Investigations in Geologic Carbon Sequestration: Multiphase Flow of CO₂ and Water in Reservoir Rocks

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Introduction

Carbon dioxide capture and sequestration (CCS) in deep geological formations has emerged over the past twenty years as an important component of the portfolio of options for reducing greenhouse emissions. Our research focuses on the fundamental science underpinning sequestration in saline aquifers and multiphase flow of $\text{CO}_2$, brine and to a lesser degree, oil. Saline aquifers have the largest sequestration capacity, as compared to oil and gas reservoirs or deep unmineable coal beds. Saline aquifers are also more broadly distributed and thus, closer to more emission sources. However, unlike oil and gas reservoirs with proven seals that have withstood the test of time, saline aquifers must be carefully characterized and monitored to assure that $\text{CO}_2$ will achieve high retention rates. Improved fundamental understanding of multi-phase flow and trapping in $\text{CO}_2$-brine systems will be needed to take advantage of this large storage capacity of saline aquifers. Important questions remain to be answered, such as, what fraction of the pore space will be filled with $\text{CO}_2$, what will be the spatial extent of the plume of injected $\text{CO}_2$, how much and how quickly will $\text{CO}_2$ dissolve in brine, and how much $\text{CO}_2$ will be trapped by capillary forces when water imbibes back into the plume and to what extent is capillary trapping permanent? Here we are developing new experimental data, new monitoring methods, and carrying out simulations to improve our ability to answer these questions. Modifications to currently accepted multiphase flow theory are being developed to provide reliable predictions of the fate and transport of $\text{CO}_2$ in the subsurface. A combination of laboratory experiments, numerical methods and analytical solutions are being developed to address these issues as shown in the schematic below (Figure 1). Interaction and iteration between these four approaches improves our ability to quickly identify and test new phenomena and approaches for accurately capturing them in quantitative models. Highlights from the past year are provided below.

Figure 1. Illustration of the 4 interrelated components of our approach to study multi-phase flow and trapping of $\text{CO}_2$. 
Numerical and Analytical Analysis of the Effects of Small Scale Heterogeneity on CO2/Brine Multiphase Flow System in Horizontal Core-Floods

A 2D semi-analytical model considering gravity and permeability heterogeneity has been developed for predicting brine displacement efficiency over a wide range of capillary numbers that provides good agreement with the simulated 3D results. The analytical derivation is general and the solution can estimate the flow regimes for horizontal core floods efficiently. An illustrative comparison between the semi-analytical solution and the results of 3-dimensional simulations including viscous, capillary, and gravity forces is shown in Figure 2.

Based on this new study, we also provide a simple parametric approach for including the influence of capillary heterogeneity on displacement efficiency of horizontal core-floods operating in the viscous dominated flow regime. The study shows that the greater the degree of heterogeneity, the lower the brine displacement efficiency. Similarly, as capillary forces increase in comparison to viscous forces, the brine displacement efficiency will also decrease. This work was published in Advances in Water Resources (Kuo and Benson, 2015).

Figure 2. Comparison between the average core saturation calculated with the 2-D semi-analytical solution and 3-D numerical simulations that include viscous, capillary and gravity forces. Examples are provided for 4 different degrees of heterogeneity.
Calculation of Capillary Pressure Curves Using Synchrotron X-Ray Micro-tomography

Previous studies have shown that rocks often have a high degree of heterogeneity in the capillary pressure curves, so-called capillary heterogeneity. While evidence of this is compelling, little data for independent quantification this is available. Since capillary heterogeneity is often observed on a scale 500 µm or less, it is difficult to use conventional methods for making capillary pressure measurements, particularly when destructive testing is undesirable. To obtain such data, we collaborated with scientists at SLAC National Accelerator Laboratory to use synchrotron X-Ray microtomography to characterize the pore space of the rock and use this data to generate capillary pressure curves for volumes as small as about 1 mm³. Due to some inherent shortcomings of existing approaches for calculating capillary pressure curves from the morphology of the pore space, we developed a new method to extract the pore sizes distribution of the porous structure directly, without approximation or complex calculation. The method uses progressive expansion of the solid surfaces to characterize the pore size distribution, and hence, the capillary pressure curve for the rock. A schematic illustrating the method is shown in Figure 3.

Figure 3. Schematic illustration of the quantitative evaluation of the pore structure using the proposed solid expansion and contraction method is shown in panels (a) and (b). Panel (c) shows the plot of the normalized accessible pore volume (the saturation percentage) versus the pore throat. The differential plot of panel (c) is shown in panel (d). The error bar is determined by analyzing the standard deviation of the experimental data from the tomographic measurement of different areas of the sample.
We have also demonstrated its capability to replicate the capillary pressure curve measured with mercury intrusion porosimetry (MIP) measurement as is illustrated in Figure 4. This work was published in Scientific Reports (Yang et al., 2015).

![Figure 4. Comparison of the capillary pressure curves as computed by mercury intrusion (colored curves) and solid contraction and expansion method (black curves, the solid and the dotted curves are the measurement over different sub-volumes of the sample).](image)

**A Non-Linear Solver for Multi-Phase Flow**

Nonlinear convergence problems in numerical reservoir simulation, especially in problems with capillary heterogeneity, can lead to unacceptably large computational time and are often the main impediment to performing simulation studies of large-scale problems. We have worked for the past 4 years to analyze and address this problem for immiscible, incompressible, two-phase flow in porous media in the presence of viscous, buoyancy, and capillary forces. Although simulation problems are multi-dimensional with large numbers of cells and variables, we find that the essence of the nonlinear behavior can be understood by studying the discretized (numerical) flux function for the interface between two cells.

The numerical flux is expressed in terms of the saturations of the two cells. Discontinuities in the first-order derivative of the flux function (referred to as kinks) and inflection lines are identified as the cause of convergence difficulty. These critical features (kinks and inflections) change the curvature of the
numerical flux function abruptly, and can lead to overshoots, oscillations, or divergence in Newton iterations. Based on our understanding of the nonlinearity, a nonlinear solver has been developed, referred to as the Numerical Trust Region (NTR) solver. The solver is able to guide the Newton iterations safely and efficiently through the different saturation ‘trust-regions’ delineated by the kinks and inflections. Specifically, overshoots and oscillations that often lead to convergence failure are avoided.

As shown in Figure 5, numerical examples demonstrate that our NTR solver (blue lines in Figure 5) has superior convergence performance compared with existing methods. In particular, convergence is achieved for a wide range of timestep sizes and Courant–Friedrichs–Lewy (CFL) numbers spanning several orders of magnitude. In addition, a discretization scheme is proposed for handling heterogeneities in capillary-pressure–saturation relationship. The scheme has a lesser degree of nonlinearity compared with the standard Single-point Phase-based Upstream weighting scheme, leading to an improved nonlinear convergence performance especially when used together with our NTR solver. Our proposed numerical solution strategy is based on the numerical flux and handles capillarity. It extends the previous work by Jenny et al. (2009)\(^1\) and Wang and Tchelepi (2013)\(^2\) significantly. This work has been published in the Journal of Computational Physics (Li and Tchelepi, 2015).

![Figure 5](image)

Figure 5. Convergence performance comparison between discretization schemes and solvers: (a) number of iterations versus timestep size; (b) number of iterations versus the maximum CFL number in the domain. The DIC scheme together with the NTR solver can converge in a variety of timestep sizes and CFL numbers with fewer iterations.

Quantification of the Influence of Capillary Heterogeneity on Buoyancy Driven Flows

As shown in Figure 6, recent advancements in experimental techniques allow quantifying sub core-scale heterogeneities in a high resolution (Krause et al., 2013 and Pini and Benson, 2013). Based on observations of heterogeneity distributions in natural core samples, we perform simulations to study the influence of sub-core-scale heterogeneities on large-scale buoyancy driven CO₂ migration during geological storage.

Figure 6. Natural heterogeneities in sandstones. Although laminations (indicated by the red arrows) are major sources of heterogeneity, the surrounding areas are also heterogeneous.

We observe that even the heterogeneities at millimeter scale can affect large-scale buoyancy-driven upward CO₂ migration. For the representative examples we study, ignoring small-scale heterogeneities can lead to an overestimation of the migration speed by a factor of two or more as illustrated in the example shown in Figure 7. To analyze the cause of such overestimation, we introduce a dimensionless heterogeneity factor to characterize different levels of heterogeneity. The influence on CO₂ migration is quantified with respect to a variety of heterogeneity factors, correlation lengths, and fluid viscosity ratios for isotropic and anisotropic media.

Our findings suggest that sub core-scale heterogeneities should not be ignored in core analysis, even for cores that appear relatively homogeneous and do not have distinguishable heterogeneity patterns. In addition, relative-permeability curves measured from core-flood experiments under high flow-rate conditions (a


common practice to eliminate capillary end-effects) should not be directly used when modeling low-flow-rate CO₂ migration if sub-core-scale heterogeneities are present. Instead, capillary-limit upscaling should be used to develop effective relative permeability curves for application under these conditions. Furthermore, for layered heterogeneity patterns commonly observed in sedimentary formations, relative permeability curves will be anisotropic as shown by the capillary-limit up-scaled relative permeability curves shown in Figure 8.

Figure 7. Saturation distributions for buoyantly drive transport of CO₂. Columns ‘A’ are the fine-scale true solution. Columns ‘B’ and ‘C’ are results of the homogenized simulations. Small-scale heterogeneities are ignored in columns B but considered in columns C by using capillary-limit upscaling. Note that columns B correspond to the industry practice that ignores small-scale heterogeneities in core analysis. While columns C match the fine-scale results accurately, columns B largely overestimate the plume speed.
Figure 8. An example of anisotropic permeability distribution and capillary-limit up-scaled relative permeability curves. While the effective relative-permeability curves are isotropic under a high-rate condition, they become anisotropic under a low flow rate due to small-scale heterogeneities.

Optimization of Monitoring for Leakage Using Pressure Sensors in Overlying Aquifers

We investigate the application of assimilating pressure data, from monitoring wells overlying a geological storage reservoir with uncertain geology, in order to locate and characterize leakages as quickly, and cheaply, as possible. A schematic of the system investigated is shown in Figure 9. We consider from one to nine monitoring wells in the overlying aquifer, and from 1 month up to 18 months of monitoring data after the CO$_2$ storage project starts. The data assimilation method makes use of the Karhunen-Loeve expansion to reduce the optimization variable space, while enabling candidate solutions to implicitly honor a Gaussian prior model, which may include hard-data. Minimizations are carried out using Particle Swarm Optimization. A total of 2000 realizations are evaluated, using stochastically generated heterogeneity fields, including the location and size of leaks. As shown in Figure 10 below, our results indicate that as little as one year of pressure monitoring data may be sufficient to locate and quantify a leak in the caprock. Similarly, we find that the accuracy in predicting leakage locations and total fluid leakage (brine plus CO$_2$) improves when there are at very least three
monitoring locations in the overlying aquifer. Beyond four monitoring wells, little improvement in quantifying the size or location of the leak is achieved. This is a very promising result and suggests that pressure monitoring can be a valuable tool for monitoring leakage.

Figure 9. Illustration of the system considered for this study of pressure monitoring optimization.

Figure 10. Top: History matches (HM) to true model fluid leakage over 30 years of CO₂ injection from 12 months of data and different numbers of monitoring wells (MW). 'Fluid' refers to both CO₂ and brine, though most of the initial leakage fluid is brine. Bottom: History matches (HM) to true model CO₂ leakage over 500 years (assuming CO₂ injection finishes after 30 years) from 12 months of data and different numbers of monitoring wells (MW). In both plots, the mass fraction is a proportion of the total injected mass of CO₂, which is 150 million tonnes.
Journal articles (published and in press)


Conference Papers


Conference Presentations and Posters

Boxiao Li, Computational Methods of Water Resources, Stuttgart, Germany (June 2014). On Small-Scale Heterogeneity and CO₂ Plume Migration in Geological Storage.

Boxiao Li, Computational Methods of Water Resources, Stuttgart, Germany (June 2014). Unconditionally Convergent Nonlinear Solver for Modeling CO₂
Sequestration.

Boxiao Li, European Conference on the Mathematics of Oil Recovery (September 2014). Nonlinear Analysis of Newton-Based Solvers for Multiphase Transport in Porous Media with Viscous and Buoyancy Forces.

Boxiao Li, International Conference on Greenhouse Gas Control, Austin, TX (October 2014). Small-Scale Heterogeneity and Buoyancy-Driven CO₂ Migration in Geological Storage.

Boxiao Li, Reservoir Simulation Symposium, Houston, TX (February 2015). Numerical Trust Region Newton Solver for Multiphase Transport in Porous Media Based on Detailed Nonlinear Analysis.

Da Huo, EGU 2014 General Assembly, Measuring Stress-dependent Fluid Flow Behavior in Fractured Porous Media

Da Huo, SPE 2014 Annual Technical Conference and Exhibition. Investigating Aperture-Based Stress-Dependent Permeability and Capillary Pressure in Rock Fractures

Da Huo, AGU 2014 Fall Meeting, Local Cubic Law Simulation of Stress-dependent Aperture-Based Permeability.
