Effect of upscaling heterogeneous domain on CO₂ trapping mechanisms

Ehsan Saadatpoor*, Steven L. Bryant, Kamy Sepehrnoori

Department of Petroleum and Geosystems Engineering, The University of Texas at Austin, 1 University Station C0300, Austin, TX 78712, USA

Abstract

We study the effect of upscaling (based on single-phase properties) on buoyancy-driven vertical flow of CO₂. The mechanism of CO₂ immobilization of interest in this situation is local capillary trapping, resulting from competition between buoyancy and capillarity in fine-scale heterogeneity. Different degrees of coarsening are considered and based on average gas saturation and mass of CO₂ in storage aquifer, these upscaling methods are found to underestimate the extent of local capillary trapping. Then, we upscale the simulation of a leak at the top seal of the aquifer after buoyancy-driven flow has stabilized, again with the single phase upscaling method. The predicted amount of escaped gas is larger for the upscaled simulations, and as such, single-phase upscaling appears to underestimate the security of CO₂ sequestration in heterogeneous formations. Using a corrected value of residual gas saturation in coarse-grid simulations is shown to give an acceptable result for the mass percent of escaped CO₂.

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Keywords: Local capillary trapping; Capillary entry pressure; Buoyancy; Residual saturation; Leakage.

1. Introduction

Assessment of capacity of the storage formation is one of the essential phases of any carbon sequestration project. Assessment of the fraction of the capacity that is stored securely, i.e., stored with negligible risk of escape, is increasingly important. Numerical simulations are widely used to estimate different modes of trapping and to analyze the risk of using the formation as a potential storage zone. In carbon sequestration in deep saline aquifers, CO₂ displaces brine during injection and may continue to migrate by buoyancy after injection ends. During the migration of bulk phase CO₂, various modes of trapping occur. In the carbon storage literature, secure trapping in deep saline aquifers is commonly categorized as residual trapping, dissolution trapping, local capillary trapping, and mineral trapping. The local capillary trapping takes place during buoyancy-driven flow through rocks with fine-scale heterogeneity [1]. This mode of trapping occurs in heterogeneous domains and can be seen across a wide range of length scales. Of particular interest is the fine-scale heterogeneity (mm to m scale) that is characteristic of many depositional environments.

* Corresponding author. Tel.: +1-512-913-5804; fax: +1-512-471-9605.
E-mail address: ehsan@mail.utexas.edu.

doi:10.1016/j.egypro.2011.02.480
Capillary trapping in correlated structures within the heterogeneity can only be seen in simulations that use homogeneous capillary pressure field. Using homogeneous capillary pressure field or even several rock types in a heterogeneous domain fails to capture local capillary trapping. However, fine-scale simulation is always costly and often impractical; therefore, an upsampling method would greatly facilitate assessment of secure storage capacity in large formations nominated for storage. In addition, the uncertainties associated with the heterogeneity modeling and the need to perform long term predictions (the order of 1000 years) make it more reasonable to assess the initial estimates based on some coarse-grid simulations. The challenge, then, is for the coarse-scale model to capture the effect of fine-scale features on the distribution of CO2. Some of these effects include whether the CO2 reaches the top seal of the storage formation, the time it takes for CO2 to reach the top seal, and the amount of CO2 leakage if a presumptive leak develops in the top seal.

Upscaling is defined as a method of converting petrophysical properties (e.g., porosity, permeability, and phase saturation) from a fine-scale grid system to a coarse-scale grid system such that the two systems are equivalent or behave as similarly as possible. This involves special considerations in heterogeneous formations in order to establish a balance between simulation time in the coarse-grid model and preservation of important dynamic behavior in the fine-grid model. Moreover, it is now known that the type of fluid displacement process also affects the quality of the upsampling method. An approach which is accurate for single phase flow may prove inadequate for viscosity-dominated multiphase flow, and an approach accurate for the latter may not work well when displacement is driven by buoyancy.

Arithmetic averaging is routinely applied to upscale the additive scalar properties such as porosity, fluid saturation, and component mole fractions. Using this averaging approach necessarily decreases the standard deviation of the frequency distribution of the property. Bigger sample volumes also bring about smaller standard deviation for the property, and more similarity to the homogeneous conditions. However, the real challenge arises for nonadditive properties, permeability and multiphase flow properties above all. The effective permeability of an upscaled heterogeneous medium is defined as the permeability of a homogeneous medium such that both provide the same flux for the given boundary conditions. Therefore, both the distribution of heterogeneities and the boundary conditions are important in upsampling of a heterogeneous medium [2]. Several methods are discussed in the literature for upsampling permeability, including power-law average, renormalization, pressure-solver method, and pseudofunction technique [3].

Residual phase saturation is another important property, particularly in operations like CO2 storage where imbibition takes place. This multiphase property has a great impact on residual trapping and the mass of escaped CO2 if the aquifer leaks through a rupture in the overlying seal. Underestimating residual saturation in an upscaled model might result in disqualification of a candidate aquifer due to wrong estimation of secure storage capacity. Overestimating it can lead to accepting a risky candidate aquifer. So finding the proper value of S_{grmax} for upscaled model can help in performing timesaving simulations in order to estimate the risk of leakage. However, still this upscaled value might not be able to capture the dynamics of the flow like distribution of different trapping mechanisms in the project.

The competition between buoyancy and capillary entry pressure which causes local capillary trapping does not depend on residual saturation. Indeed, the salient feature of local capillary trapping is that the most of the saturations in the accumulations are far above residual. Nevertheless, treating the CO2 held in local capillary traps as though it were a residual phase has some appeal. If a suitably upscaled or equivalent value of residual saturation can be found, then incorporating that value into commercial and research codes being used for sequestration simulations and risk assessment is straightforward. The challenge here is to account for the range of possible displacement behavior. We anticipate that the correlation length of the small-scale heterogeneity will affect the equivalent residual saturation. More complicated is the behavior of CO2 in local capillary traps after a leak develops in the overlying seal. If the CO2 is connected to CO2 which has risen under buoyancy to accumulate at the top of a structure, then the amount that remains in the trap after a leak is a stochastic function of the leak location [4]. If the CO2 in the local trap is not connected to the accumulation, then it will not be displaced, regardless of whether or not the seal leaks. Thus, process dynamics for local capillary trapping strongly influence the upsampling method.

In this work, first we study the effect of upsampling based on single-phase properties on buoyancy-driven vertical flow of CO2. Porosity and absolute permeability are upscaled, then used to scale the endpoint capillary pressures using Leverett scaling group. Relative permeabilities and reference capillary pressure curve are kept unchanged for the upscaled model. Different degrees of coarsening are considered and results are analyzed based on average gas.
saturation and mass of CO₂ in storage aquifer. Then, simulation of a leak at the top seal of the aquifer is upscaled, again with the single phase upscaling method, and the results are analyzed. Finally, using a corrected value of residual gas saturation in coarse-grid simulation is shown to give an acceptable result for the mass percent of escaped CO₂.

2. Simulation model

The Computer Modeling Group’s GEM simulator is used in this study. Dissolution of CO₂ in brine as well as residual trapping of CO₂ is considered, but geochemical reactions are not used and mineral trapping is neglected.

We use a simplified aquifer model to study the dynamic behavior of buoyancy-driven flow of CO₂ during post-injection phase. The two-dimensional aquifer is 400 ft wide. A large saturation of CO₂ emplaced at the bottom of the aquifer represents the distribution of CO₂ at the end of the injection phase that is done low into the aquifer. Aquifer temperature is held constant at 140°F and initial pressure is assumed to be 2,265 psi at 5,300 ft reservoir depth. Both values are typical values of a conventional deep saline aquifer in the Gulf Coast. The base case is run with a 1 ft by 1 ft fine grid system.

The Peng-Robinson equation of state is used to model fluid properties. This equation is tuned for H₂O-CO₂ system by Kumar et al. [5] using experimental data for density and solubility over a wide range of pressures, temperatures, and salinities related to deep saline aquifers. The brine salinity of 100,000 ppm is assumed for the aquifer. The Pedersen correlation is used for viscosity of brine phase [6].

A synthetic heterogeneous permeability field is generated for 40,000 grid blocks of the base case. The permeability field has a log-normal distribution with a mean value of 190 md. The standard deviation of natural logarithm of permeability is 1.23. Correlation length is 50 ft in the horizontal direction, but uncorrelated in the vertical direction. The permeability field is assumed to be isotropic. Based on this permeability field, porosity and relative permeability hysteresis parameters (irreducible water saturation and maximum residual gas saturation) are generated using Holtz equations [7]. Porosity is generated for every grid block, but a single value is estimated for relative permeability hysteresis parameters.

The Brooks-Corey capillary pressure model is used in this study [8]. A reference curve with capillary entry pressure of 1.2 psi and compatible with relative permeability hysteresis parameters is generated and assigned to the average permeability of the field. Then, this reference capillary pressure curve is scaled for every grid block via Leverett scaling group,

\[ P_{c2}(S_w) = P_{c1}(S_w) \frac{k_1}{k_2} \frac{\phi_2}{\phi_1}. \]  

Therefore, the permeability and porosity of the heterogeneous domain are affecting the drainage capillary pressure curves, making the capillary entry pressure field heterogeneous. The capillary pressure hysteresis is neglected in this work considering its small impact compared to hysteresis in gas relative permeability.

To study the security of storage, we assume another aquifer is located above the storage aquifer and a 1 ft shale layer acts as the top seal that separates the two aquifers. (The thin barrier is for convenience; previous work has shown its thickness does not affect the ultimate amount of leakage.) A prescribed amount of CO₂ is emplaced into the storage formation as an initial condition and is allowed to accumulate below the top seal after 50 years of buoyancy-driven flow. Then a fracture appears in the top seal. The CO₂ is now subject to an open path through the upper aquifer. The leak is 2 ft wide and gives enough space to both the CO₂ and brine to move past each other in different directions, if they do so.

3. Upscaling

In this work, we use single phase upscaling to upscale the single phase properties of the model, namely porosity and permeability. The calculated values of porosity and permeability are used to calculate the drainage capillary pressure curve for new coarse grid blocks by scaling the original capillary pressure curve via the Leverett scaling group, equation (1). The relative permeability curve and maximum residual gas saturation are assumed to be constant for the whole system regardless of upscaling. This assumption will be shown to be impractical and will need to be changed during the upscaling process.
We use the arithmetic average of the original grid blocks as the equivalent porosity of the coarse grid block:

\[ \phi_e = \frac{\sum_{i=1}^{n}(V_{p_i}\phi_i)}{\sum_{i=1}^{n}V_{p_i}}, \]  

(2)

where \( \phi_e \) is effective porosity of the coarse grid block, \( V_p \) is pore volume, \( \phi \) is porosity, subscript \( i \) denotes the \( i \)’th original grid block, and \( n \) is the total number of original grid blocks in the coarse grid block.

Geometric averaging is shown to be the best method of approximating effective permeability regardless of the type of permeability distribution [9]. In practice, for horizontal and vertical flow, arithmetic averages and geometric averages are used, respectively [2]. Therefore, we also use geometric mean to upscale permeability in our study of the buoyancy-driven vertical flow of CO₂:

\[ k_e = (\prod_{i=1}^{n} k_i)^{1/n}, \]  

(3)

where \( k_i \) is the permeability of the \( i \)’th original grid block in the upscaled sample.

4. Results and discussion of simulations

4.1. Upscaling and local capillary trapping

Twenty-two ft of CO₂-saturated layers are assumed to be present at the bottom of the 110 ft high 2D aquifer at the beginning of post-injection relaxation period. The CO₂ then moves upward due to the buoyancy effect while competing with capillary forces. Figure 1 shows gas saturation profile after 50 years of buoyancy-driven flow in the original fine grid system as well as upscaled systems with different levels of coarsening. In all cases buoyant flow is almost at steady state.

In the original 1×1 ft fine grid, Figure 1(a), large saturations (yellow and orange pixels) of gas have remained below local capillary barriers throughout the flow path. These accumulations constitute the local capillary trapping.

Figure 1(b) through (e) show the saturation profile for upscaled system with coarse grid blocks of 2×2 ft, 4×4 ft, 10×10 ft, and 20×20 ft, respectively. Even in Figure 1(b) with grid blocks of 2×2 ft, the CO₂ does not follow the same preferential flow paths as in original grid. This shows that conventional upsampling of a permeability field with large correlation length compared to the block size will substantially change a buoyancy-driven multiphase displacement. This is because local capillary barriers are large and tend to induce horizontal flow. The existence of the barriers is due to local variation in permeability which is diminished by conventional upsampling. Thus, upsampling opens new vertical flow paths which the gas follows; hence, the saturation distribution substantially changes.

As can be seen in Figure 1(b) through (e), as the degree of coarsening increases, the amount of local capillary trapping decreases. In Figure 1(c) some local capillary trapping can still be seen. In Figure 1(d) the gas displacement still shows the heterogeneity of the domain but no local capillary trapping; instead the behavior is almost identical to that when capillary pressure is homogeneous throughout a heterogeneous domain. Figure 1(e) shows little evidence of heterogeneity. Although this approaches the grid size needed for field-scale simulations, the comparison with fine-scale simulations shows that the dynamics of the behavior have completely changed after upsampling.

Table 1 shows the average saturation and mass of CO₂ in the top 88 ft of the storage aquifer, seen in Figure 1, after 50 years of buoyant flow. As discussed earlier, as the extremes of permeability are smeared by upsampling, the behavior becomes more homogeneous and less CO₂ is trapped in local capillary traps inside the emplacement zone, so the average gas saturation above the emplacement zone slightly increases. This is clearer when we see a similar trend for the total mass of CO₂ in the same zone. An equal amount of CO₂ in the storage zone for 10×10 and 20×20 grid blocks shows that local capillary trapping has been suppressed in this level of upsampling.

<table>
<thead>
<tr>
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<th>1×1</th>
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<th>4×4</th>
<th>10×10</th>
<th>20×20</th>
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<tr>
<td>Average gas saturation</td>
<td>9.9%</td>
<td>10.6%</td>
<td>10.2%</td>
<td>11.0%</td>
<td>10.9%</td>
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<tr>
<td>Mass of aqueous CO₂</td>
<td>2.7</td>
<td>2.7</td>
<td>4.6</td>
<td>5.6</td>
<td>5.3</td>
</tr>
<tr>
<td>Mass of scCO₂</td>
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<td>16.2</td>
<td>15.3</td>
<td>15.1</td>
<td>14.9</td>
</tr>
<tr>
<td>Total Mass of CO₂</td>
<td>17.9</td>
<td>18.9</td>
<td>19.9</td>
<td>20.7</td>
<td>20.2</td>
</tr>
<tr>
<td>% of originally emplaced CO₂</td>
<td>54.1%</td>
<td>57.3%</td>
<td>60.3%</td>
<td>62.7%</td>
<td>63.4%</td>
</tr>
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Table 1. Average gas saturation and mass of CO₂ (in tonnes) in the storage formation above the initial emplacement zone for cases seen in Figure 1, after 50 years of buoyant flow.
4.2. Upscaling and gas column height

In Figure 1(a) with the original fine grid, the CO₂ has risen to a height of 30 ft below the seal at steady state. All of the emplaced CO₂ is trapped in the form of residual, dissolution, or local capillary trapping without any risk of leakage. Although in Figure 1(b) more CO₂ has made its way to the storage zone, it goes through some horizontal flow paths and the gas column height is still the same for both. This level of upscaling has maintained the model’s ability to predict the gas column height.

Figure 1. Gas saturation profile of the base case with 22 ft of initially emplaced CO₂ after 50 years (a) with 1×1 ft fine grid system with 50 ft horizontal correlation length. The grid and single phase flow properties are upscaled to blocks of (b) 2×2 ft, (c) 4×4 ft, (d) 10×10 ft, and (e) 20×20 ft. In (a) and (b) CO₂ has risen to a height of 30 ft below the seal, while in (c) and (d) CO₂ has risen to the top seal and in (e) it has just passed mid-way toward the top.
In contrast, upscaling to coarser grid blocks has changed the prediction. Comparison with Figure 1(c) and (d) shows that some local capillary barriers are lost as a result of upscaling; hence, the CO₂ has found a narrow high permeable channel with low entry pressure at the right side of the domain that acts as a connecting path to the top seal. This introduces the risk of undesired CO₂ movement, either migration beyond an authorized zone or leakage through an unexpected leak in the seal. Thus, the simulation in (c) and (d) would overestimate the risk associated with this amount of storage.

4.3. Upscaling and gas leakage

The results of leak simulation are shown in Figure 2. Initially, 62 ft of CO₂-saturated layers are emplaced at the bottom of the 150 ft high aquifer and arrive at steady state after 50 years of relaxation. Then a leak is developed at 110 ft to the left of the domain. We assume that a leak at this position gives the mean value of gas leakage from this formation. The gas saturation profile after 50 years of leak development (i.e., 100 years after injection) is shown in Figure 2 for the original and upscaled grid blocks. In all of the grids, the 1 ft thick shale layer is constructed by 1×1 ft grid blocks and the 2 ft wide leak is located at the exact same position in this layer. In 20×20 ft grid, the blocks at the top and bottom of the leak are refined to have the CO₂ flow through the narrow leak.

In Figure 2(a) with the original fine grid, while a lot of CO₂ is trapped below the wide horizontal local capillary barriers inside the storage formation, there is a path for CO₂ to reach the top seal at the left side of the domain and no CO₂ has reached the top right of the domain. In Figure 2(b), again the loss of these wide horizontal local capillary barriers has made it possible for CO₂ to invade the top right zone as well. The saturation profile and swept zone substantially changes with more upscaling, as can be seen in Figure 2(c) through (e).

Table 2 quantifies the amount of CO₂ escaped through the leak as mass percent of originally emplaced CO₂. Remarkably smaller masses of CO₂ escape in the original fine grid block compared to the upscaled grids. Again, the loss of several major horizontal local capillary barriers in the upscaling process can be the reason. This shows that even a small degree of coarsening can disturb the risk assessment calculations and estimations, although it might still be helpful in predicting some flow behavior like gas column height.

4.4. Effective residual saturation

As we saw in preceding simulations, single phase upscaling cannot be used for CO₂ storage applications where there is a special interest in gas column height and amount of gas leakage. Some multiphase flow property should also be involved in upscaling process in order to use it for risk assessment purposes. Here we examine the potential of maximum residual gas saturation as a candidate. We try to find an effective residual gas saturation for the upscaled grid that leads to same amount of escaped gas due to presumptive leakage as in the original fine grid after 100 years (13.3% in Table 2). Table 3 and Table 4 show the results for 4×4 ft and 10×10 ft block size, respectively. As can be seen in Figure 3, mass of escaped CO₂ has a linear relationship with $S_{grmax}$ in the upscaled simulations.

The upscaling has two different effects on the dynamics of CO₂ flow. Decreasing the degree of heterogeneity causes the elimination of local capillary barriers which decreases the mass of local capillary trapping. However, it also increases the sweep efficiency, and hence, increases the mass of residual trapping. The maximum residual gas

<table>
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<th>$S_{grmax}$ Base</th>
<th>0.325</th>
<th>0.345</th>
<th>0.350</th>
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</thead>
<tbody>
<tr>
<td>Mass of escaped CO₂</td>
<td>18.7</td>
<td>13.8</td>
<td>12.6</td>
</tr>
<tr>
<td>% of orig. emplaced CO₂</td>
<td>19.7</td>
<td>14.6</td>
<td>13.4</td>
</tr>
</tbody>
</table>

Table 3. Mass of escaped CO₂ (in tonnes) at 50 years after leakage in top seal for different values of $S_{grmax}$. Grid blocks are 4×4 ft.

<table>
<thead>
<tr>
<th>$S_{grmax}$ Base</th>
<th>0.325</th>
<th>0.345</th>
<th>0.350</th>
</tr>
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<tbody>
<tr>
<td>Mass of escaped CO₂</td>
<td>17.8</td>
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<td>18.3</td>
<td>15.1</td>
<td>13.5</td>
</tr>
</tbody>
</table>

Table 4. Mass of escaped CO₂ (in tonnes) at 50 years after leakage in top seal for different values of $S_{grmax}$. Grid blocks are 10×10 ft.
saturation needs to increase and decrease in order to compensate for these effects, respectively. Therefore, the net effect is not the same for different cases. Here for the large correlation length of 50 ft, the $S_{gr max}$ should decrease for coarser grid block to give the same value of escaped gas, which means the effect of sweep efficiency is dominant. Saadatpoor et al. [10] show that in case of a 5 ft correlation length, the $S_{gr max}$ should increase for coarser grid block to give the same value of escaped gas.

![Figure 2](image-url)

Figure 2. Gas saturation profile of leakage case with 62 ft of initially emplaced CO$_2$ after 50 years of leakage (a) with 1×1 ft fine grid system. The grid and single phase flow properties are upscaled to blocks of (b) 2×2 ft, (c) 4×4 ft, (d) 10×10 ft, and (e) 20×20 ft.
5. Conclusion

Considering the effect of heterogeneous capillary pressure in heterogeneous formations gives rise to local capillary trapping as capillary barriers induce the flow paths of buoyant CO₂. Hence, local capillary trapping is dependent on the heterogeneity of the domain. The well-known single phase upscaling approaches used in reservoir engineering reduce the extremes of permeability, especially if upscaling is conducted in uncorrelated directions (vertical in our 2D domains). Therefore, the heterogeneity of the domain and the local capillary trapping decrease. As the degree of coarsening increases, the resulting domains display more homogeneous behavior.

Upscaling above the limits of correlation length of heterogeneity is misleading in the risk assessment of a carbon sequestration project. Even well below this limit, the upscaling still may not preserve the dynamics of buoyant flow when correlation length is large compared to the original block size. A new method of upscaling is needed for CO₂ storage applications, like capacity assessment or risk analysis. Such a method should change the multiphase flow properties in a way that enables estimation of the storage capacity or amount of leakage in a CO₂ storage project. Considering the effect of residual gas saturation on the amount of trapping in storage aquifer, one can think of residual gas saturation as a proper candidate for this method of upscaling. A decrease of variance in the permeability field (as a result of upscaling) has opposing effects on value of effective residual saturation. On one hand, it causes a decrease in local capillary trapping; hence, promoting an increase in residual saturation to make up for this effect. On the other hand, the resulting domain is more homogeneous and a larger area of the domain is invaded by gas; therefore, a decrease in residual saturation is needed to adjust for this effect. The net result could be either a larger value of effective residual saturation (see results for a permeability field with 5 ft correlation length [10]) or a smaller value as was the case in this work. Overall, to get a more precise risk assessment of a project with an economical coarse-grid model the effective residual saturation can be employed.

Acknowledgments

We are grateful to the sponsors of the Geologic CO₂ Storage Industrial Associates Project at The University of Texas at Austin: BP, Chevron, ConocoPhillips, ExxonMobil, Foundation CMG, Landmark Graphics, Luminant, Shell, and Statoil.

References