Fast Assessment of CO₂ Plume Characteristics Using a Connectivity Based Proxy

ABSTRACT

During the operation of a geological carbon storage project, it is crucial to estimate the uncertainty in the flow characteristics of injected CO₂. However, because a large suite of geological models are probable given sparse static data, it is impractical to conduct full physics flow simulations in the entire suite in order to quantify the uncertainty in CO₂ plume migrations. We propose a fast connectivity based proxy that approximates a CO₂ plume migration in a 3-dimensional heterogeneous reservoir during an injection period where viscous forces are dominant over capillary forces. The geological models are ranked based on the extent of the approximated CO₂ plumes. By selecting a representative group of models among the ranked models, the uncertainty in the spatial and temporal characteristics of the CO₂ plume migrations can be quickly quantified. We saved about 90% of the computational cost of quantifying the uncertainty in the extent of CO₂ plumes using the connectivity based proxy.

1. INTRODUCTION

In a geological carbon storage project, one of the critical questions is whether injected CO₂ will remain confined within a permitted zone (Jeong et al., 2013). In order to answer this question, the spatial and temporal characteristics of the CO₂ plume should be estimated before CO₂ is injected. However, because sparse data would be available to characterize aquifers, a large suite of subsurface models has to be considered in order to account for the significant uncertainty associated with the geology of the storage formation. Senel and Chugunov (2013) assessed the uncertainty of injection performance and the extent of CO₂ plumes in a CO₂ storage site in Illinois Basin. They ran a full

1 physics simulator for 200 cases described using different reservoir parameters. However,
2 an excessive computational cost is incurred in order to conduct full physics simulations
3 over a large suite of subsurface models. Fast alternatives to full physics simulators have
4 been researched to alleviate the computational cost of predicting CO₂ plume migrations.

5 The fastest way to approximate the buoyant flow of CO₂ plumes is to analytically
6 or semi-analytically solve a simplified form of the governing equations describing the
7 CO₂ migrations. In these approaches, the physics and the description of fluid and rock
8 properties are simplified. The analytical solutions for a CO₂ plume migration are useful to
9 screen potential CO₂ storage sites. Nordbotten et al. (2005) presented an analytical
10 solution for the height of CO₂ column, and a semi-analytical solution for the pressure
11 distribution as a function of time and radial distance from an injector. Mathias et al.
12 (2009) developed an analytical solution to the temporal and spatial pressure distribution.
13 Vilarrasa et al. (2013) presented a semi-analytical solution that considers the effect of a
14 non-uniform injection rate along the entire aquifer interval. However, these existing
15 analytical and semi-analytical solutions are applicable to homogeneous rock. Thus they
16 are inappropriate for approximating a CO₂ plume migration when the heterogeneity of the
17 rock properties such as facies, permeability, and porosity significantly influences the CO₂
18 plume migration.

19 Vertical-equilibrium (VE) models save the computational cost of predicting a CO₂
20 plume migration by simulating flow in the vertically averaged model instead of a fully 3-
21 dimensional model. The key assumption of the VE models is that brine and CO₂ attain
22 vertical equilibrium instantaneously due to strong buoyancy forces (Guo et al., 2014).
23 Under such an assumption, the lateral migration of the plume is solved numerically over
24 the vertically averaged 2D domain of the reservoir and subsequently, the vertical
25 migration of the plume is solved analytically. The VE models thus provide 3-dimensional

1 results for CO₂ saturations (Nilsen et al., 2011). Bandilla et al. (2014) showed that the
2 CO₂ plumes for the Sleipner L9 model computed using their VE models are in good
3 agreement with those computed using a fully 3-dimensional model. However, the
4 vertically coarsened model still needs to be simulated. Court et al. (2012) reported that
5 the VE models are inappropriate for formations that have low vertical permeability, large
6 thickness, or brine and CO₂ that have a small contrast in density. In such cases, the
7 vertical equilibrium between brine and CO₂ is not established along the thickness of the
8 formation. In addition, the vertical equilibrium assumption does not work properly when
9 a CO₂ plume migration is controlled by 3-dimensional heterogeneity. This will be shown
10 in the verification section of the connectivity based proxy.

11 Bhowmik et al. (2014) applied a random walk to diagnose flow of CO₂ plumes in
12 heterogeneous aquifer models. The random walker approximates migration paths as well
13 as flow responses by stochastically transitioning walkers from one location to the next.
14 The random walker is a Markov process and it requires the current state of the walkers in
15 order to predict their next state. The transitions of a large number of walkers over a fairly
16 large grid is not only required, but these transitions also have to be modeled sequentially
17 adding to the computational time.

18 Invasion percolation theory can be used to simulate the invasion of slow moving
19 immiscible fluids when viscous forces are negligible compared to capillary and gravity
20 forces (Carruthers, 2003). In this theory a fluid invades or percolates into porous media if
21 the fluid pressure is greater than the threshold capillary pressure. However, invasion
22 percolation theory is not valid when CO₂ is injected at a high rate because viscous forces
23 are dominant over capillary forces (Cavanagh, 2013; Singh et al., 2010).

24 Streamline simulation offers rapid modeling of fluid displacements in
25 heterogeneous porous media. Kovscek and Wang (2005) showed that an analytic

streamline-based proxy can provide a good approximation of the ratio of oil recovery to injected CO₂ volume in a large set of heterogeneous reservoir models during CO₂ enhanced oil recovery. However, the streamline proxy has two disadvantages in approximating a CO₂ plume migration. First, the streamline proxy cannot reproduce the buoyancy effect between two fluids with different densities (Thiele and Batycky, 2015). Second, a pressure equation must be solved at least once to calculate the streamlines using the potential field (Sharifi et al., 2014). Even a one-time calculation demands high computational cost in a geological model with millions of cells.

Sethian (1996) introduced the fast-marching method (FMM) to quickly compute the position of monotonically advancing fronts. FMM has been recently applied to approximate reservoir drainage volume (Sharifi et al., 2014; Xie et al., 2015). FMM is a computationally efficient method to approximate fluid movements in heterogeneous porous media. However, it cannot reproduce the buoyant flow of a CO₂ plume.

In this study, we propose a fast connectivity based proxy to approximate a CO₂ plume migration in 3-dimensional reservoir models with heterogeneity in facies, permeability, and porosity during an injection period where viscous forces are dominant over capillary forces. CO₂ plume migration is governed by advective and buoyant forces during the injection period while dissolution, diffusion, and density-driven convection processes take over during the post-injection period (Darcis et al., 2011). In particular, density-driven convection can cause downward migration of the CO₂ plume in the form of fingers that have the opposite flow direction to the buoyant flow direction (Zhang, 2013). This study is aimed at approximating a CO₂ plume migration only during the injection period.

The connectivity based proxy has advantages over the previous proxies in terms of the computational cost and accuracy because it considers the buoyant flow of a CO₂

1 plume without any complicate pressure calculations. CO₂ plume migrations in a synthetic
2 aquifer model computed using the connectivity based proxy are compared to those
3 computed using a full physics simulator, CMG-GEM (CMG, 2012) for various
4 combinations of injection periods, injection rates, a CO₂ density, a CO₂ viscosity, the
5 degree of rock heterogeneity, permeability of cap rock, and topology of the aquifer. The
6 full physics simulations are also compared to the CO₂ plume migrations computed using
7 FMM and a VE model. The connectivity based proxy is also verified for two field cases.
8 Lastly, we will show that the uncertainty in the extent of CO₂ plumes in a large suite of
9 geological models can be quickly quantified using the connectivity based proxy.

10 **2. SCALED CONNECTIVITY ANALYSIS**

11 Connectivity analysis measures how connected a well is to every grid cell in a
12 discrete rendition of the reservoir model. The migration of an injected fluid can be
13 approximated using connectivity analysis by simply assuming that an injected fluid
14 reaches a grid cell with better connectivity earlier. However, connectivity analysis based
15 on only reservoir static properties such as porosity and permeability has to be modified to
16 account for buoyant force. In this section, we investigate further why connectivity
17 analysis cannot reproduce the buoyant flow behavior of a CO₂ plume and a remedy for
18 the problem is presented.

19 **2.1. Connectivity analysis**

20 Hird and Dubrule (1998) presented a way to calculate the least resistive path from
21 wells to grid cells and they defined the cost of the least resistive path as connectivity. The
22 resistivity between two neighboring grid cells is calculated knowing their average
23 effective permeability, the cross-sectional area to flow, and the distance between two

adjacent grid cells. They obtained a good correlation between connectivity and water breakthrough times in 2-dimensional cross section models.

Hirsch and Schuette (1999) introduced principles of graph theory to quickly assess connectivity of reservoir models. They postulated that grid cells are connected by edges, and the edge weights are computed using reservoir parameters that impact connectivity such as porosity and permeability. They computed effective horizontal permeability, and determined connected components using graph theory concepts.

Pardo-Igúzquiza and Dowd (2003) developed a computer program for estimating connectivity in a 3-dimensional model. Once an indicator map that defines a permeable phase or lithofacies is available, their program calculates some connectivity statistics such as minimum, mean, and maximum lengths of connected components.

De Lima et al. (2012) characterized well-to-reservoir and well-to-well connectivity in fractured reservoir models using the methods presented by Hirsch and Schuette (1999). They used the ratio of pore volume to transmissibility between neighboring grid cells as an edge weight, which is one of Hirsch and Schuette's suggestions. This edge weight can be also interpreted as the time needed to fill the given pore volume with a fluid of unit viscosity under a unit potential difference (De Lima et al., 2012).

$$\text{Edge weight} = \frac{\text{Average pore volume}}{\text{flow rate from Darcy's law}} = \frac{\sqrt{Vp_i Vp_j}}{T_{i,j} \cdot \frac{\Delta\Phi}{\mu}} = \frac{\sqrt{Vp_i Vp_j}}{T_{i,j}} \dots\dots\dots \text{Equation (1)}$$

The subscript i and j are the indices of grid cells, V_p is pore volume, $\Delta\Phi$ is the potential difference between grid cells i and j , μ is the fluid viscosity, $T_{i,j}$ is the transmissibility between grid cells i and j . ΔP and μ are dropped from the final

expression because they have unit values. $T_{i,j}$ of two regular cells connected along the x-direction is given by (Donnez, 2007):

$$T_{i,j} = \frac{T_i \cdot T_j}{T_i + T_j} \text{ where } T_i = k_{x,i} \frac{\Delta y \cdot \Delta z}{\Delta x_i/2} \text{ and } T_j = k_{x,j} \frac{\Delta y \cdot \Delta z}{\Delta x_j/2} \dots\dots\dots \text{Equation (2)}$$

T_i and T_j are transmissibilities computed corresponding to half the cell. k_x is the absolute permeability in the x-direction. Δx , Δy , and Δz are the cell sizes in the x-, y-, z-directions, respectively. $T_{i,j}$ is the harmonic average of T_i and T_j . $T_{i,j}$ of non-regular cells is calculated using the equations that Donnez (2007) provides.

A smaller edge weight implies a shorter time to fill the grid cells or the shorter travel time of the fluid between the grid cells. The connectivity from a source to a grid cell is the sum of the edge weights along the shortest path, which is computed using Dijkstra's algorithm (Fredman and Tarjan, 1987). In other words, the connectivity is the shortest time to travel from the source to the grid cell. The proposal is to use this approach to approximate the migration of injected fluid. The procedure of calculating fluid displacement using connectivity analysis (CA) is as follows:

- i) Calculate edge weights between neighboring grid cells using Equation (1)
- ii) Calculate connectivity using Dijkstra's algorithm
- iii) Sort grid cells in ascending order of connectivity
- iv) Fill an unfilled grid cell with the smallest connectivity with as much fluid as the product of the cell volume, porosity, and average injected fluid saturation
- v) Repeat the 4th step until the filled total volume equals the injected volume

A method to compute the average injected fluid saturation will be discussed later. The key assumption is that the injected fluid migrates faster to a grid cell with better connectivity. The migrated region is calculated by truncating the flow path such that the

1 saturated volume of the intersected grid cells equals the volume of the injected fluid.
 2 Each intersected grid cell is assigned a binary value: either saturated with the injected
 3 fluid or not.

4 CA is applied to a two-dimensional case as shown in Figure 1(a), where the
 5 dimensions of the grid system are 201 by 201 by 1 and the dimensions of the grid cell are
 6 5m by 5m by 2m. The porosity is constant, 0.2. CO₂ is injected at the center of the aquifer
 7 at 500 m³/day for a duration of 10 years. The reservoir is described using a single layer in
 8 the vertical direction. Figure 1(b) shows the CO₂ plume migration computed by a
 9 compositional numerical simulator (CMG-GEM). In Figure 1(c), redder means better
 10 connectivity and shorter travel time. In Figure 1(b) and Figure 1(c), CO₂ migrates earlier
 11 to grid cells indicated in red, which have smaller connectivity. Because of the manner in
 12 which connectivity is computed, the CO₂ plume migration is mainly governed by
 13 permeability heterogeneity. Compared to Figure 1(b), CA provides a good approximation
 14 for the CO₂ migration along the north-south permeable direction as shown in Figure 1(d).

(c) Connectivity (1000 days) (d) CO₂ migration by CA

1 Figure 1 Log₁₀ of permeability for a 2D case, corresponding CO₂ saturation computed
2 using CMG-GEM, and corresponding results of CA. The unit of the axes is meters.

3 Now CA is applied to a three-dimensional case as shown in Figure 2 where the z-
4 axis is exaggerated by a factor of 10. The dimensions of the grid system are 201 by 201
5 by 10 and the dimension of an individual grid cell is 5m by 5m by 2m. CO₂ is injected at
6 the center of the aquifer and 15m below the aquifer top at 6,000m³/day for a period of 2
7 years.

8
9
10 Figure 2 Log₁₀ of permeability (md) of a 3D case. The unit of the axes is meters. The z-
11 axis is exaggerated by a factor of 10.

12 Contrary to the 2D case, the CO₂ plume simulated using CMG-GEM in Table 1
13 exhibits buoyant characteristics. After the injected CO₂ migrates vertically in the vicinity
14 of the injection well, it spreads horizontally. However, the CO₂ plume approximated
15 using CA does not exhibit such buoyant behavior.

16 Table 1 Comparison of CO₂ migration by CMG-GEM and CA using Equation (1) in
17 the geological model shown in Figure 2. The unit of the axes is meters. The
18 z-axis is exaggerated by a factor of 10.

	CO ₂ saturation by CMG-GEM	Connectivity (years)	CO ₂ migration by CA
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1 In order to take the buoyancy effect into account, the potential difference caused
2 by viscous and gravity forces should be considered in Equation (1). The relative
3 permeability of CO₂ should be also considered in the transmissibility term because the
4 edge weight represent the travel time of CO₂ when two fluids are flowing concurrently.
5 Likewise, the CO₂ volume should be used instead of the pore volume. Thus Equation (1)
6 for the edge weight is extended to Equation (3):

$$\begin{aligned}
 \text{Modified Edge weight} &= \frac{\text{Average } CO_2 \text{ volume}}{CO_2 \text{ flow rate from Darcy's law}} \\
 &= \frac{\overline{\mu_{CO_2}} \hat{S}_{CO_2} \sqrt{Vp_i \cdot Vp_j}}{\hat{k}_{r,CO_2} T_{ij} [\Delta P_{ij} + (\overline{\rho_{brine}} - \overline{\rho_{CO_2}}) g \Delta h_{ij}]} \dots\dots\dots \text{Equation (3)}
 \end{aligned}$$

7 The i and j are cell indexes, $\overline{\mu_{CO_2}}$ average CO₂ viscosity in aquifer conditions, ΔP
8 pressure difference, $\overline{\rho_{brine}}$ average brine density in aquifer conditions, $\overline{\rho_{CO_2}}$ average
9 CO₂ density in aquifer conditions, g gravity constant, Δh depth difference between the
10 i -th and j -th cells. $\hat{S}_{CO_2}$ and $\hat{k}_{r,CO_2}$ are the CO₂ saturation and the CO₂ relative
11 permeability at the end point of the CO₂ relative permeability curve. ΔP is the pressure
12 difference between the i -th and j -th grid cells. The procedure to calculate ΔP will be
13 discussed later.

Now the connectivity is calculated for the 3D model shown in Figure 2 using Equation (3) instead of Equation (1). The results obtained using Equation (3) are shown in Table 2. In the results of the full physics flow simulation shown in Table 2, it is evident that the CO₂ plume exhibits strong buoyancy caused by the density difference between CO₂ and water. The CO₂ plume vertically migrates to upper layers and then horizontally spreads within the top layer. CA corresponding to Equation (3) considers buoyant force, but the spread of the CO₂ plume in all layers along the vertical migration path is more similar to a cylinder rather than a wedge as depicted by the full physics flow simulation result. However, in the full physics simulation, CO₂ mostly migrates in the vertical direction with high velocity in the vicinity of the injection well before reaching the top layer. The reason why CA cannot reproduce the buoyant behavior is discussed in the next section and then, a modified connectivity analysis that reproduces the buoyant flow will be presented.

Table 2 Comparison of CO₂ migration by CMG and CA using Equation (3) in the geological model shown in Figure 2. The unit of the axes is meters. The z-axis is exaggerated by a factor of 10.

	CO ₂ saturation by CMG-GEM	Connectivity (years)	CO ₂ migration by CA
Areal view
Slice at i=101

2.2. Scaled Connectivity Analysis

Let us study a simple example to investigate why connectivity analysis cannot reproduce the flow pattern corresponding to buoyant flow. Figure 3 shows an example of tracing the migrated regions along a cross-section using the original connectivity analysis. In Figure 3(a), the bracketed numbers in the grid cells and the numbers on the arrows represent the indices of the grid cells and the edge weights, respectively. The vertical edge weight is 1 and the horizontal edge weight is 100. The edge weights in the vertically downward direction are infinite because the potential differences are negative in that direction. The total injected amount is 5 grid cells and the saturated blocks are colored in yellow. The connectivities of the grid cells are presented in Figure 3(b). For example, the shortest paths from the injector to the grid cell (7) are INJ-(3)-(6)-(7), INJ-(3)-(4)-(7), and INJ-(1)-(4)-(7). The paths are different, but the costs or the connectivities to the grid cell (7) are the same, $1+1+100=102$. In Figure 3(b), the connectivities are truncated with the injected volume in the order of the connectivity values. The grid cells with the top five connectivities (0, 1, 2, 100, 101) are marked as the grid cells contacted by the migrating CO₂ plume.

Figure 3 An example of connectivity analysis

However, Figure 3(c) shows the expected plume migration when buoyancy is dominant. The original approach is inappropriate for representing buoyant flow. This is because a fluid does not migrate along the shortest path in terms of the sum of travel

times between neighboring grid cells. In fact, the movement of the CO₂ plume is strongly affected by the local gradient at each location of the plume and the movement is in the direction of the maximum gradient. In Figure 3(c), most of the fluid migrates vertically rather than horizontally at first because there is big difference between the two edge weights, 1 and 100 in the vicinity of the injector. The injected fluid rapidly migrates to the top layer, and then the fluid migrates horizontally in the top layer along the local minimum edges, which is colored orange in Figure 3(c). For example, an edge weight of 1 is the minimum adjacent to the injector location, and an edge weight of 1 is also the minimum at the next location of the plume (middle left). Then an edge weight of 100 is the minimum at the top left because the edge weight in the downward direction is infinite. Again an edge weight of 100 is the minimum at the next locations (top middle and top right). The actual migration follows the path of local minimum edges. Thus CA is modified so that the shortest paths contain the local minimum edges as many as possible.

Scaled connectivity analysis (SCA) scales edge weights with the local minimum edge weight so that fluid migrates along the edge with the local minimum edge weight at each grid cell. In SCA, the minimum edge weight among the neighboring edges is found and then the edge weights are divided by the minimum edge weight. In Figure 4, the minimum edge weight is 2 and then the edge weights are scaled by dividing all the edge weights to that block by 2.

Figure 4 An example of locally scaled edge weights

Figure 5 shows the result of scaled connectivity analysis for the example in Figure 3. Table 3 shows the sequential steps of calculating the shortest path from INJ to the grid cell (8) in the scaled graph in Figure 5. As shown in Figure 5, the truncated connectivity in the scaled graph reproduces the local minimum path. As is evident, by scaling edge weights with their local minimum, the buoyant flow behavior is reproduced.

Figure 5 Result of scaled connectivity analyses for the example shown in Figure 3
Table 3 Sequential steps of calculating the shortest path from INJ to the grid cell (8) in shown Figure 5

Current grid cell	Connected grid cells	Connected edge weights	Local minimum edge weight	Scaled edge weights	Next grid cell
INJ	(1), (3)	100, 1	1	100, 1	(3)
(3)	(4), (6)	100, 1	1	100, 1	(6)
(6)	(7)	100	100	1	(7)
(7)	(6), (8)	100, 100	100	1, 1	(8)

There are three differences between connectivity analysis and scaled connectivity analysis. The first difference is to calculate connectivity in a scaled graph instead of the original graph. The second difference is to use a modified Dijkstra's algorithm that calculates the cumulative sum of original edge weights along the shortest path computed in a scaled graph. The last difference is that the modified Dijkstra's algorithm rejects the path along which the travel time is greater than a critical time computed based on the injection period. The modified Dijkstra's algorithm can save computation time by ignoring paths that are infeasible given the specified time.

2.3. Procedure of SCA

The procedure of approximating CO₂ plume migration using SCA is as follows:

- i) Calculate a radial pressure gradient at the centroid of each cell using the following equation:

$$\frac{dP}{dr} = \frac{Q_{CO_2} \overline{\mu_{brine}}}{2\pi r \bar{k} \bar{h}} \dots \dots \dots \text{Equation (4)}$$

- ii) Calculate edge weights between neighboring grid cells using Equation (3)
- iii) Change negative edge weights to infinity (implying that flow cannot occur against gravity)
- iv) Scale edge weights with their local minimums
- v) Calculate scaled connectivity using the modified Dijkstra's algorithm
- vi) Fill grid cells with an injected fluid in the order of the scaled connectivity such that the filled total volume equals the injected volume

In Equation (3) and Equation (4), $\overline{\mu_{CO_2}}$, $\overline{\rho_{CO_2}}$, $\overline{\mu_{brine}}$, and $\overline{\rho_{brine}}$ can be obtained from a full physics simulation result or thermo-dynamically calculated under bottom hole conditions.

Equation (4) is the analytical solution for the pressure gradient in the radial flow in homogeneous rock under steady state flow conditions (Ahmed, 2006). In Equation (4), P is pressure and r is the distance from an injector. Q_{CO_2} is the flow rate in aquifer conditions, $\overline{\mu_{brine}}$ average viscosity of brine in aquifer conditions, $\bar{k}$ average permeability, $\bar{h}$ average thickness of the aquifer.

In SCA, $\bar{k}$ is used to approximate the pressure gradient in Equation (4). Because $\bar{k}$ is likely to be related to the permeability in the CO₂ swept zone, $\bar{k}$ might be changed according to operating conditions such as injection time and injection rate. An arithmetic average can be attempted first for $\bar{k}$ in Equation (4). However, $\bar{k}$ should be manually

1 adjusted until SCA gives a good approximation of a full physics simulated CO₂ plume
 2 migration. Our final goal is not to obtain a good approximation of a CO₂ plume migration
 3 for only one geological model, but to acquire proxy responses that represent CO₂ plume
 4 migrations in a large suite of geological models. The adjustment of $\bar{k}$ is conducted for
 5 only one geological model, and then the adjusted $\bar{k}$ is also used for the other models that
 6 have the same geological setting for permeability and porosity such as mean and
 7 variogram.

8 The steady state pressure solution corresponding to flow in a cylindrical
 9 homogenous medium is given by (Ahmed, 2006):

$$P = P_{wf} + \frac{Q\mu}{2\pi kh} \log \frac{r}{r_w} \dots\dots\dots \text{Equation (5)}$$

10 Where P_{wf} is the well bottom hole pressure, r is a radial distance from the well, r_w is
 11 a well radius. In this solution to the pressure equation in radial coordinates, two grid cells
 12 that are located at a considerable distance, d_{ij} , from each other might have small pressure
 13 drop across them if they are separated by a small radial distance. This implies that the
 14 edge weights along the radial direction will be small while in other directions, the edge
 15 weights will be large. This in turn causes the shortest paths to be always in the radial
 16 direction and the final approximation of plume migration to have a radial shape.
 17 Consequently, we propose a modified expression for the pressure drop as:

$$\Delta P_{ij} = \frac{\left. \frac{dP}{dr} \right|_i + \left. \frac{dP}{dr} \right|_j}{2} d_{ij} \dots\dots\dots \text{Equation (6)}$$

18 Where d_{ij} is the distance between the grid cells i and j . In Equation (6), the distance
 19 between two neighboring grid cells is used instead of the radial distance to consider the
 20 effect of heterogeneity in directions other than the radial direction.

1 Brine viscosity is used in Equation (4) instead of CO₂ viscosity even though CO₂
2 is injected. The velocity of CO₂ plume is controlled by pre-existing brine even if CO₂ is
3 much less viscous than brine because the aquifer is filled with brine. Thus brine viscosity
4 is more appropriate than the CO₂ viscosity to approximate the pressure gradient.

5 The edge weight in Equation (3) is the time needed to fill the given pore volume.
6 The maximum pore volume filled with CO₂ is the pore volume times the CO₂ saturation
7 at the end point of the CO₂ relative permeability curve. Thus the end point of the CO₂
8 relative permeability curve is used for $\hat{S}_{CO_2}$ and $\hat{k}_{r,CO_2}$.

9 The gravity term, $\Delta(\rho gh)_{ij}$, in Equation (3), assumes that $\Delta\rho g$ is constant and
10 Δh depends on the vertical locations of two adjacent grid cells. If the face in contact with
11 the two adjacent cells is between the center of the two adjacent cells, as shown in Figure
12 6(a) and (b), then Δh is calculated as the depth (z_1) of the starting cell minus the depth
13 (z_2) of the ending cell. In Figure 6(b), the negative gravity term means the direction from
14 the starting cell to the ending cells is opposite to the buoyant flow direction. If the sum of
15 a pressure difference and a negative gravity term is still negative, then the edge weight
16 becomes infinite, which means CO₂ cannot move from the starting cell to the ending cell.
17 If the face is located either above, or below the depth to the center of the two adjacent
18 cells, as shown in Figure 6(c) to (f), then the flow paths may be in a direction opposite to
19 buoyant flow. The flow path in the direction opposite to buoyant flow should have a
20 disadvantage because it is hard to migrate against gravity. Thus in these cases, Δh is the
21 negative depth difference between the face and the cell center instead of the depth
22 difference between the starting and ending cells.

Figure 6 Examples of calculating Δh in a 2D cross section

Flow in the up-dip direction is preferred more than in the down-dip direction in a CO_2 migration because of strong buoyancy effect. However, a small down-dip angle such as 1° does not make significant changes in CO_2 plume migrations in most of aquifers that have a much larger horizontal extent than the vertical extent. Although a CO_2 plume can migrate to small down-dip angles, those can make the potential term, $\Delta\Phi = \Delta P_{ij} + \Delta(\rho gh)_{ij}$, in Equation (3) negative. The negative potential term is adjusted using Equation (7) and Equation (8) in order to allow the down-dip flow of CO_2 plume. In Equation (7) and Equation (8), a dip angle of two adjacent grid cells is denoted as α . $\alpha_{\min}$ is the minimum down-dip angle ignoring the buoyant force and $\alpha_{\max}$ is the maximum down-dip angle factoring the buoyant force. If a down-dip angle is less than $\alpha_{\max}$, then the effect of the negative buoyant force is reduced as shown in Equation (7)

1 and Equation (8). ω is the power in the power model of Equation (7) to control the
 2 shape of the interpolated curve. The effect of the negative buoyant force varies according
 3 to the structure in vicinity of a cell, but it is simply interpolated as formulated in Equation
 4 (7). Figure 7 shows the change in the down dip factor as a function of ω . $\omega = 1$
 5 represents the linear regression between $\alpha_{\min}$ and $\alpha_{\max}$. $\alpha_{\min}$, $\alpha_{\max}$, and ω are
 6 aquifer-structure-dependent parameters. They should be adjusted when SCA does not
 7 reproduce the down dip migration in a full physics simulation. However, good results are
 8 obtained in the examples of this study with $\alpha_{\min} = 1^\circ$, $\alpha_{\max} = 5^\circ$, and $\omega = 0.5$.

$$\text{down dip factor} = \begin{cases} 0, & 0 < \alpha \leq \alpha_{\min} \\ \left(\frac{\alpha - \alpha_{\min}}{\alpha_{\max} - \alpha_{\min}} \right)^\omega, & \alpha_{\min} < \alpha < \alpha_{\max} \\ 1, & \text{otherwise} \end{cases} \dots\dots\dots \text{Equation (7)}$$

$$\Delta\Phi = \Delta P_{ij} + \text{down dip factor} \cdot \Delta(\rho gh)_{ij} \dots\dots\dots \text{Equation (8)}$$

Figure 7 Down dip factor as a function of ω

11 As mentioned in the previous section, the modified Dijkstra's algorithm rejects
 12 paths that have connectivity greater than a certain time. This time is different from an
 13 injection period because the edge weights are calculated using approximate parameters
 14 such as viscosity, density, and pressure gradients. This cutoff time is obtained by adding
 15 50% of the injection duration in order to account for errors that the approximations

1 results in. The modified Dijkstra's algorithm therefore ignores paths that have the
2 connectivity larger than one and half times of an injection period.

3 In the last step, grid cells are sorted in the order of their scaled connectivity. Each
4 grid cell can have CO₂ as much as the product of its volume, porosity, and average CO₂
5 saturation ($\overline{S_{CO_2}}$). The grid cells are filled with CO₂ until the cumulative CO₂ volume is
6 equal to the total volume of injected CO₂ in aquifer conditions. $\overline{S_{CO_2}}$ should be adjusted
7 to better CO₂ plume migration computed by a full physics simulator in one of many
8 probable geological models. A small $\overline{S_{CO_2}}$ results in a large CO₂ plume in SCA while a
9 large $\overline{S_{CO_2}}$ results in a small CO₂ plume. Several $\overline{S_{CO_2}}$ are attempted until a SCA
10 approximation matches an observed CO₂ plume. Good matches are obtained in most of
11 the examples of this study with the CO₂ saturation at the end point in a CO₂ relative
12 permeability curve for $\overline{S_{CO_2}}$.

13 Before SCA is applied to a large suite of geological models, $\bar{k}$, $\overline{S_{CO_2}}$, $\alpha_{\min}$,
14 $\alpha_{\max}$, and ω are adjusted for a few small and synthetic models. $\bar{k}$ that is influenced by
15 the degree of heterogeneity is manually adjusted unless an SCA approximation computed
16 using an arithmetic average of permeability is in good agreement with a full physics
17 simulated CO₂ plume migration. $\overline{S_{CO_2}}$ should be increased or decreased when the size of
18 the CO₂ plume in a SCA approximation is large or small compared to its full physics
19 simulation, respectively. The aquifer-structure-dependent parameters should be adjusted
20 when SCA does not reproduce the down dip migration in a full physics simulation.

21 **3. VERIFICATION OF SCA**

22 The objective of SCA is to quickly approximate CO₂ plume migrations rather than
23 to delineate it as accurately as possible in heterogeneous porous media. In this section,
24 the application of SCA for approximating CO₂ plume migrations is verified under

different operating conditions, fluid properties, aquifer structures, and rock heterogeneity. SCA is also compared against a full physics simulator (CMG-GEM) and other proxies for CO₂ plume migrations.

3.1. Base case

The aquifer shown in Figure 2 is used as a base case. The input data of SCA shown in Table 4 are used for the base case. The initial average pressure and temperature of the aquifer is 18,145 kPa and 75 °C, respectively. The fluid properties are obtained from the CMG-GEM results at the injector or they are calculated corresponding to the conditions at the injector. The permeability shown in Figure 8 follows a log normal distribution with mean 1.3880 and standard deviation 0.6376 of log₁₀ permeability. As shown in Figure 8, the major correlation direction is north-south. The major, minor and vertical correlation lengths are 250 m, 50 m and 15 m, respectively. The permeability is generated using the sequential Gaussian simulation in SGeMS (Remy et al., 2011). The porosity is assumed to be constant at 0.2. Capillary pressure is ignored and Figure 9 shows the relative permeability curves of brine and CO₂. The boundary is connected to an infinite aquifer.

Table 4 Input data of SCA for the base case

Aquifer structure	Size	1,005 m * 1,005 m * 20 m
	Dimensions of a grid cell	5 m * 5 m * 2 m
Operating conditions	Injection period	2 years
	Injector location	(i, j, k) = (101, 101, 3)
	Injection rate	11214.5 kg/day
Rock and fluid properties in aquifer conditions	Average permeability	67 md
	Average porosity	0.2
	CO ₂ saturation at the end point	0.7
	CO ₂ relative permeability at the end point	0.8
	Average CO ₂ viscosity	0.0332 cp
	Average CO ₂ density	411.3 kg/m ³

	Average brine viscosity	0.3786 cp
	Average brine density	1007 kg/m ³
	Average CO ₂ saturation	0.7
Others	Minimum downdip	1°
	Maximum downdip	5°
	Power of downdip factor	0.5

1

2 Figure 8 Different views and histogram of log₁₀ permeability (md) field shown in Figure
3 2. The axis unit in (a) and (b) is in meters. The z-axis is exaggerated by a factor of 10.

4

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Figure 9 Relative permeability of CO₂ and water in the base case

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Table 5 shows scaled connectivity and connectivity computed by SCA for the base case. Table 6 shows CO₂ plume migration computed using SCA and CMG-GEM in the base case. In the CMG-GEM results, CO₂ migrates longer in the north-south direction than the east-west direction along the major correlated direction of permeability. This implies the spatial distribution of permeability is the main factor that determines

1 CO₂ plume migration. SCA presents an approximation of CO₂ plume horizontal
 2 migration similar to the full physics simulation results. The wedge-shaped migration of
 3 CO₂ plume in the slice at $i = 101$ of Table 6 is reproduced in the results of SCA. SCA
 4 does not capture the small horizontal migration in the second layer, but the SCA proxy
 5 does perform adequately to quantify the uncertainty in dominant migration paths.

6 Table 5 Scaled connectivity and connectivity in the base case. The unit of the axes is
 7 meters. The z-axis is exaggerated by a factor of 10.

8 Table 6 Comparison of CO₂ migration by SCA and CMG-GEM in the base case. The unit
 9 of the axes is meters. The z-axis is exaggerated by a factor of 10.

3.2. Injection period

Table 8 shows the CO₂ plume migration after CO₂ is injected during 1 year while the injection period is 2 years in the base case. SCA reproduces the CO₂ plume migration that is horizontally shorter than in the base case.

Table 7 Comparison of CO₂ migration by SCA and CMG-GEM for 1 year. The unit of the axes is meters. The z-axis is exaggerated by a factor of 10.

Table 8 shows the CO₂ plume migration after CO₂ is injected for 4 years. 80 md is used in this case for $\bar{k}$ in the approximate pressure gradient equation (Equation (4)) instead of 67 md, which is the arithmetic average. Because Equation (4) is an approximation of the spatially and temporally different pressure gradients, $\bar{k}$ should be adjusted if operating conditions such as an injection period are changed.

In Table 8, the east part of the SCA approximation does not have the CO₂ plume migration in the south direction. This is because the impermeable zone in the east part shown in Figure 8 impedes the CO₂ flow. However, the overall shape of the SCA approximation and the CMG-GEM result is still similar.

Table 8 Comparison of CO₂ migration by SCA and CMG-GEM for 4 years. The unit of the axes is meters. The z-axis is exaggerated by a factor of 10.

	SCA	CMG-GEM (S_{CO_2})
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3.3. Injection rate

Table 9 and Table 10 show the results of SCA and CMG-GEM corresponding to half and double of the CO₂ injection rate in the base case, respectively. In the double injection rate case, 80 md is used for $\bar{k}$ in Equation (4) instead of the arithmetic average of permeability.

The horizontal migrations approximated by SCA in Table 9 and Table 10 are slightly different from those of the CMG-GEM results, but SCA captures the essence of the horizontal migrations of CO₂ plumes at the half and double injection rates.

In Table 9, the wedge-shaped vertical migration in the CMG-GEM result is reproduced in the SCA approximation. As shown for the slice i=101 in Table 6 and Table 10, the double injection rate case has longer horizontal migration in each layer than the base case. This is because the higher injection rate leads to higher pressure gradient. In the SCA result for the double injection rate case, CO₂ also spreads longer horizontally in each layer.

Table 9 Comparison of CO₂ migration by SCA and CMG-GEM for half injection rate case. The unit of the axes is meters. The z-axis is exaggerated by a factor of 10.

	SCA	CMG-GEM (S_{CO_2})
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1 Table 10 Comparison of CO₂ migration by SCA and CMG-GEM for double injection rate
2 case. The unit of the axes is meters. The z-axis is exaggerated by a factor of
3 10.

4 3.4. Density and viscosity

5 In this case, SCA and CMG-GEM results are compared when the aquifer has the
6 higher initial pressure (28145 kPa) than the base case (18145 kPa). If the initial pressure
7 increases, then the density and viscosity of CO₂ increase. The density and viscosity of
8 CO₂ for the SCA input data increase from 411.3 kg/m³ and 0.0332 cp used in the base
9 case to 735.7 kg/m³ and 0.0622 cp. The size of the CO₂ plume in this case is smaller than
10 that in the base case because the total volume and the mobility of the injected CO₂

1 decrease. SCA reproduces such the spatial characteristics of the small CO₂ plume for this
 2 case as shown in Table 11.

3 Table 11 Comparison of CO₂ migration by SCA and CMG-GEM for higher CO₂ density
 4 and viscosity. The unit of the axes is meters. The z-axis is exaggerated by a
 5 factor of 10.

6 **3.5. Rock heterogeneity**

7 Table 12 shows CO₂ migration in homogeneous rock that has the mean of log₁₀
 8 permeability as the base case. SCA reproduces the buoyant flow in the cross-sectional
 9 view. However, SCA fails to reproduce the radial migration of the CO₂ plume because it
 10 does not consider diagonal connections such as the north-east/south-west directions. It is
 11 not appropriate to apply SCA to analyze displacement in homogeneous rock, but the goal
 12 of this study is to quantify the uncertainty in CO₂ displacement in heterogeneous rock.

13 Table 12 Comparison of CO₂ migration by SCA and CMG-GEM for homogeneous rock.
 14 The unit of the axes is meters. The z-axis is exaggerated by a factor of 10.

	SCA	CMG-GEM (S_{CO_2})
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However, permeability in most of reservoirs is not homogeneous. The most common measure of permeability heterogeneity is V_{DP} , the Dykstra-Parsons coefficient (Jensen, 2000):

$$V_{DP} = \frac{k_{0.50} - k_{0.16}}{k_{0.50}} \dots\dots\dots \text{Equation (9)}$$

where $k_{0.50}$ is the median of permeability and $k_{0.16}$ is the 0.16 quantile of permeability. V_{DP} in most reservoirs ranges from 0.5 to 0.9 where $V_{DP} = 0$ means homogeneous (Willhite, 1986).

Now SCA is tested in four heterogeneous permeability fields. The four heterogeneous permeability fields are generated by normalizing $\log_{10}$ permeability of the base case and back-transforming them with the same mean and the different standard deviations, 0.5, 0.7, 0.9, and 1.5 times of the standard deviation of the base case. The 2nd and 3rd rows in Table 13 show the areal view and histogram of $\log_{10}$ permeability in the four permeability fields. V_{DP} of the four permeability fields are 0.52, 0.65, 0.73, and 0.89 and V_{DP} in the base case is 0.77.

The 4th and 5th rows in Table 13 are the arithmetic averages and adjusted $\bar{k}$ of the four permeability fields. As discussed before, $\bar{k}$ in the approximate pressure gradient equation (Equation (4)) should be adjusted if reservoir model parameters are changed.

The arithmetic average of an entire permeability field is a good reference for $\bar{k}$. However, the arithmetic average is not always a good representation of heterogeneous rock because the behaviors of produced or injected fluid are not only mostly affected by permeability near a well, but the spatial distribution of permeability is also complicated.

The CMG-GEM results (the 7th row) in Table 13 show the CO₂ plume migrations according to V_{DP} . As V_{DP} becomes higher, the CO₂ plume spreads longer in the north-south direction and it is more affected by permeability heterogeneity. As shown the areal views of SCA and CMG-GEM in Table 13, SCA reproduces the overall trend in the shape of the CO₂ plume simulated by CMG-GEM. In this regard, SCA fails to reproduce the radial migration of the CO₂ plume in the homogeneous model, but SCA is successful in capturing the spatial characteristics of the CO₂ plumes in the heterogeneous models whose V_{DP} lie in the normal range.

Table 13 Comparison of CO₂ migration by SCA and CMG-GEM for four heterogeneous permeability fields

	$V_{DP}=0.52$	$V_{DP}=0.65$	$V_{DP}=0.73$	$V_{DP}=0.89$
Log ₁₀ k (md)
Histogram of log ₁₀ k (md)
Arithmetic k	32 md	41 md	56 md	207 md
Adjusted $\bar{k}$	50 md	50 md	65 md	Not adjusted

3.6. Cap rock

As shown in Figure 10, the 3th layer from the top is modeled as a shale barrier in this variation of the base case. It is investigated if SCA reproduces a CO₂ leakage through the shale barriers according to the permeability of the shale barriers.

Figure 10 Cross-sectional view (i=101) of log₁₀ permeability (md) in the base case with shale barriers. The unit of the axes is meters. The z-axis is exaggerated by a factor of 10.

Table 14 shows the CO₂ migration when the shale barrier has a permeability of 0.01 md. Even though the permeability of the shale barrier is small, CO₂ migrates through the shale barrier. The CO₂ saturation above the shale barriers is small, but considering the short injection period (2 years), CO₂ cannot be confined safely below the shale barrier. SCA captures the horizontal extent of the plume migration in the top layer as well as the vertical migration of the CO₂ plume.

Table 14 Comparison of CO₂ migration by SCA and CMG-GEM for shale barriers with 0.01 md. The unit of the axes is meters. The z-axis is exaggerated by a factor of 10.

1 Reducing the permeability of the shale barrier to 0.001 md prevents a CO₂
2 leakage as shown in Table 15. SCA represents the vertical migration as well as the
3 horizontal migration of the CO₂ plume.

4 Table 15 Comparison of CO₂ migration by SCA and CMG-GEM for shale barriers with
5 0.001 md. The unit of the axes is meters. The z-axis is exaggerated by a
6 factor of 10.

3.7. Topology of the aquifer

SCA is applied to three folded aquifer layers where amplitudes in the vertical direction are added to the structure in the base case. Figure 11 shows the $\log_{10}$ permeability distribution in the three structures. The spatial distribution of permeability is identical to that in the base case. The medium and strong amplitudes in Figure 11(b) and Figure 11(c) are four times and eight times larger than the weak amplitudes in Figure 11(a), respectively.

Figure 11 $\log_{10}$ permeability (md) in three aquifer models with variable topology. The unit of the axes is meters. The z-axis is exaggerated by a factor of 10.

Compared to the base case, the weak amplitudes in the vertical direction shown in Figure 11(a) do not make significant variation in the CO_2 plume migration as shown in the CMG-GEM results for the weak amplitudes of Table 16. The CO_2 plumes for the base case and the case with medium amplitudes have slightly different shape in the south and east regions, but they are still almost the same despite the medium amplitudes. This implies that the structural patterns shown in Figure 11(a) and Figure 11(b) do not have strong influence on the CO_2 plume migrations. For the weak and medium amplitudes, the SCA approximations are similar to the CMG-GEM results in the vertical and horizontal migrations.

Table 16 Comparison of CO_2 migration by SCA and CMG-GEM for the three aquifer structures shown in Figure 11. The unit of the axes is meters. The z-axis is exaggerated by a factor of 10.

1 Compared to the weak and medium amplitudes, the CO₂ plume migration
2 computed using CMG-GEM for the strong amplitudes is quite different from that for the
3 base case as shown in Table 16. This means the structural pattern in the strong amplitudes
4 has stronger influence on the CO₂ plume migration than those in the weak and medium
5 amplitudes. SCA reproduces the vertical migration and the longer horizontal migration
6 along the north-south direction, but it does not reproduce the frontal shapes exactly
7 compared to the weak and medium amplitudes. In this regards, SCA might not work
8 properly when structural heterogeneity has significant influence on a CO₂ plume

migration. Unfortunately, we cannot know if SCA works for a complex structure before applying because there is no direct way to measure how much influence structural heterogeneity has on a CO₂ plume migration. However, the final goal of SCA is to provide approximate CO₂ plumes for a large suite of geological models. We can judge if SCA works for the complex structure by comparing the results of SCA and a full physics simulator in one model of the suite.

3.8. Other proxies

In this case, two proxies, the fast marching method (FMM) and a vertical equilibrium (VE) model, are applied to the base case and the case with the shale barrier, and then their results are compared with those using CMG-GEM. For the VE model, the co2lab module in the Matlab Reservoir Simulation Toolbox (MRST) is used (Lie et al., 2011).

In the left column in Table 17, the diffusive time of flight to every grid cell is calculated using FMM. The diffusive time of flight implies the arrival time of a pressure wave (Kulkarni et al., 2001). The diffusive time of flight does not imply the arrival time of injected CO₂, but here we investigate if FMM can consider the buoyant effect. The grid cells are filled with CO₂ in the order of the diffusive time of flight as much as the volume of injected CO₂. As shown in Table 17, FMM does not reproduce the buoyant flow of CO₂ plume because it is not designed to consider the buoyancy effect between two fluids.

Table 17 CO₂ migration by FMM in the base case. The unit of the axes is meters. The z-axis is exaggerated by a factor of 10.

	Diffusive time of flight years	Approximation of CO ₂ plume	CMG-GEM (S_{CO_2})
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Table 18 and Table 19 show the migration of CO₂ plume calculated using VE and CMG-GEM for the base case and the shale barrier case, respectively. In Table 18, the result of VE for the base case is acceptable because the VE model is able to correctly represent the buoyant migration of the CO₂ plume, and the horizontal migration due to permeability heterogeneity. However, VE overestimates CO₂ saturations in the east-southern region of the reservoir compared to the result of CMG-GEM. The vertically averaged permeability shown in Table 20 is higher in the east-southern zone than the permeability of the top layer in the base case shown in Figure 8(a) and this causes the CO₂ plume computed using the VE model to spread more in the east-southern zone.

VE is applied to the cap rock case where the whole 3rd layer from the top has a shale barrier of permeability equal to 0.001 md as shown in Figure 10. The shale barrier has constant permeability and consequently, the vertically averaged permeability is similarly impacted at all locations in the reservoir. This is evident in the map of the vertically averaged permeability shown in Table 20 where the observed permeability features look virtually the same. For this reason, the CO₂ migration computed by VE in the cap rock case is almost identical to that in the base case. VE is therefore unable to capture the influence of the shale barrier on the vertical migration of the CO₂ plume. In

1 this regard, VE is inappropriate to represent the CO₂ plume migration affected by vertical
2 heterogeneity.

3 Table 18 Comparison of CO₂ migration by VE and CMG-GEM for the base case. The
4 unit of the axes is meters. The z-axis is exaggerated by a factor of 10.

5 Table 19 Comparison of CO₂ migration calculated by VE and CMG-GEM for the cap
6 rock case where there is a shale barrier of permeability 0.001md. The unit of
7 the axes is meters. The z-axis is exaggerated by a factor of 10.

8 Table 20: Vertically averaged log₁₀ permeability for the cases in Table 18 and Table 19.
9 The unit of the axes is meters.

	Vertically averaged log ₁₀ peambility in the base case	Vertically averaged log ₁₀ peambility in the cap rock case
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4. APPLICATION TO FIELD CASES

4.1. The Johansen model

The Johansen Formation is a candidate site for geological CO₂ storage located in the south-western coast of Norway (Eigestad et al., 2009). The data set for the Johansen Formation is available online. SCA is applied to approximate a CO₂ migration in the Johansen Formation and it is compared to the results of a full physics simulator, CMG-GEM.

The grid system of the Johansen model is 100 by 100 by 11. The typical cell size is 500 m by 500 m, and its thickness varies from 16 to 24 m. Figure 12 shows the structure and faults of the Johansen model where the red means a fault and the yellow means an active cell. A major fault is located in the middle of the Johansen model along the north-south direction. The boundaries which do not face a boundary fault are connected to an aquifer allowing brine displacement. The initial average pressure and temperature of the aquifer are 31,310 kPa and 94 °C, respectively.

Figure 12 Structure and faults of the Johansen model. The unit of the axes is meters. The z-axis is exaggerated by a factor of 10.

The Johansen model has shale layers at the top and bottom, and sandstone layers in the middle, which is the Johansen Formation. The first row in Table 21 shows $\log_{10}$ horizontal permeability and porosity of the entire 3D model including the shale layers at the bottom and top. The ratio of vertical to horizontal permeability is 0.1. The horizontal permeability of the shale layers are 0.01 md and 0.1 md at the top and bottom, respectively. The porosity of the shale layers is constant, 0.1. The second row in Table 21 shows $\log_{10}$ horizontal permeability and porosity of sandstone in the Johansen Formation. The horizontal permeability and porosity of the Johansen Formation range from 64 to 1,660 md and from 0.10 to 0.29, respectively. CO₂ is injected at (48,48) over the Johansen Formation during 500 years.

Table 21 Log₁₀ horizontal permeability and porosity of the Johansen model. The unit of the axes is meters. The z-axis is exaggerated by a factor of 10.

Figure 13 shows the relative permeability curves of CO₂ and water in the Johansen model. The end point values in the relative permeability curve of CO₂ are used for $\hat{S}_{CO_2}$ and $\hat{k}_{r,CO_2}$ in Equation (3). Table 22 contains the input parameters for SCA. The fluid properties are obtained from the CMG-GEM results at the injector.

Figure 13 Relative permeability in the Johansen model

Table 22 Input data of SCA for the Johansen model

Aquifer structure	Average thickness	103.5194 m
Operating conditions	Injection period	500 years
	Injector location	(i, j, k) = (48, 48, 6) ~ (48, 48, 10)
	Injection rate	14,000 m ³ /day in aquifer conditions
Fluid properties in aquifer conditions	CO ₂ saturation at the end point	0.9
	CO ₂ relative permeability at the end point	0.2142
	Average CO ₂ viscosity	0.058 cp
	Average CO ₂ density	700 kg/m ³
	Average brine viscosity	0.3027 cp
	Average brine density	1014.5 kg/m ³
	Average CO ₂ saturation	0.9
Others	Minimum downdip	1°
	Maximum downdip	5°
	Power of downdip factor	0.5

The right column in Table 23 shows the 3D, top, and cross-sectional views of CO₂ migration after 500 years computed by CMG-GEM. SCA is able to reflect the migration

1 of the CO₂ plume to both the eastern and western regions adjacent to the main fault. The
2 CO₂ plume spreads to the longest extent in the east direction because the eastern regions
3 are updip. The CO₂ plume in the updip direction will continue to move to the north and
4 east directions because of buoyancy even though CO₂ is no longer injected. As shown in
5 the slices at $i = 48$ and $j = 48$, SCA captures the spatial features of the CO₂ plume that
6 migrates farthest away in the east direction.

7 Table 23 Comparison of CO₂ migration by SCA and CMG-GEM in the Johansen model.
8 The unit of the axes is meters. The z-axis is exaggerated by a factor of 10.

4.2. The Sleipner L9 model

The Sleipner L9 model is a benchmark model for the topmost layer of the Utsira formation in the Sleipner gas field where CO₂ has injected since 1999 (Singh et al., 2010). The data set for the Sleipner L9 model was released by Statoil in 2011. The approximation of the CO₂ migration in the Sleipner L9 model computed by SCA is compared with the full physics simulation result presented by Singh et al (2010).

The grid system of the Sleipner L9 model is 65 by 119 by 43. The lateral cell size is 50 by 50 m, and its thickness ranges from 0.0745 to 1 m. Table 24 shows the log₁₀ horizontal permeability and porosity of the entire model and the sandstone layers. The sandstone layers are between the top and bottom shale layers. The shale layers act like no flow boundaries and the lateral boundaries have constant pressure (Bandilla et al., 2014). The horizontal and vertical permeabilities range from 1692 to 1977 md and from 482 to 564 md, respectively. As shown in the sand permeability of Table 24, the shallower zone has higher porosity and permeability than the deeper zone.

Table 24 Log₁₀ horizontal permeability and porosity of the Sleipner L9 model. The unit of the axes is meters. The z-axis is exaggerated by a factor of 20.

Table 25 includes the input data for SCA for the Sleipner L9 model. The initial aquifer pressure (105 bar) and the bottom hole temperature (48°C) that Alnes et al. (2011) presented are used to calculate the properties of the CO₂ plume within SCA. Especially, we used the bottom hole temperature instead of the initial aquifer temperature (35.5°C) for SCA because it takes some time for the injected CO₂ to cool down to the initial aquifer temperature. The CO₂ density gradually changes from 461.5 kg/m³ at the bottom-hole temperature to 810.3 kg/m³ at the initial aquifer temperature as CO₂ moves far from the injector. However, the CO₂ density (461.5 kg/m³) at the bottom-hole temperature is used to reproduce the fast movement to the top layer of the buoyant CO₂ plume at the injector in SCA. Thus the viscosity and density of CO₂ and brine are thermodynamically calculated at the initial aquifer pressure and the bottom-hole temperature.

Table 25 Input data of SCA for the Sleipner L9 model for 2008

Aquifer structure	Average thickness	11.3 m
Operating conditions	Injection period	10 years
	Injector location	(i, j, k) = (36,75,36)
	Injection rate at the initial aquifer conditions	290 kg/day
	Total injected volume at the initial aquifer conditions	2453608 m ³
Fluid properties in aquifer	CO ₂ saturation at the end point	0.89
	CO ₂ relative permeability at the end point	0.75

conditions	Average CO ₂ viscosity	0.035 cp
	Average CO ₂ density	461.5 kg/m ³
	Average brine viscosity	0.567 cp
	Average brine density	993 kg/m ³
	Average CO ₂ saturation	0.89
Others	Minimum downdip	1°
	Maximum downdip	5°
	Power of downdip factor	0.5

The solid line in Figure 14 shows the cumulative mass of the injected CO₂ that Singh et al. (2010) used in the Sleipner L9 model. The dashed line with asterisks in Figure 14 represents the average mass rates from 1999 to 2008, which are the cumulative masses divided by the injection periods. CO₂ plume migrations should be approximated using SCA for multiple times (1999, 2001, 2002, 2004, 2006, 2008), but the average mass rate is not constant and it continues to increase as the dashed line with asterisks in Figure 14 shows. However, pressure gradients are calculated at a constant flow rate because steady state is assumed in SCA. Thus one that represents the varying flow rate should be chosen for each year. When SCA was conducted with the average mass rates corresponding to the multiple times, the SCA approximations had the longer and larger extent of the plumes. This is because the average mass rate causes the pressure gradients to be overestimated because the average mass rate increases sharply. Therefore the median of the average mass rates is used to calculate the pressure gradients instead of the average mass rate. The dashed line with squares in Figure 14 represents the median mass rates from 1999 to 2008 and they are the median values in the average mass rates from 1999 to their years. For example, the average mass rates are 114.16, 171.23, 190.26, and 228.31 for 1999, 2001, 2002, and 2004, respectively. The median mass rate for 2004 is the median of 114.16, 171.23, 190.26, and 228.31. The median mass rate for each year is used to calculate the pressure gradients in each year. The end point of the CO₂ relative

1 permeability curve that Singh et al. (2010) provides is used for $\hat{S}_{CO_2}$ and $\hat{k}_{r,CO_2}$ in
 2 Equation (3).

3
 4 Figure 14 Cumulative masses, average mass rates, and median mass rates of injected CO₂
 5 in the Sleipner L9 model from 1999 to 2008 (Singh et al., 2010)

6 Singh et al. (2010) provided the results of ECLIPSE 300 (©Schlumberger)
 7 simulation in the Sleipner L9 model from 1999 to 2008. Table 26 shows the results
 8 obtained using SCA for the Sleipner L9 model for the same duration. SCA reproduces the
 9 migration of the CO₂ plume along the north-south direction observed in ECLIPSE 300
 10 results presented by Singh et al. (2010). SCA captures the spatial features of the CO₂
 11 plume that migrates to a longer extent in the north-east region than in the north-west
 12 region. In SCA, the migration to the north-west region is overestimated compared to the
 13 ECLIPSE 300 results. However, SCA presents similar approximations in terms of the
 14 shape and size of the CO₂ plume during all the periods compared to the ECLIPSE 300
 15 results.

16 Table 26 CO₂ plume migrations computed by ECLIPSE 300 and SCA for the Sleipner L9
 17 model from 1999 to 2008

ECLIPSE 300 results presented by Singh et al. (2010)
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5. QUANTIFICATION OF UNCERTAINTY IN CO₂ MIGRATION USING SCA

The final goal of this study is to quickly quantify the uncertainty in the spatial features of CO₂ plumes over a large suite of heterogeneous models. However, it takes a tremendous computation cost to run a full physics simulator in the large suite of the models. The uncertainty can be quickly quantified through a ranking process using a proxy (Ballin et al., 1992; Deutsch and Srinivasan, 1996; Scheidt and Caers, 2009). A fast proxy, SCA, is used to compute CO₂ plume migrations in the large suite instead of the full physics simulator. The models are ranked based on the extent of the approximated CO₂ plumes and then they are sampled with an interval. The sampled models are considered as the representatives of the entire suite. The uncertainty in the spatial features of CO₂ plumes are quickly quantified by conducting full physics simulations in the representative models instead of the entire suite.

The procedure of the ranking process using SCA is as follows:

- i) Approximate the CO₂ plume migration in a suite of models using SCA

- 1 ii) Calculate the extent of the CO₂ plumes in the north, south, east, and west
- 2 directions in the proxy results
- 3 iii) Rank and sort the models based on the proxy extent of the CO₂ plumes
- 4 iv) Sample representative models with an interval
- 5 v) Run a full physics simulator in the representative models
- 6 vi) Calculate the P10, P50, P90 quantiles of the extent of the CO₂ plumes in the
- 7 north, south, east, and west directions based on the full physics simulation
- 8 results in the representative models

9 The ranking process is applied to two cases: a variogram based modeling case and
10 an object modeling case. Geological models for the two cases are generated based on a
11 variogram based modeling technique and an object modeling technique, respectively.
12 SCA is applied to quantify the uncertainty in the extent of CO₂ plumes in geological
13 models generated using two different geostatistical techniques.

14 **5.1. Variogram based modeling case**

15 In this case, 400 heterogeneous geological models are generated using the
16 sequential Gaussian simulation and the sequential Gaussian co-simulation, which are
17 variogram based techniques. Table 27 shows the details of the three different
18 distributions of porosity and horizontal permeability in the 400 models. In the case names
19 of Table 27, short and long mean short and long correlation lengths, and NS and EW
20 mean the north-south and east-west correlation directions. The horizontal-to-vertical
21 permeability is 0.1.

22 Table 27 Three kinds of geological models in the variogram based modeling case

Number of models	200 models	100 models	100 models
Dataset name	Short NS	Long NS	Long EW
Mean and standard deviation of ϕ	(0.2, 0.05)	(0.2, 0.04)	(0.2, 0.04)

Minimum and maximum of ϕ	(0.05, 0.35)	(0.1, 0.3)	(0.1, 0.3)
Mean and standard deviation of $\log_{10} k$	(2.5, 0.35)	(2, 0.53)	(2, 0.53)
Minimum and maximum of $\log_{10} k$	(1.6, 3.4)	(0.8, 3.2)	(0.8, 3.2)
Major correlated direction of ϕ and k	North-south	North-south	East-west
Correlation lengths of ϕ and k in terms of cells	(20, 15, 5)	(40, 10, 3)	(40, 10, 3)
Correlation of ϕ and k	0.8	0.7	0.7

Figure 15 shows the aquifer structure. The grid system is 151 by 151 by 10 and the cell size is 100 m by 100 m by 5 m. A CO₂ injector is located at the center of the aquifer. The boundary is connected to an infinite aquifer allowing brine displacement. The relative permeability curves shown in Figure 9 are used.

Figure 15 Aquifer structure in the variogram based modeling case. The unit of the axes is km. The z-axis is exaggerated by a factor of 20.

Table 28 shows the input data of SCA. The fluid properties are obtained from the CMG-GEM results. Different average permeabilities are used for the three datasets when the pressure gradients are calculated using Equation (4). 1500 md is used for the short NS and 500 md is used for the long NS and the long EW. This is because as described in Table 27, the long NS and long EW have the same cumulative distribution of permeability, but their distribution is different from that in the short NS.

1

Table 28 Input data of SCA for the variogram based modeling case

Aquifer structure	Size	15.1 km * 15.1 km * 50 m
	Dimensions of a grid cell	100 m * 100 m * 5 m
Operating conditions	Injection period	3 years
	Injector location	(i, j, k) = (101, 101, 3) ~ (101, 101, 5)
	Injection rate	20,000 m ³ /day in bottom hole conditions
Fluid properties in aquifer conditions	CO ₂ saturation at the end point	0.7
	CO ₂ relative permeability at the end point	0.8
	Average CO ₂ viscosity	0.0445 cp
	Average CO ₂ density	545 kg/m ³
	Average brine viscosity	0.3538 cp
	Average brine density	1008 kg/m ³
	Average CO ₂ saturation	0.4
Others	Minimum downdip	1°
	Maximum downdip	5°
	Power of downdip factor	0.5

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In Table 29, the CO₂ plumes in the CMG-GEM results migrate along the 45° counter-clockwise, the north-south, and the east-west permeable features near the injector in the three models. The CO₂ plume in the long EW is smaller than the short NS and the long NS because the permeable zones near the injector in the top layer of the long EW are smaller than the others. SCA reproduces such spatial characteristics of the CO₂ plumes in the CMG-GEM results.

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Table 29 Porosity, log₁₀ horizontal permeability, SCA result, CMG-GEM result in each dataset of the variogram based modeling case. The unit of the axes is km. The z-axis is exaggerated by a factor of 20.

1 The extent of the CO₂ plume in the north, south, east, and west directions are
 2 measured in order to rank the 400 models. Figure 16 shows the extent of the CO₂ plume
 3 in the north, south, east, and west directions calculated by CMG-GEM and SCA in the
 4 400 models. The correlations between these results in the 400 models are 0.91, 0.84,
 5 0.88, and 0.87 in the north, south, east, and west directions, respectively. In the CMG-
 6 GEM results, the extent of the CO₂ plume from the injector in each direction is calculated
 7 in the zone that has CO₂ saturation greater than 0.01.

Figure 16 Scatter plots of the extent of the CO₂ plume from the injector in the north, south, east, and west directions in the CMG-GEM and SCA results

The 10% of the 400 models are sampled based on the extent of the CO₂ plume computed using SCA in each direction. The P10, P50, and P90 of the extent in each direction are calculated in the full physics simulation results of the sampled 40 models. Figure 17 shows the cumulative distribution function (CDF) of the plume extent in the four directions based on the CMG-GEM results and the P10, P50, and P90 of the plume extent computed in the sampled 40 full physics simulation results. As shown in Figure 17, the P10, P50, and P90 values in the sampled models are close to the full physics results.

Figure 17 Cumulative distribution functions and quantiles of the CO₂ plume lengths in the CMG-GEM results and the samples selected based on the SCA results

It takes about 700 seconds and 2.2 seconds to run CMG-GEM and SCA in a model, respectively. The parallel version of the CMG-GEM simulator was run on 6 processors, but a single processor was used for SCA. The total computational cost is $400 * 700 / 3600 = 77.78$ hours for the ranking process using CMG-GEM and $(400 * 2.2 + 40 * 700) / 3600 = 8.02$ hours for the ranking process using SCA. About 90% of the computational cost is saved in computing P10, P50, and P90 by ranking the 400 models using SCA.

As shown in Figure 18, SCA captures the overall spatial characteristics of the mean profile of the CO₂ saturations computed using CMG-GEM. In Figure 18 (a), the red rectangles connect the P10, P50, and P90 quantiles of the extent of the CO₂ plumes in the north, south, east, and west directions estimated on the basis of the 40 models sampled from the SCA results. The small, medium, and large rectangles represent P10, P50, and

1 P90, respectively. The red rectangles cover the extent of the CO₂ plume in the CMG-
 2 GEM results.

3 Figure 18 Means of CMG-GEM CO₂ saturations and SCA approximations in 400
 4 models. The unit of the axes is km.

5 **5.2. Object based modeling case**

6 Issautier et al. (2014) pointed out that variogram-based modeling techniques (or
 7 two-point statistics techniques) fail to reproduce CO₂ storage capacity for fluvial
 8 reservoirs with high sinuosity because they ignore the connectivity characteristics of
 9 fluvial sand channels. In this case, we see if SCA works for fluvial models generated
 10 using an object modeling technique (Bridge and Leeder, 1979; Deutsch and Wang, 1996;
 11 Keogh et al., 2007).

12 For this object modeling case, we use the model parameters of the base case in the
 13 section 3.1. such as the aquifer structure shown in Figure 11(a), the operation conditions,
 14 the fluid properties, and the relative permeability curves shown in Figure 9. Thus the
 15 input data for SCA are the same to those in Table 4. Only different geological models are
 16 used. The model is assumed to have a north-south oriented fluvial depositional
 17 environment shown in Figure 19. In Figure 19, yellow is sand and the background is
 18 shale. The horizontal permeability and porosity of sand and shale are 300 md, 0.2 and 1

md, 0.1, respectively. The ratio of horizontal and vertical permeabilities is 0.1. 200 fluvial models are generated using the TiGenerator in SGeMS (Boucher et al., 2010). The thickness is 5 vertical grid cells and the width is 15 lateral grid cells. CO₂ is injected at (i, j, k) = (101, 101, 3) at 18,690.8 kg/day during 1 year. All of the 200 models have sand facies at the injector location. The boundary is connected to an infinite acting aquifer where fluid displacement is allowed.

Figure 19 A fluvial geological model. The unit of the axes is meters. The z-axis is exaggerated by a factor of 20.

Figure 20 shows the results of SCA and CMG-GEM in the geological model shown in Figure 19. In this model, there is no sand facies near the injector at $k = 9$ and 10 where the k index at the top is 10 . The 8th layer is the top most layer where the injector is connected to the sand facies. Thus the CO₂ plume vertically migrates up to the 8th layer and then starts to spread horizontally in the 8th layer. As shown Figure 20(b) and (c), SCA reproduce the spatial features of the CO₂ plume that migrates along the permeable zone in the 8th layer.

Figure 20 Sand facies in the $k = 8$ slice through the 3D reservoir model, SCA result, and CO₂ saturation computed by CMG-GEM in that slice obtained after performing the simulation on the 3D model shown in Figure 19. The unit of the axes is meters. The z-axis is exaggerated by a factor of 20.

The extent of the CO₂ plume from the injector in the north, south, east, and west directions are calculated using the results obtained by SCA and CMG-GEM. In the CMG-GEM results, the extent of the CO₂ plume is the maximum distance from the injector in each direction in the zone that has CO₂ saturation greater than 0.01. Figure 21 shows the extent of the CO₂ plumes in the north, south, east, and west directions in the CMG-GEM and SCA results. In Figure 21, the x-axis and the y-axis represent the results in SCA and CMG-GEM, respectively. The correlations computed using the 200 fluvial models are 0.52, 0.65, 0.74, and 0.73, respectively. The correlations in the north and south directions are smaller than those in the east and west directions. This is because the variations in the extent of the plume in the north and south directions are smaller than those in the other two directions as shown Figure 21. The main orientation of the channels is the north-south direction, and most of the models have the CO₂ plume extending in those directions. In contrast, the plume migration in the east and west directions depends on the sinuosity of the channel bodies connected to the injector. For this reason, the permeable zones have larger variations in the east and west directions

1 than in the north and south directions. These variations are greater than the resolution of
 2 the SCA model and consequently the correlations in the east and west directions are
 3 better.

4 Figure 21 Scatter plots of the extent of the CO₂ plume from the injector in the north,
 5 south, east, and west directions in the CMG-GEM and SCA results

6 The 200 models are ranked in the order of the extent of the CO₂ plume computed
 7 using SCA and then 10% of the 200 models are sampled (corresponding to equally
 8 spaced quantiles of the cdf of the plume front distance from the injector). The P10, P50,
 9 and P90 of the plume extent are computed by running the full physics simulator, CMG-
 10 GEM, on the 20 sampled models. Figure 22 shows the cumulative distribution function
 11 (CDF) of the plume extent in different directions based on the CMG-GEM results and the
 12 P10, P50, and P90 of the plume extent computed in the sampled 20 full physics

1 simulation results. As shown in Figure 22, the P10, P50, and P90 values for the plume
 2 extent in the sampled models are close to the full physics results.

3 Figure 22 Cumulative distribution functions and quantiles of the CO₂ plume lengths
 4 based on the CMG-GEM results and the samples selected based on the SCA results

5 It takes about 2500 seconds and 4 seconds to run CMG-GEM and SCA using a
 6 geological model, respectively. The parallel version of the CMG-GEM simulator was run
 7 on 6 processors, but a single processor was used for SCA. The total computational cost
 8 for the CMG-GEM simulation is $200 * 500 / 3600 = 138.89$ hours and $(200 * 0.7 + 20 * 500) / 3600 = 14$ hours for SCA. About 90% of the computational cost is saved in
 9 estimating P10, P50, and P90 using SCA.
 10

In Figure 23(a) and (b), the migration of the CO₂ plume in the north and south directions are slightly overestimated in the mean profile computed using the SCA approximations compared to that by the CMG-GEM. In Figure 23(a), the red rectangles connect the P10, P50, and P90 estimates for the extent of the plume in the north, south, east, and west directions estimated using the sampled 20 models. The red rectangles cover most of the CO₂ saturated zone in Figure 23(a).

(c) Mean (>0.01) of CO₂ saturations computed using CMG-GEM in 200 models

(d) Mean (>0.01) of approximations computed using SCA in 200 models

Figure 23 Means of CMG-GEM CO₂ saturations and SCA approximations in 200 models. The unit of the axes is meters. The z-axis is exaggerated by a factor of 20.

6. CONCLUSIONS

The final goal of this study is to quickly quantify the uncertainty in the spatial and the temporal features of CO₂ plume migrations. However, it is impractical to run a full physics simulator on a large suite of geological models. We propose a fast alternative method named SCA for approximating the CO₂ plume migrations, and to save the computational cost of quantifying the uncertainty in the CO₂ plume migrations.

In SCA, adjacent grid cells are assumed to be connected with edges and the edge weight are defined as a travel time. SCA scales the edge weights with their local minimum in order to reproduce a CO₂ plume flowing along the locally minimum edges because of strong buoyancy. The scaled connectivity that is the cost of the shortest path

1 from an injector in the scaled graph is used to determine the sequence in which grid cells
2 are filled with CO₂.

3 SCA was validated by changing several conditions in the base case. Results that
4 were close to the full physics responses were obtained corresponding to variations in an
5 injection period, an injection rate, a CO₂ density, a CO₂ viscosity, the degree of rock
6 heterogeneity, permeability of a cap rock. SCA presented better approximations than CA,
7 the fast marching method, and the vertical equilibrium model in the heterogeneous cases.
8 However, SCA does not work properly when the rock heterogeneity is weak or the
9 aquifer structure has an overwhelming influence on a CO₂ plume migration.

10 SCA was applied to two real field cases, the Johansen model and the Sleipner L9
11 model. In both of the cases, SCA captured the spatial and temporal characteristics of the
12 CO₂ plumes.

13 SCA was used to quickly quantify the uncertainty in the extent of CO₂ plumes in
14 models that are described using two-point statistics and fluvial models with strong
15 sinuosity. In the cases, SCA provided the accurate proxy responses that reflect the plume
16 migration in the different directions. The initial suite of geological models was ranked
17 and sampled based on the proxy responses. The P10, P50, and P90 of the full physics
18 simulation in the sampled models were calculated. About 10% of the total computational
19 cost was required to quantify the P10, P50, and P90 responses bracketing the uncertainty
20 in the extent of the CO₂ plumes in each direction.

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