environments with a rich research history. Other methods that might achieve this are structure-imitating techniques, although models generated with these methods generally consider larger domains equivalent to reservoir-scale, with a focus on spatial inter-relationships of various facies (e.g. point bar, crevasse splay, channel, etc.). Models used here focus on smaller scale features that might exist within each of those depositional lithologies.

Fig. 1 Spatial arrangement of bedding structures for the eight sedimentary models generated with modified Matlab™ script used in this study. The numerical grids (XYZ) consist of 495×400×142 cells, corresponding to (0.99×0.8×0.28) m³.

2.2. Grain size characterization

Threshold capillary pressure, P_{th} , also defined as displacement or entry pressure, is a key parameter controlling the migration pathway of CO₂, especially when flow occurs in the capillary limit [Saadatpoor *et al.*, 2010]. To make our study applicable to actual field settings, we consider a range of values that are expected in unconsolidated clastic reservoirs. Based on textural parameters such as grain size and grain sorting, *Beard and Weyl* [1973] classified 54 artificially mixed unconsolidated sands into eight grain-size subclasses and six sorting groups. Following previous work of *Meckel et al.* [2015], we used this classification to extrapolate realistic P_{th} values and populate each BAM with different degrees of textural contrast between matrix and laminae values, as characterized by the difference in the mean of the distributions used for each.

The grain size is subsequently used to calculate P_{th} (in kPa) using equation 3 from *Berg* [1975]:

$$P_{th} = 16.3 \times \frac{\gamma}{d_{50}} \quad (3)$$

Where 16.3 is a geometric constant that also incorporates unit conversion, γ is interfacial tension in N/m, and d_{50} is median grain diameter, in millimeters. In this study we consider 0.03 N/m for CO₂-H₂O system, representative for reservoirs at approximately 10 MPa and 35 °C [Chiquet *et al.*, 2007].

Each of the facies shown in **Fig. 2** has a lognormal grain size distribution and is described by the median diameter (d_{50}) and the Trask sorting coefficient (S_o). We convert these grain size distributions to analogous capillary threshold pressure distributions as described below.

The Trask sorting coefficient (S_o) is defined as the square root of the ratio of the 25th to the 75th percentile of the cumulative density function of the lognormal distribution:

$$S_o = \sqrt{\frac{d_{25}}{d_{75}}} \quad (4)$$

Where d is grain size in millimeters.

Since the grain sizes are often log normally distributed [Folk, 1966], the logarithm of the grain size (D) will be normally distributed and is given as:

$$D = \log(d) \quad (5)$$

Then, substituting 5 into 4, the Trask sorting coefficient can be re-written as:

$$S_0 = e^{\frac{D_{25}-D_{75}}{2}} \quad (6)$$

For a normal distribution, the quantile function is defined as:

$$D = \mu + \sigma\sqrt{2}\text{erf}^{-1}(1 - 2p) \quad (7)$$

Where μ is the mean, σ is the standard deviation and p is the cumulative probability.

The mean of the normal distribution is given by the logarithm of the median of the lognormal distribution:

$$\mu = \log(d_{50}) \quad (8)$$

Substituting 7 and 8 into 6, we solve for the standard deviation σ of the normal distribution. Then, using the calculated mean and the standard deviation, for cumulative probabilities from 0 to 0.999, we calculate the inverse CDF which gives the values of the normal distribution. Since these are logarithmic values, the antilog gives back the lognormally distributed grain sizes in millimeters. These values are then substituted in equation 3 to obtain log-normally distributed P_{th} values.

The main input parameters for the numerical models are the arithmetic mean ($m.$) and standard deviation ($s.d.$) of the log-normally distributed P_{th} PDF of matrix and laminae values, which are calculated as follows:

$$m. = e^{\left(\mu + \frac{1}{2}\sigma^2\right)} \quad (9)$$

$$s.d. = e^{\left(\mu + \frac{1}{2}\sigma^2\right)} \sqrt{e^{(\sigma^2)} - 1} \quad (10)$$

Where μ is the mean and σ is the standard deviation of P_{th} PDF on a logarithmic scale.

Fig. 2 The library of 54 facies used for assignment of P_{th} values to matrix and laminae in the eight BAMs. Each facies has a specific distribution of grain sizes described by a median value (columns) and sorting category (rows). Sorting is given in terms of Trask coefficient S_o and ϕ scale [Folk and Ward, 1957]. These facies are characteristic of a wide range of clastic depositional processes and environments. For example, very fine grained, well sorted silt reflects upper point bar deposits of fluvial deposits, poorly sorted coarse sand reflects channel thalwegs, and very well sorted medium sand typically occurs in shoreface environments. Permeabilities for these materials range from 471 Darcy (extremely well sorted upper coarse sand, upper left) to 50 mD (very poorly sorted upper coarse silt, lower right) (Beard and Weyl [1973], their Table 6). To illustrate the methodology used for generating different textural contrasts, three cases are shown where MUCSa represents the matrix facies and MUMSa, MUFSa, and MUVFSa are used for the laminae of cases 26, 27, and 28, respectively.

2.3. Lithologic variability

In reservoir characterization, geological heterogeneity is generally measured by coefficients of variation that consider the central tendency of the property of interest (e.g. P_{th}) across the medium. The bimodality of P_{th} distribution, however, represents a key controlling parameter in this study and needs to be reflected in coefficients that are used to predict capillary trapping capacity. To characterize the textural contrast between matrix and laminae for each modeling scenario, we introduce the dimensionless parameter, δ :

$$\delta = \frac{|\mu_1 - \mu_2|}{\sigma} \quad (11)$$

Where μ_1 and μ_2 are the means (on a logarithmic scale) and σ is the standard deviation of P_{th} PDF assigned to of the matrix and lamina, respectively, and σ is the mean standard deviation of P_{th} PDF (also on a logarithmic scale) assigned to the laminae. Since the pairings of matrix and laminae share the same sorting category for all the examples presented here, hence the same standard deviation of the P_{th} PDF, only one σ appears at the denominator of equation 11. As it will be shown in the Discussion section, the δ parameter appears to correlate well with the average model saturation predicted across a large range of different textural contrasts. More importantly, the variables involved in the quantification of δ are directly available from the classification of *Beard and Weyl* [1973] and simple to gather in the field or from a core description. To visually illustrate the influence of different facies combinations on textural contrast between matrix and laminae, **Fig. 3** shows the resulting P_{th} PDFs for the three example cases presented in **Fig. 2**. As mentioned above, with the purpose of representing realistic depositional environments, grain sizes assigned to matrix facies are always coarser than grain sizes assigned to the laminae. Also, an attempt was made to represent a large part of the ensemble of possible combinations by selecting 40 different matrix-laminae cases (**S.I. 1**, **S.I. 2**, and **S.I. 3**). These cases can be grouped in a 5 by 8 matrix, having sorting categories as rows, and textural contrast between matrix (in blue) and laminae (in red) as columns (**S.I. 4**).

As it will be demonstrated in the next sections, the baffle effect exerted by the laminae on the buoyant plume is closely related to the bimodal character of the P_{th} PDF and it manifests itself with different plume distributions across the eight BAMs.

Fig. 3 Three different textural contrasts created by assigning constant P_{th} PDF to matrix (in this case Moderately Sorted Upper Coarse Sand, or MUCSa, in blue) and changing P_{th} PDF of laminae (in this case showing Upper Medium Sand > Upper Fine Sand > Upper Very Fine Sand, from low to high P_{th} , in red). The complete set of 40 cases is available in the supplementary information.

3. Numerical model

Based on seismic observations gathered at the Sleipner storage site [Chadwick *et al.*, 2010] following injection of a large volume of CO₂ in a brine-bearing sedimentary formation, continuous-phase high-saturation plumes can be structurally trapped underneath low permeability baffles in a stacked layer configuration. At the cm-m scale, a hypothetical scenario resembling the one in **Fig. 4** can be approximated to a porous medium underlain by a virtually infinite source zone of CO₂. An analog approach for representing such boundary condition has been previously adopted in numerical simulations of CO₂ migration dominated by capillarity and buoyancy [Bryant *et al.*, 2008; Saadatpoor *et al.*, 2010; Ren *et al.*, 2015]. In a similar fashion, we found our numerical model on the assumption that, during post-injection, pressure gradients have dissipated and the migration of CO₂ is mainly controlled by 1) the density difference between the two phases and 2) the spatial arrangement of facies with contrasting P_{th} within the reservoir.

The IP simulations are carried out with Permedia™'s Static Migration model, which despite its original scope of capturing the transport processes of secondary oil migration, has been recently proved capable of matching certain aspects of CO₂ migration [Cavanagh and

Haszeldine, 2014]. Permedia is a commercial simulator that utilizes a gravity destabilized macroscopic IP modeling scheme. Traditional IP algorithms model pore scale fluid displacement processes where drainage and imbibition can be modeled as bond and site percolation, respectively. Permedia utilizes a macroscopic approach [Kueper and McWhorter, 1992; Ioannidis et al., 1996; Glass and Yarrington, 2003; Yang et al., 2013], where the lattice sites/cells are considered to be a macroscopic block with averaged capillary entry pressures instead of as a single pore. Permedia accounts for buoyancy thereby allowing the formulation of gravity destabilized flow scenarios. Commonly used IP models that account for gravity do so by implementing a simple vertical gradient proportional to the height of the cell above the base layer [Meakin et al., 1992]. This is based on the assumption that the invading phase forms a continuous and connected path across the domain. Since this does not accurately represent the physics and actually the invading phase undergoes fragmentation, in Permedia the buoyancy pressure is calculated dynamically from the top of the connected/active cluster [Carruthers, 1998]. These connected clusters formed due to backfilling at capillary barriers are called ‘accumulations’. The rest of the plume consists of stringers that are classified as ‘migration pathways’. Permedia also allows bicontinua of fluids to occupy each grid block. However, unlike other IP models which use the P_c - S curve to determine the saturation at each cell [Kueper and McWhorter, 1992], in Permedia the cells that form the accumulation are assigned non-wetting phase saturation equal to $1-S_{wc}$ (connate water saturation) and the migration pathways are assigned critical/residual non-wetting saturation. Fragmentation due to capillary forces is implemented by assuming that snap-off occurs in migration pathways where the oil saturation is just enough to form a spanning cluster. Snap-off occurs when the pore to throat size ratio is small i.e. when low entry pressure cells are surrounded by high entry pressure cells [Carruthers, 1998]. As such, the specific simulator used is not dissimilar from many modified IP simulators.

Fig. 4 Problem conceptualization of the invasion percolation approach. Seismic image of the Sleipner CO₂ plume (left) shows accumulation of CO₂ at high saturations underneath shale layers, which can be simplified to a planar source boundary condition underneath a porous medium at the mesoscale (cm-m).

Prior to carrying out IP simulations, a representative elementary volume (REV) with dimensions of $(0.202 \times 0.202 \times 0.202) \text{ m}^3$ is extracted from the center of each BAM. The methodology followed used to identify the size of the REV combined the approach followed by *Bear* [1972] and *Nordahl and Ringrose* [2008] and is described with more detail in Appendix A. To exemplify the implementation of lithologic variability into the BAM, **Fig. 5** shows one realization of the P_{th} field applied to four of the eight REV considered in this study after being populated with values representative of matrix-laminae case 28 (MUCSa-MUVFSa). Although it is worth nothing that the laminae are very thin (1-3 gridblocks) compared to the bulk thickness of the cross-bedded model (101 gridblocks), we expect that the amount of trapped CO₂ within the laminae will be minimal. In fact, once the average threshold pressure of a lamina is reached by the non-wetting phase pressure building up underneath it, the plume will have enough energy to penetrate and quickly reach the overlying coarser zone (matrix). In other words, the large part of plume trapping is likely to be achieved as a result of the backfilling process within the matrix.

Regarding the variability of threshold pressure distribution within matrix and laminae, no specific correlation structure was applied, although a different seed of the random number generator was automatically assigned to each of the 200 realizations to convert the user-specified PDFs into cell attributes. The numerical grid consists of approximately one million cells with dimensions of $(2 \times 2 \times 2) \text{ mm}^3$, which are analogous to the measurement scale of a probe-permeameter device [*Nordahl et al.*, 2005] and are consistent with the scale at which P_{th} values

are accounted for. Closed boundary conditions are applied to all the faces of the numerical domain. To recreate an infinite source of CO₂ at the bottom of the REV, we apply an injection volume 69x larger than the pore volume (1.65 L, assuming constant porosity of 0.2). Despite the volumetric constrain of the source, however, we disregard any CO₂ volume calculation and emphasize the final distribution of the plume, which will be evaluated in terms of cells invaded at percolation normalized by the total number of cells:

$$\langle S_{CO_2} \rangle = \frac{\text{cells invaded}}{\text{total cells}} \quad (12)$$

Fig. 5 Representative Elementary Volumes for four (of eight total) BAMs after being populated with P_{th} values sampled from PDF of case 28 (MUCSa-MUVFSa).

As suggested by Oldenburg *et al.* [2015], the spatial discretization of the model represents the characteristic length over which the displacing phase front advances sequentially.

Consequently, the interplay of buoyancy and capillary forces can be quantified by means of the Bond number:

$$Bo = \frac{\Delta\rho g r^2}{\gamma} \quad (13)$$

Where $\Delta\rho$ is the density difference between the two phases, g is the gravitational constant, r is the characteristic length, and γ is the surface tension between the two phases. After applying values in agreement with those measured at reservoir conditions by *Chiquet et al.* [2007] ($\Delta\rho=300 \text{ kg/m}^3$, $\gamma=0.03 \text{ N/m}$) and average grain diameters from the 40 lithologic variability scenarios we obtain Bond numbers between 2.3×10^{-4} and 6.9×10^{-2} . Such range defines the intersection of flow regimes representative of invasion percolation and CO_2 sequestration, according to *Cinar and Riaz* [2014].

The stochastic nature of geological heterogeneity requires IP simulations to be carried out across a range of P_{th} fields for each textural contrast scenario. The small computational burden of this modelling approach allows doing so by random sampling the P_{th} PDF and creating 200 equiprobable P_{th} realizations. On the one hand, this methodology permits a quick assessment of the average storage capacity at the REV scale from the knowledge of textural contrast between matrix and laminae facies. On the other hand, the uncertainty of model predictions can be quantified by evaluating the standard deviation of simulation results.

To exemplify the impact of threshold pressure heterogeneity on plume migration, IP simulation results in **Fig. 6** show CO_2 distribution at percolation for one P_{th} field realization (random seed=1234) and three different textural contrasts applied to BAM #5. Despite the lack of time-dependence of the IP method, invasion sequences such as the ones presented in **Fig. 6** can give insights into the predominant processes controlling CO_2 distribution within the porous medium, such as migration via low-saturation stringers or trap backfilling at higher saturation.

Although limited to three cases, **Fig. 6** illustrates the influence of P_{th} PDF overlap (**Fig. 3**) on the magnitude of the baffle effect exerted by the laminae over the final CO_2 distribution. As one can expect by intuition, more local capillary trapping will distinguish cases with more separation between P_{th} PDFs of matrix and laminae (e.g. case 28). As opposed to the high saturation due to this backfilling behavior, when the overlap between the two PDFs increases (e.g. case 26), the laminae P_{th} distribution will lose correlation and the plume will favor a

stringer-like migration. As a matter of fact, this is the overall trend emerging from IP simulations carried out across a large number of textural contrast combinations. However, as we report in **Fig. 7**, the relationship between average model saturation and textural contrast parameter δ is nonlinear and affected by the spatial arrangement of the laminae.

Fig. 6 P_{th} fields of matrix and laminae lithofacies populated following the corresponding PDF shown in **Fig. 3**. The increasing textural contrast represented by δ leads to different responses in terms of displacement patterns and plume trapping as can be observed from invasion sequences of CO_2 across BAM #5 (dark blue and dark red colors represent early and late invasion, respectively, while the same color scale used in **Fig. 5** is used to denote P_{th} field in the background).

4. Discussion

Following a systematic approach accounting for a wide range of textural contrasts we assessed the hypothesis that the fraction of rock invaded by CO_2 at percolation is correlated with the P_{th} contrast between matrix and laminae and with the geometry of the sedimentary model. We believe that this approach can lead to more accurate predictive estimates of storage capacity in sedimentary formations with respect to other estimation methods based on static assumptions. The contrast is defined by the parameter introduced in equation 11, which is calculated for the 40 cases mentioned earlier. We are aware of the fact that some extreme cases are geologically

unlikely, especially the ones involving laminae with extremely poor grain sorting, which translate into questionably large variances. Also, in some cases, $\delta > 50$ may be unreasonable from a depositional process perspective. For the sake of completeness and to explore fundamental aspects, however, we included in our analysis a range of contrasts that in some cases may exceed the limits of reality. **Fig. 7** shows the correlation between percentage of model invaded by the plume and the parameter δ , plotted against the average model saturation predicted by equation 14.

$$\langle S_{CO_2} \rangle(\delta) = C_4 + \frac{C_1 - C_4}{1 + \left(\frac{\delta}{C_3}\right)^{C_2}} \quad (14)$$

The nonlinearity of the correlation seems to be well captured by the 4-parameter regression model that constrain the minimum and maximum asymptotes with coefficients C_1 and C_4 , respectively. While coefficient C_1 has no role in differentiating the eight BAMs, the maximum average model saturation represented by coefficient C_4 shows higher variability and a strong dependence on the depositional architecture of the geological model. Interestingly, the influence of each architecture is manifested at textural contrasts denoted by $\delta > 3$, which can be related to differences in median grain sizes between matrix and laminae ranging from about 0.4 mm (e.g. between EWUCSa and EWUMSa) to about 0.7 mm (e.g. between PUCSa and PUMSa). Similar contrast in grain size have been observed by *Meckel* [2013] in sedimentary relief-peels from fluvial depositional environments.

Given the strong anisotropy of the medium, we can expect considerably different saturation trends if the CO_2 flow direction is parallel or sub-parallel to the laminae. However, we consider that a sub-horizontal orientation of the sedimentary model represents the most common scenario encountered in the subsurface to include in our simulations.

Fig. 7 Influence of P_{th} contrast between matrix and laminae on average model saturation (expressed as percentage of cells invaded by CO_2 plume).

Overall, the predictions of the non-linear parametric model indicate a satisfactory fit with the average number of cells invaded by the plume calculated from 200 realizations for each matrix-laminae case, leading to coefficients of determination between 0.9288 and 0.978 (**Table 2**). Regardless of the metric used to characterize the statistical distance between PDFs of matrix and laminae, this study aims at identifying trends in trapped CO_2 volumes as a function of textural contrast and bedform architecture.

As it can be observed from **Fig. 7**, average numerical results represented by dots follow a scattered distribution, especially at high textural contrasts between matrix and laminae. In an attempt to understand this poorly constrained behavior, we analyze the effect of P_{th} PDF on the percentage of cells invaded by the plume by breaking down the results into each grain sorting category (**Fig. 8**). The resulting plots representative of BAM #5 and #63 shows how each sorting category affects the distribution of the results along the x-axis, where higher standard deviations (e.g. Poorly Sorted) constrain the results to lower contrast values. Remarkably, the Extremely

Well Sorted category follows a trend that is quite separated from the rest of the data. This tendency suggests that 1) the parameter δ does not integrate all the factors affecting the average model saturation over the entire range of textural contrast, and 2) the scarce overlap between matrix and laminae P_{th} PDF due to small standard deviations generates saturation trends that do not reach stable plateaus within realistic textural contrasts.

Fig. 8 Average model saturation results for two BAMs #5 showing different trends corresponding to each sorting category.

Table 2 Fitting parameters for the regression model and coefficient of determination for each bedform model. R^2 values are estimated using mean square errors between regression model and average IP simulation results, represented by points in **Fig. 7**.

	Min. saturation asymptote, C_1	Slope factor, C_2	Inflection point, C_3	Max. saturation asymptote, C_4	Coefficient of determination, R^2
# 3	3.23	5.11	3.49	72.43	0.97
# 5	2.88	4.04	2.69	51.84	0.92
# 13	3.25	3.71	2.82	57.75	0.94
# 19	3.03	5.12	3.51	48.68	0.96
# 27	3.07	3.62	2.69	36.15	0.90
# 36	2.48	4.37	2.71	36.08	0.88
# 42a	2.74	4.17	3.08	68.59	0.97
# 63	2.72	4.05	3.02	69.53	0.98

5. Concluding remarks

The ability to anticipate fluid saturations resulting from buoyant flow in heterogeneous clastic materials has been greatly advanced through this research. It is clear that the contrast in average grain size between matrix and laminae (overall degree of lithologic heterogeneity) can have a profound influence on CO₂ saturation. The range of saturation from a homogenous sand (low matrix-laminae P_{th} contrast; $\delta < 3$) to a similar architecture but with large contrast ($\delta > 20$) could be as much as 30 or 40%. Sedimentary descriptors such as grain size and bedform architecture can be related to depositional environments, which are typically inferred from well log (Gamma, SP) motifs in the subsurface. The presented work is an effort to understand the influence of bedform-scale (cm-to-m) heterogeneity on CO₂ saturation in geological reservoirs experiencing buoyant fluid flow. By means of IP simulations through three-dimensional sedimentary models we considered a range of possible textural contrasts with the goal of detecting trends in trapping behavior. Ultimately, the fraction of trapped CO₂ plume is revealed to be controlled by both sedimentary architecture and P_{th} contrast between matrix and laminae. We suggest that anticipated saturations of candidate reservoirs can be constrained using diagnostic descriptive sedimentology criteria related to interpreted depositional environments.

These saturation results have significant implications for two topics of great importance for CCS: 1) CO₂ storage capacity assessment, 2) subsurface seismic imaging.

Van der Meer [1992] recognized that the CO₂ storage process is “affected by many individual mechanisms: fluid properties at reservoir conditions, specific conditions of the rock matrix and depositional environment of the geological formation”. Further, he noted that mobility aspects would reduce the pore volume accessed by the CO₂, a concept termed *theoretical effective pore volume* and eventually codified as *storage efficiency* (typically represented as ‘E’). In his early work, *Van der Meer* [1992] assumed that perhaps 2% of the total pore volume would be accessed by the CO₂, although the determination of that factor was informal until *Van der Meer* [1995] formalized it. This concept of storage efficiency has been arguably the most debated aspect of storage capacity assessment since then. These early concepts are reflected in the early capacity work in both Canada [*Bachu et al.*, 1994], USA [*Bergman and Winter*, 1995], and in every regional storage capacity atlas developed since (where E is typically quite low). The saturations we present for small-scale heterogeneous models are not appropriate

for applying to regional assessments (too much lithologic heterogeneity at coarse stratigraphic scales), but are likely to be useful for understanding reservoir-scale performance. Small scale heterogeneity may elevate saturation well above 5%, and is likely to be instrumental in limiting long-term migration.

Seismic imaging has been demonstrated to be a useful tool for documenting and understanding fluid flow in CO₂ injections associated with carbon capture and storage (i.e. Sleipner, Snohvit, In Salah, Weyburn, Frio, Cranfield, Decatur). The seismic response (e.g. Gassman fluid substitution) is well described for idealized models of saturation. We believe there is an inherent limitation in the theoretical approaches, in that they do not incorporate realistic saturation distributions [Behzadi *et al.*, 2011], such as those illustrated here. This is primarily because the non-idealized and realistic saturation distributions do not lend themselves to theoretical solutions. A recognition of this limitation by the seismic research community has led to a number of theoretical patchy saturation models [White, 1975] to improve conformance with field data, yet they remain theoretical. It is suggested that a more complete understanding of seismic response will result from investigating low saturations with realistic 3D distributions. The focus on realistic saturations is important because any undesired migration of CO₂ out of an injection interval is likely to manifest in a range of saturations dependent on lithology and depositional environment. It is suggested that the use of large (multi-meter scale) models at high resolution with realistic saturations may allow forward seismic modeling to better constrain anticipated subsurface seismic response.

Acknowledgements

This work was supported entirely by the Center for Frontiers of Subsurface Energy Security, an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Basic Energy Sciences under Award # DE-SC0001114.

6. Appendix A

Prior to charging the porous medium with CO₂ through IP simulations, we evaluated spatial scale effects on variation of heterogeneity in order to determine the appropriate representative elementary volume (REV) for the numerical domain. The purpose of this analysis is twofold: 1) to save computational time by selecting models with efficient grid sizes and 2) to

relate average storage capacity predictions with grid block volumes that can be considered for a future upscaling study. The property of the medium we target for REV identification is the matrix to laminae ratio, which is analogous to the net-to-gross sand/shale ratio [Flett *et al.*, 2007] and merely represents the volumetric fraction of flow baffles within each BAM. As previously pointed out by other authors [Ma *et al.*, 2008], we consider this property to significantly affect the overall distribution of CO₂ under quasi-static buoyant flow. However, we also recognize the important role played by the geometrical arrangement of each BAM, as manifested by the range in maximum CO₂ saturation, once exceeded a certain textural contrast between matrix and laminae.

To calculate the matrix to laminae ratio for each BAM illustrated in **Fig. 1**, cubic subsets with progressively larger dimensions are extracted from the center of the full size 495×142×400 cells model and plotted as a function of sample volume. Data presented in **Fig. 9** show a common behavior converging towards constant plateaus, indicating $8.24 \times 10^{-3} \text{ m}^3$ as a potential effective medium volume for approximating matrix to lamina ratio heterogeneity at larger scales. For the BAMs involved in this study, matrix to lamina ratios range between 0.81 and 0.94 for # 27 and # 3, respectively. Remarkably, we found no direct correlation between this metric and the plateau values (parameter D in equation 14) exhibited by the numerical results shown in **Fig. 7**, suggesting a more complex relationship between geometric arrangement of laminae and average model saturations achieved by IP simulations.

Fig. 9 Matrix to laminae ratio as a function of sample volume. Each sample volume corresponds to a cubic subset extracted from the middle of the full size BAM.

References

- Altman, S. J., et al. (2014), Chemical and Hydrodynamic Mechanisms for Long-Term Geological Carbon Storage, *J Phys Chem C*, 118(28), 15103-15113.
- Bachu, S., W. D. Gunter, and E. H. Perkins (1994), Aquifer Disposal of CO₂: Hydrodynamic and Mineral Trapping, *Energy Convers Manage*, 35(4), 269-279.
- Barth, G. R., T. H. Illangasekare, and H. Rajaram (2003), The effect of entrapped nonaqueous phase liquids on tracer transport in heterogeneous porous media: laboratory experiments at the intermediate scale, *J Contam Hydrol*, 67(1-4), 247-268.
- Bear, J. (1972), *Dynamics of fluids in porous media*, xvii, 764 p. pp., American Elsevier Pub. Co., New York.
- Beard, D. C., and P. K. Weyl (1973), Influence of Texture on Porosity and Permeability of Unconsolidated Sand, *Am Assoc Petr Geol B*, 57(2), 349-369.
- Behzadi, H., V. Alvarado, and S. Mallick (2011), CO₂ saturation, distribution and seismic response in two-dimensional permeability model, *Environ Sci Technol*, 45(21), 9435-9441.
- Behzadi, H., V. Alvarado, and R. Lynds (2012), Modeling CO₂ saturation distribution in eolian systems, *International Journal of Greenhouse Gas Control*, 11, 110-116.

- Berg, R. R. (1975), Capillary Pressures in Stratigraphic Traps, *Aapg Bulletin-American Association of Petroleum Geologists*, 59(6), 939-956.
- Bergman, P. D., and E. M. Winter (1995), Disposal of Carbon-Dioxide in Aquifers in the Us, *Energ Convers Manage*, 36(6-9), 523-526.
- Berkowitz, B., and R. P. Ewing (1998), Percolation theory and network modeling applications in soil physics, *Surv Geophys*, 19(1), 23-72.
- Boggs, S. (2012), *Principles of sedimentology and stratigraphy*, 5th ed., xiii, 585 p. pp., Pearson Prentice Hall, Upper Saddle River, N.J.
- Bryant, S. L., S. Lakshminarasimhan, and G. A. Pope (2008), Buoyancy-Dominated Multiphase Flow and Its Effect on Geological Sequestration of CO₂, *Spe J.*, 13(4), 447-454.
- Carruthers, D. (1998), Transport modelling of secondary oil migration using gradient-driven invasion percolation techniques, 210 pp, Heriot-Watt University.
- Carruthers, D. (2003), Modeling of Secondary Petroleum Migration Using Invasion Percolation Techniques, in *Multidimensional Basin Modeling*, edited by S. D. a. R. Marzi, pp. 21-37, AAPG/Datapages Discovery Series.
- Carruthers, D., and P. Ringrose (1998), Secondary oil migration: oil-rock contact volumes, flow behaviour and rates, *Geological Society, London, Special Publications*, 144(1), 205-220.
- Catalan, L., X. W. Fu, I. Chatzis, and F. A. L. Dullien (1992), An Experimental-Study of Secondary Oil Migration, *Aapg Bulletin-American Association of Petroleum Geologists*, 76(5), 638-650.
- Cavanagh, A. J., and R. S. Haszeldine (2014), The Sleipner storage site: Capillary flow modeling of a layered CO₂ plume requires fractured shale barriers within the Utsira Formation, *International Journal of Greenhouse Gas Control*, 21, 101-112.
- Celia, M. A., and J. M. Nordbotten (2009), Practical modeling approaches for geological storage of carbon dioxide, *Ground Water*, 47(5), 627-638.
- Chadwick, A., et al. (2010), Quantitative analysis of time-lapse seismic monitoring data at the Sleipner storage operation, *The Leading Edge*, 29(2), 170-177.
- Chandler, R., J. Koplik, K. Lerman, and J. F. Willemsen (1982), Capillary Displacement and Percolation in Porous-Media, *J Fluid Mech*, 119(Jun), 249-267.
- Chiquet, P., J. L. Daridon, D. Broseta, and S. Thibeau (2007), CO₂/water interfacial tensions under pressure and temperature conditions of CO₂ geological storage, *Energ Convers Manage*, 48(3), 736-744.
- Choi, J.-H., Y. Seol, R. Boswell, and R. Juanes (2011), X-ray computed-tomography imaging of gas migration in water-saturated sediments: From capillary invasion to conduit opening, *Geophys Res Lett*, 38(17).

Cinar, Y., and A. Riaz (2014), Carbon dioxide sequestration in saline formations: Part 2-Review of multiphase flow modeling, *J Petrol Sci Eng*, 124, 381-398.

Corbett, P. W. M., P. S. Ringrose, J. L. Jensen, and K. S. Sorbie (1992), Laminated Clastic Reservoirs: The Interplay of Capillary Pressure and Sedimentary Architecture, in *SPE Annual Technical Conference and Exhibition*, edited, Society of Petroleum Engineers, Washington, D.C.

Corradi, A., P. Ruffo, A. Corrao, and C. Visentin (2009), 3D hydrocarbon migration by percolation technique in an alternate sand–shale environment described by a seismic facies classified volume, *Mar Petrol Geol*, 26(4), 495-503.

Cox, D. L., S. J. Lindquist, C. L. Bargas, K. G. Havholm, and R. M. Srivastava (1994), Integrated Modeling for Optimum Management of a Giant Gas Condensate Reservoir, Jurassic Eolian Nugget Sandstone, Anschutz Ranch East Field, Utah Overthrust (U.S.A.), in *Stochastic Modeling and Geostatistics*, edited by J. M. Y. a. R. L. Chambers, pp. 287-321, AAPG Comput. Appl. Geol.

Dembicki, H., and M. J. Anderson (1989), Secondary Migration of Oil - Experiments Supporting Efficient Movement of Separate, Buoyant Oil Phase Along Limited Conduits, *Aapg Bulletin-American Association of Petroleum Geologists*, 73(8), 1018-1021.

England, W. A., A. S. Mackenzie, D. M. Mann, and T. M. Quigley (1987), The Movement and Entrapment of Petroleum Fluids in the Subsurface, *J Geol Soc London*, 144, 327-347.

Flett, M., R. Gurton, and G. Weir (2007), Heterogeneous saline formations for carbon dioxide disposal: Impact of varying heterogeneity on containment and trapping, *J Petrol Sci Eng*, 57(1-2), 106-118.

Folk, R. L. (1966), A Review of Grain-Size Parameters, *Sedimentology*, 6(2), 73-93.

Folk, R. L., and W. C. Ward (1957), Brazos River Bar: a study in the significance of grain size parameters, *Journal of sedimentary petrology*, 27(1), 3-26.

Frette, V., J. Feder, T. Jossang, and P. Meakin (1992), Buoyancy-Driven Fluid Migration in Porous-Media, *Phys Rev Lett*, 68(21), 3164-3167.

Gasda, S. E., H. M. Nilsen, and H. K. Dahle (2013), Impact of structural heterogeneity on upscaled models for large-scale CO₂ migration and trapping in saline aquifers, *Adv Water Resour*, 62, 520-532.

Gershenson, N. I., R. W. Ritzi, D. F. Dominic, M. Soltanian, E. Mehnert, and R. T. Okwen (2015), Influence of small-scale fluvial architecture on CO₂ trapping processes in deep brine reservoirs, *Water Resour Res*, 51(10), 8240-8256.

Glass, R. J., and L. Yarrington (1996), Simulation of gravity fingering in porous media using a modified invasion percolation model, *Geoderma*, 70(2-4), 231-252.

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

Glass, R. J., S. H. Conrad, and W. Peplinski (2000), Gravity-destabilized nonwetting phase invasion in macroheterogeneous porous media: Experimental observations of invasion dynamics and scale analysis, *Water Resour Res*, 36(11), 3121-3137.

Graue, A. (1994), Imaging the Effects of Capillary Heterogeneities on Local Saturation Development in Long Corefloods, *SPE Drilling & Completion*, 9(01), 57-64.

Green, C. P., and J. Ennis-King (2010), Effect of Vertical Heterogeneity on Long-Term Migration of CO₂ in Saline Formations, *Transp. Porous Media*, 82(1), 31-47.

Green, C. P., and J. Ennis-King (2013), Residual Trapping Beneath Impermeable Barriers During Buoyant Migration of CO₂, *Transp. Porous Media*, 98(3), 505-524.

Green, C. P., and J. Ennis-King (2015), Estimating Breakthrough Time During Buoyant Migration of CO₂ in a Reservoir Containing Impermeable Barriers, *Transp. Porous Media*, 107(1), 281-298.

Hartkamp-Bakker, C. A. (1991), Capillary Oil Entrapment in Crossbedded Sedimentary Structures of Fluvial Sandstone Reservoirs, in *66th Annual Technical Conference and Exhibition of the Society of Petroleum Engineers*, edited, Society of Petroleum Engineers, Dallas, TX.

Hesse, M. A., and A. W. Woods (2010), Buoyant dispersal of CO₂ during geological storage, *Geophys Res Lett*, 37.

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

Jung, B., G. Garven, and J. R. Boles (2014), Effects of episodic fluid flow on hydrocarbon migration in the Newport-Inglewood Fault Zone, Southern California, *Geofluids*, 14(2), 234-250.

Kjonsvik, D., J. Doyle, and T. Jacobsen (1994), The Effects Of Sedimentary Heterogeneities On Production From A Shallow Marine Reservoir - What Really Matters?, in *SPE Annual Technical Conference and Exhibition*, edited, Society of Petroleum Engineers, New Orleans, Louisiana.

Knackstedt, M. A., and L. Paterson (2009), Invasion Percolation, in *Encyclopedia of Complexity and Systems Science*, edited by A. R. Meyers, pp. 4947-4960, Springer New York, New York, NY.

Koltermann, C. E., and S. M. Gorelick (1996), Heterogeneity in sedimentary deposits: A review of structure-imitating, process-imitating, and descriptive approaches, *Water Resour Res*, 32(9), 2617-2658.

- Kortekaas, T. F. M. (1985), Water/Oil Displacement Characteristics in Crossbedded Reservoir Zones, *Soc Petrol Eng J*, 25(06), 917-926.
- Krevor, S. C. M., R. Pini, B. X. Li, and S. M. Benson (2011), Capillary heterogeneity trapping of CO₂ in a sandstone rock at reservoir conditions, *Geophys Res Lett*, 38.
- Kueper, B. H., and D. B. McWhorter (1992), The use of macroscopic percolation theory to construct large-scale capillary pressure curves, *Water Resour Res*, 28(9), 2425-2436.
- Kuo, C. W., and S. M. Benson (2015), Numerical and analytical study of effects of small scale heterogeneity on CO₂/brine multiphase flow system in horizontal corefloods, *Adv Water Resour*, 79, 1-17.
- Lenormand, R., E. Touboul, and C. Zarcone (1988), Numerical-Models and Experiments on Immiscible Displacements in Porous-Media, *J Fluid Mech*, 189, 165-187.
- Li, B. X., and S. M. Benson (2015), Influence of small-scale heterogeneity on upward CO₂ plume migration in storage aquifers, *Adv Water Resour*, 83, 389-404.
- Luo, X. R., J. Yu, L. P. Zhang, Y. Yang, R. Y. Chen, Z. K. Chen, and B. Zhou (2007), Numerical modeling of secondary migration and its applications to Chang-6 member of Yanchang Formation (Upper Triassic), Longdong area, Ordos Basin, China, *Sci China Ser D*, 50(2), 91-102.
- Luo, X. R., F. Zhang, S. Miao, W. Wang, Y. Huang, B. Zhou, D. Loggia, and G. Vasseur (2004), Experimental verification of oil saturation and losses during secondary migration, *Journal of Petroleum Geology*, 27(3), 241-251.
- Luo, X. R., C. Z. Hu, Z. Y. Xiao, J. Zhao, B. S. Zhang, W. Yang, H. Zhao, F. Y. Zhao, Y. H. Lei, and L. K. Zhang (2015), Effects of carrier bed heterogeneity on hydrocarbon migration, *Mar Petrol Geol*, 68, 120-131.
- Ma, J. S., G. D. Couples, and A. R. Gardiner (2008), Numerical modeling of the fluid flow impact of thin baffle laminae in cross bedding, *Water Resour Res*, 44(4).
- Meakin, P., J. Feder, V. Frette, and T. Jo (1992), Invasion percolation in a destabilizing gradient, *Phys Rev A*, 46(6), 3357.
- Meakin, P., G. Wagner, A. Vedvik, H. Amundsen, J. Feder, and T. Jøssang (2000), Invasion percolation and secondary migration: experiments and simulations, *Mar Petrol Geol*, 17(7), 777-795.
- Meckel, T. A. (2013), Digital Rendering of Sedimentary-Relief Peels: Implications for Clastic Facies Characterization and Fluid Flow, *J Sediment Res*, 83(5-6), 495-501.
- Meckel, T. A., S. L. Bryant, and P. R. Ganesh (2015), Characterization and prediction of CO₂ saturation resulting from modeling buoyant fluid migration in 2D heterogeneous geologic fabrics, *International Journal of Greenhouse Gas Control*, 34, 85-96.

Meckel, T. A., P. G. Krishnamurthy, and L. Trevisan (in review), A method to generate small-scale, high-resolution 3D sedimentary bedform architecture models representing realistic geologic facies.

Mikes, D., and J. Bruining (2006), Standard flow cells to incorporate small-scale heterogeneity (crossbedding) in a reservoir model, *Mar Petrol Geol*, 23(9-10), 979-993.

Mouche, E., M. Hayek, and C. Mügler (2010), Upscaling of CO₂ vertical migration through a periodic layered porous medium: The capillary-free and capillary-dominant cases, *Adv Water Resour*, 33(9), 1164-1175.

Neufeld, J. A., and H. E. Huppert (2009), Modelling carbon dioxide sequestration in layered strata, *J Fluid Mech*, 625, 353-370.

Nordahl, K., and P. S. Ringrose (2008), Identifying the Representative Elementary Volume for permeability in heterolithic deposits using numerical rock models, *Math Geosci*, 40(7), 753-771.

Nordahl, K., P. S. Ringrose, and R. J. Wen (2005), Petrophysical characterization of a heterolithic tidal reservoir interval using a process-based modelling tool, *Petrol Geosci*, 11(1), 17-28.

Oldenburg, C. M., S. Mukhopadhyay, and A. Cihan (2015), On the use of Darcy's law and invasion-percolation approaches for modeling large-scale geologic carbon sequestration, *Greenhouse Gases: Science and Technology*, 6(1), 19-33.

Pickup, G. E., and C. Y. Hern (2002), The development of appropriate upscaling procedures, *Transp. Porous Media*, 46(2-3), 119-138.

Pickup, G. E., P. S. Ringrose, J. L. Jensen, and K. S. Sorbie (1994), Permeability tensors for sedimentary structures, *Math Geol*, 26(2), 227-250.

Polak, S., Y. Cinar, T. Holt, and O. Torsaeter (2015), Use of low- and high-IFT fluid systems in experimental and numerical modelling of systems that mimic CO₂ storage in deep saline formations, *J Petrol Sci Eng*, 129, 97-109.

Rabinovich, A., K. Itthisawatpan, and L. J. Durlofsky (2015), Upscaling of CO₂ injection into brine with capillary heterogeneity effects, *J Petrol Sci Eng*, 134, 60-75.

Rasmussen, B. (1997), Fluorescent growth bands in irradiated-bitumen nodules: Evidence of episodic hydrocarbon migration, *Aapg Bulletin-American Association of Petroleum Geologists*, 81(1), 17-25.

Ren, B., S. L. Bryant, and L. W. Lake (2015), Quantifying Local Capillary Trapping Storage Capacity Using Geologic Criteria, in *Carbon Management Technology Conference*, edited, Sugar Land, Texas.

Riaz, A., and Y. Cinar (2014), Carbon dioxide sequestration in saline formations: Part I-Review of the modeling of solubility trapping, *J Petrol Sci Eng*, 124, 367-380.

Ringrose, P. S., and P. W. M. Corbett (1994), Controls on two-phase fluid flow in heterogeneous sandstones, *Geological Society, London, Special Publications*, 78(1), 141-150.

Ringrose, P. S., E. Skjetne, and C. Elfenbein (2003), Permeability Estimation Functions Based on Forward Modeling of Sedimentary Heterogeneity, in *SPE Annual Technical Conference and Exhibition*, edited, Denver, Colorado.

Ringrose, P. S., A. W. Martinus, and J. Alvestad (2008), Multiscale geological reservoir modelling in practice, *Geological Society, London, Special Publications*, 309(1), 123-134.

Ringrose, P. S., K. S. Sorbie, P. W. M. Corbett, and J. L. Jensen (1993), Immiscible flow behaviour in laminated and cross-bedded sandstones, *J Petrol Sci Eng*, 9(2), 103-124.

Rubin, D. M. (1987), Cross-bedding, bedforms, and paleocurrents, in *Society of Economic Paleontologists and Mineralogists*, edited, p. 187, Concepts in Sedimentology and Paleontology.

Rubin, D. M., and C. L. Carter (2005), Bedforms and Cross-Bedding in Animation, U.S. Geological Survey.

Saadatpoor, E., S. L. Bryant, and K. Sepehrnoori (2010), New Trapping Mechanism in Carbon Sequestration, *Transp. Porous Media*, 82(1), 3-17.

Siddiqui, F. I., and L. W. Lake (1992), A dynamic theory of hydrocarbon migration, *Math Geol*, 24(3), 305-327.

Sylta, Ø. (1993), New techniques and their applications in the analysis of secondary migration, paper presented at Basin modelling: advances and applications: proceedings of the Norwegian Petroleum Society conference, 13-15 March 1991, Stavanger, Norway/edited by AG Doré et al. Dokumentet er del av serien Special publication (Norsk petroleumssforening).

Sylta, Ø., J. I. Pedersen, and M. Hamborg (1998), On the vertical and lateral distribution of hydrocarbon migration velocities during secondary migration, *Geological Society, London, Special Publications*, 144(1), 221-232.

Thomas, M. M., and J. A. Clouse (1995), Scaled Physical Model of Secondary Oil Migration, *Aapg Bulletin-American Association of Petroleum Geologists*, 79(1), 19-29.

Toussaint, R., K. J. Måløy, Y. Méheust, G. Løvoll, M. Jankov, G. Schäfer, and J. Schmittbuhl (2012), Two-Phase Flow: Structure, Upscaling, and Consequences for Macroscopic Transport Properties, *Vadose Zone J*, 11(3).

Trevisan, L., R. Pini, A. Cihan, J. T. Birkholzer, Q. Zhou, and T. H. Illangasekare (2015), Experimental analysis of spatial correlation effects on capillary trapping of supercritical CO₂ at the intermediate laboratory scale in heterogeneous porous media, *Water Resour Res*, 51(11), 8791-8805.

Van der Meer, L. G. H. (1992), Investigations Regarding the Storage of Carbon-Dioxide in Aquifers in the Netherlands, *Energ Convers Manage*, 33(5-8), 611-618.

Van der Meer, L. G. H. (1995), The CO₂ Storage Efficiency of Aquifers, *Energ Convers Manage*, 36(6-9), 513-518.

van Lingen, P. P., J. Bruining, and C. P. J. W. van Kruijsdijk (1996), Capillary Entrapment Caused by Small-Scale Wettability Heterogeneities, *SPE Reservoir Engineering*, 11(02), 93-100.

Vasseur, G., X. R. Luo, J. Z. Yan, D. Loggia, R. Toussaint, and J. Schmittbuhl (2013), Flow regime associated with vertical secondary migration, *Mar Petrol Geol*, 45, 150-158.

Welte, D. H., T. Hantschel, B. P. Wygrala, K. S. Weissenburger, and D. Carruthers (2000), Aspects of petroleum migration modelling, *J Geochem Explor*, 69, 711-714.

White, J. E. (1975), Computed seismic speeds and attenuation in rocks with partial gas saturation, *Geophysics*, 40(2), 224-232.

Wilkinson, D., and J. F. Willemsen (1983), Invasion Percolation - a New Form of Percolation Theory, *J Phys a-Math Gen*, 16(14), 3365-3376.

Wilson, C. E., A. Aydin, L. B. Durlofsky, A., and D. T. Brownlow (2011), Use of outcrop observations, geostatistical analysis, and flow simulation to investigate structural controls on secondary hydrocarbon migration in the Anacacho Limestone, Uvalde, Texas, *Aapg Bull*, 95(7), 1181-1206.

Yan, J. Z., X. R. Luo, W. M. Wang, R. Toussaint, J. Schmittbuhl, G. Vasseur, F. Chen, A. L. Yu, and L. K. Zhang (2012), An experimental study of secondary oil migration in a three-dimensional tilted porous medium, *Aapg Bull*, 96(5), 773-788.

Yang, Z., L. Tian, A. Niemi, and F. Fagerlund (2013), Upscaling of the constitutive relationships for CO₂ migration in multimodal heterogeneous formations, *International Journal of Greenhouse Gas Control*, 19, 743-755.