Investigations in Geologic Carbon Sequestration: Multiphase Flow of CO₂ and water in reservoir rocks

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Abstract

Understanding the multiphase flow properties of CO$_2$ and water in porous media is essential for successful large-scale geologic CO$_2$ storage. Optimizing the design and operation of injection projects will depend on knowledge of injectivity, trapping capacity, distribution of CO$_2$ in the subsurface and overall areal extent of the subsurface plume. It is increasingly recognized that the capillarity and relative permeability of CO$_2$-water systems cannot be ignored for accurate simulations ranging from the sub-core to the basin scale. The Benson lab’s research program aims at improving our understanding on the dynamics of multiphase flow in porous media. The research work integrates experimental investigations and numerical simulations, thus allowing for a direct link between observations in the lab and the physics of the multiphase displacement process. In this context, current available models can be validated and/or extended so as to include a more accurate description of the physical processes involved.

The current experimental data set that deals with multiphase flow properties of the water-CO$_2$ system at reservoir conditions is limited. Accordingly, there is a limited understanding of multiphase properties, such as capillary pressure, relative permeability, and residual trapping. In the present study, multiphase flow characterization tests are presented on four sandstone rocks with distinct rock lithologies: a Berea sandstone and three reservoir rocks from formations into which CO$_2$ injection is either currently taking place or is planned. Drainage relative permeability and residual gas saturations were measured at reservoir conditions using the steady-state method in a horizontal core-flooding apparatus with fluid distributions observed using X-ray Computed Tomography (CT). The dataset is completed with absolute permeability and capillary pressure curves. A direct link could be established between petrological and the observed flow properties of the rocks. Moreover, this comprehensive data set allows addressing some of the major uncertainties common in these type of studies. For instance, a defining characteristic of the CO$_2$-water system is the low viscosity of the CO$_2$, which results in low CO$_2$ saturations during multiphase flow conditions and poor displacement efficiency during conditions of single phase flow through a partially saturated medium.

An important step in the understanding of the physics of the multiphase process is to demonstrate the ability to replicate laboratory experiments using numerical simulations. In the context of this work, this is defined as simulating the experimentally measured CO$_2$ saturation distributions within a rock core and the average pressure drop across the core under different fluid injection scenarios. The simulations are conducted using TOUGH2-MP, a commercially available numerical simulation program for multi-phase fluid in porous media. The method presented relies on the calculation of the permeability distribution at the sub-core scale, whose details were included in the previous report. Additionally, a unique capillary pressure curve is assigned to each grid block by scaling the equation with the corresponding porosity and permeability values. Two different rock cores are used in the analysis, namely Berea sandstone and a rock from the Otway Basin Pilot Project in Australia, these being representative of a homogeneous and heterogeneous core, respectively. A good agreement between simulations and experiments could be achieved, both in terms of spatial distribution and saturation values, thus showing that indeed experiments performed in the laboratory can be described
within an acceptable degree of accuracy. As an important corollary of this study, the uniqueness of the calculated permeability distribution is demonstrated.

Having shown the capability to describe core-flooding experiment, TOUGH2 can be used as a predictive tool for studying the effects of sub-core scale heterogeneity and flow rate on brine displacement efficiency and relative permeability. Again, a Berea core is considered and steady state multiphase flow injection is simulated at different fractional flows of CO$_2$ and at various injection flow rates. Heterogeneity is included in the model by considering three porosity-permeability relations with different correlation coefficients. A wide range of capillary and gravity numbers representative of those expected for a typical sequestration project is used to investigate the complexity of the physical forces in the core floods, namely viscous, capillary and buoyancy forces. It is shown that gravity is important at low flow rates, whereas heterogeneity significantly affects the saturation distribution at relatively high flow rates. Low flow rates and low fractional flow of CO$_2$ always lead to low displacement efficiencies with any kind of heterogeneities. This type of study provides useful insight for the design of relative permeability experiments.

In numerical simulations, a trade-off exists between grid resolution and computational speed. Highly efficient and accurate simulators are needed to capture the behavior of the system at the spatial resolution of the experiments. The Stanford General Purpose Research Simulator (GPRS) is explored as a new option. Equipped with robust solvers, GPRS is much faster than TOUGH2 in solving common reservoir simulation problems. Moreover, its flexible structure allows for the incorporation of new physics, should it be necessary. Of particular interest is the capillary heterogeneity, which, as described above, plays an important role in controlling the multiphase flow in porous rocks. In this work, modifications have been made in GPRS to include this effect and the ability of GPRS in tackling complicated multiphase flow dynamics is demonstrated. In this respect, the major challenge is to deal with discontinuities in the saturation distribution across cell boundaries that possess different capillary pressures. The Fully Implicit Method (FIM) with single point phase-based upwinding resolves the saturation field correctly, preserving the continuity of fluxes and the correct upstream directions. The ability and the efficiency of GPRS for modelling two-phase flow problems at the presence of strong capillary heterogeneity is demonstrated using small yet challenging examples. Comparisons between the numerical simulations and high-resolution CO$_2$ core flooding experiments are performed, showing a reasonably good agreement with the experiments and the TOUGH2 simulations.

Parallel to a growing capability of the numerical simulations to describe the physics at the sub-core scale, the precision of the experimental data that describe fluid distribution within a rock core has to increase, too. In the case of the CO$_2$-water system, one of the main limits of X-ray CT is the noise associated with the images, this being mainly caused by the relatively small density contrast between the two fluid phases as compared to the contrast between any one of the fluids and the rock. A methodology is presented to assess the error on a pixel-by-pixel level of the CT measurement and it is applied to a CO$_2$/water core-flooding experiment in a Berea sandstone. Three approaches are investigated aimed at reducing the uncertainty associated to the estimated porosity
and saturation values at the pixel level, namely the averaging over multiple scans taken at identical positions, coarsening and the utilization of iodine solutions. The comparison among these three approaches provides guidelines for designing experiments aimed at the quantitative estimation of the distribution of CO$_2$ and water at the sub-core scale. The successful implementation of the method opens the path to new challenging experiments such as the measurement of capillary pressure distribution curves within the core. Efforts in this direction are justified by the ultimate goal of improving our understanding on the dynamics of multiphase flow at the sub-core scale and on the role of heterogeneities on the distribution of CO$_2$ and water in the pore space of a reservoir rock.
1. Introduction

Carbon dioxide capture and sequestration (CCS) in deep geological formations has emerged over the past fifteen years as an important component of the portfolio of options for reducing greenhouse emissions. Four commercial projects now operating provide valuable experience for assessing the efficacy of CCS—sequestering about 4-5 Mt of CO$_2$ annually. If CCS is implemented on the scale needed for large reductions in CO$_2$ emissions, a billion tonnes or more of CO$_2$ will be sequestered annually—a 200 fold increase over the amount intentionally sequestered annually today. Effectively sequestering these large volumes will require building a strong scientific foundation of the coupled hydrological-geochemical-geomechanical processes that govern the long term fate of CO$_2$ in the subsurface. In addition, we will need methods to characterize and select sequestration sites, subsurface engineering to optimize performance and cost, safe operations, monitoring technology, remediation methods, regulatory oversight, and an institutional approach for managing long term liability.

Our research focuses on the fundamental science underpinning sequestration in saline aquifers. Saline aquifers have the largest sequestration capacity, as compared to oil and gas reservoirs or deep unminable 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 to assure that CO$_2$ will achieve high retention rates. Improved fundamental understanding of multi-phase flow and trapping in 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 CO$_2$, what will be the spatial extent of the plume of injected CO$_2$, how much and how quickly will CO$_2$ dissolve in brine, and how much CO$_2$ will be trapped by capillary forces when water imbibes back into the plume and to what extent is capillary trapping permanent? How quickly and by which methods can CO$_2$ leakage into shallow drinking water aquifers be remediated? What are the necessary properties of seals? And, if CO$_2$ is leaking how can detect this, either deep in the surface or at the land surface. Here we are developing new experimental data and carrying out simulations to improve our ability to answer these questions. As our research progresses, we will assess which, if any, modifications to currently accepted multiphase flow theory are needed and to develop approaches for reliably predicting field-scale performance.

Our laboratory is carrying out core-scale multi-phase flow experiments and reservoir-scale simulations to investigate the fundamental processes that underpin these questions. We are conducting transient and steady state core-flood experiments at representative reservoir pressure and temperatures. Each set of experiments involves co-injecting CO$_2$ and brine at a range of fractional flows and a number of different total flow rates. X-ray CT scanning is used to map the spatial distribution of CO$_2$ and brine. Detailed petrophysical analysis of the core is used to obtain 3-dimensional maps of porosity, permeability and capillary pressure. Rock properties are used to provide insight into the influence of spatial heterogeneity on the distribution of CO$_2$ and brine in the cores. Rock properties are also used as input to carry out high resolution numerical simulations of the core flood experiments. In addition, traditional steady state relative permeability measurements have been made during drainage and imbibition. As our
research progresses, we will assess which, if any, modifications to multiphase flow theory are needed to replicate the experiments and develop approaches for up-scaling laboratory measured relative permeability curves for use in reservoir-scale simulations.

Illustration of the 4 interrelated components of our approach to study multiphase flow and trapping in saline aquifer.
2. Multiphase flow properties of CO$_2$ and water in sandstone rocks at reservoir conditions

Investigators
Sam Krevor, Postdoctoral Researcher, Ronny Pini, Postdoctoral Researcher, Lin Zuo, Graduate Researcher, Sally Benson, Professor, Department of Energy Resources Engineering, Stanford University

Introduction
Understanding the multiphase flow properties of CO$_2$ and water in porous media is essential for successful large-scale geologic CO$_2$ storage. Optimizing the design and operation of injection projects will depend on expectations about the distribution of CO$_2$ in the subsurface, knowledge of injectivity, and estimates of the capacity of permanent trapping processes. It is increasingly understood that the capillarity of the CO$_2$-water system in porous media cannot be ignored for accurate simulations ranging from the sub-core scale to the basin scale [1]. The distribution of CO$_2$ in the subsurface, including column height in contact with the caprock and the surface extent of the plume, is dependent on capillary pressure-saturation relationships, and the relative permeability function [2]. Small variations in relative permeability can lead to a wide range in injectivity, and will contribute in determining the number of wells required to meet an overall injection goal [3]. Low injectivity is a well-known but poorly understood phenomenon in CO$_2$ enhanced oil recovery processes, and may be due to poorly characterized relative permeability functions [4]. CO$_2$ trapping as a free phase residual fluid is governed by hysteresis in the relative permeability curves between drainage and imbibition processes and will play a large role in determining the storage security of a project [5, 6]. For all of these reasons, it is crucial to have high quality data and a firm understanding of the results of experiments investigating multiphase flow properties of capillary pressure, relative permeability, and residual trapping.

We have performed multiphase flow characterization tests using water and supercritical CO$_2$ with four sandstone rocks representing a range of reservoir characteristics. Capillary pressure, drainage relative permeability, and residual gas trapping have been observed with flow experiments performed at 50°C and 1300 psi pore pressure, representative of high pressures and moderate temperatures seen in the subsurface. Flow experiments were performed using the steady state relative permeability method with x-ray CT imaging. With this method, the results are independent of the assumptions necessary to justify the use of Buckley-Leverett theory. The absence of common problems in core flooding experiments such as capillary end effects and gravity fluid segregation can also be confirmed through x-ray imaging. The main goal of this work is to derive important petrophysical flow parameters for a range of sandstone rock types at reservoir conditions including sufficient observation and analysis to address major uncertainties common in these types of characterizations.

Materials and Methods

Materials: Four sandstone rock cores, 5.08cm in diameter, were used representing a range of reservoir properties and rock types. Table I summarizes various properties of the
rocks and Figure 1 shows the variation in porosity of each rock along the length of the cores. A Berea was used because of its utility in making comparisons with other studies. Three other rocks, one each from the Paaratte formation in Southern Australia, the Mt. Simon in Illinois, and the Tuscaloosa massive sand from Alabama are from target reservoirs where large volume CO$_2$ injection pilot projects are either underway or under development.

Table 1: Properties of the rocks used in this study

<table>
<thead>
<tr>
<th>Name</th>
<th>Porosity [-]</th>
<th>Absolute Permeability [mD]</th>
<th>Flow rate [ml/min]</th>
<th>Length [cm]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Berea</td>
<td>22.1</td>
<td>914</td>
<td>15</td>
<td>10</td>
</tr>
<tr>
<td>Paaratte</td>
<td>28.3</td>
<td>1156</td>
<td>15</td>
<td>9.5</td>
</tr>
<tr>
<td>Mt. Simon</td>
<td>24.4</td>
<td>7.5</td>
<td>10</td>
<td>9.6</td>
</tr>
<tr>
<td>Tuscaloosa</td>
<td>23.6</td>
<td>220</td>
<td>15</td>
<td>10.8</td>
</tr>
</tbody>
</table>

Figure 1: Average porosity along the length of the cores used in the experiments.

Core flooding setup: The core flooding apparatus is a modified version of a setup described in a previous study [1]. A schematic is shown in Figure 2. The rock sample is wrapped in a sleeve with layering from the core outwards of heat-shrinkable teflon, nickel foil, another layer of heat-shrinkable teflon, and a viton rubber sleeve and placed in an aluminum core holder. Two high accuracy pressure transducers (Oil filled Digiquartz Intelligent Transmitter, Model 9000-3K-101) are tapped into the core holder with pressure measured at the inlet and outlet faces of the core. A displacement pump (Teledyne Isco, Model 260D) injects water around the sleeve to create the overburden pressure. Two electric heaters heat the water inside the confining fluid to maintain the core at the experimental temperature. Two dual-pump systems are used to inject water and CO$_2$ in the core sample (Teledyne Isco, Model 500D). The systems are composed of two pumps connected with a set of electric valves. The dual pump configuration provides continuous fluid delivery by synchronizing the pump and refill strokes so that one pump is always delivering fluid. The refill and delivery of each pump is automated through a
controller. The bodies of the CO₂ pumps are surrounded by water-regulated temperature jackets and CO₂ was kept at a constant temperature of 50°C during the experiments so that delivery rates from the CO₂ pumps corresponded to flow rates in the core. Before entering the core, CO₂ and water pass through a heat exchanger heated to the experimental temperature. The fluids combine in the lines prior to the core holder and then enter the core. After flowing through the core, the CO₂ and water are separated in a TEMCO AMS-900 high pressure two-phase separator. The separator includes an electronic pulser receiver and uses acoustic signals to constantly monitor the volume of fluids in the separator. CO₂ from the top of the separator returns to the CO₂ pumps as they refill, whereas water passes through a pressure regulating pump (Teledyne Isco, Model 1000D) that is set to deliver or receive as is necessary to maintain the fluid pressure at the set condition. In this way, the pressure at the outlet of the core is maintained at the experimental pressure of 1300 psi throughout the experiment. The water pumps refill from the pressure regulating pump. In this configuration, CO₂ and water can recirculate through the core for as long as is necessary to achieve steady state equilibrium with respect to fluid saturations in the core.

![Figure 2: Schematic of the core flooding setup used in this study.](image)

**Experimental procedure:** Steady state relative permeability tests were performed to derive the relative permeability-saturation relationship for the water-CO₂ system in each core at 50°C and 1300 psi pore pressure. The cores were vacuum dried at 70°C and at 70% constant humidity overnight and subsequently placed in the core holder. For all of the experiments, the outlet end of the core was maintained at a constant pressure of 1300 psi and a constant pressure of 1700 psi was maintained in the confining fluid, or a confining overpressure of 400 psi relative to the pore fluid. The fluid lines and core are flushed with CO₂ at the beginning of the experiment to remove air from the system. The core is then pressurized with CO₂ up to 1300 psi. At this point, a CT scan is taken of the core to provide the background scan of the core 100% saturated with CO₂. Subsequently CO₂ is vented from the core which is allowed to depressurize back to atmospheric pressure.
Next, water with no dissolved CO$_2$ is introduced to the core and several pore-volumes are flooded at atmospheric pressure. Then the water is pressurized in the core and at least 10 pore volumes of water with no dissolved CO$_2$ are flooded through the core at low flow rates. It is assumed that remnant free-phase CO$_2$ dissolves into the fresh water. It is at this time that absolute water permeability measurements are made. A background scan is then made of the core saturated 100% with water. This background scan is used in the calculation of porosity. The core is subsequently sealed by closing valves and maintained at experimental pressures and temperatures while water and CO$_2$ are circulated together through lines that bypass the core at 1300 psi. The dissolution of CO$_2$ into the water is monitored by watching for a decrease and subsequent stabilization of the mass balance of free-phase CO$_2$ in the system. Equilibration is generally established in this setup after 7 hours of circulation. After the two phases are in equilibrium, CO$_2$ circulation is stopped and valves sealing off the core are opened to allow for water circulation through the core. After at least 5 pore volumes of CO$_2$-saturated water have gone through the core, a background CT scan is taken. At this point there are CT scans of the core with air at atmospheric pressure, with 100% of the pore space filled with CO$_2$ at experimental pressure and temperature, with 100% of the pore space filled with water with no dissolved CO$_2$ at experimental pressure and temperature, and with 100% of the pore space filled with water saturated with dissolved CO$_2$ at experimental pressure and temperature.

**Relative permeability:** Relative permeability is obtained by simultaneously circulating CO$_2$ and water through the core at controlled flow-rates ($q_i$), observing the pressure drop across the core ($\Delta P$), and taking x-ray CT scans to obtain CO$_2$ saturation $S$, i.e.

$$q_i = -\frac{A k_{ij}(S) \Delta P}{\mu_i L}$$

$A$ and $L$ are the cross-section and length of the core, respectively, $\mu_i$ is the fluid viscosity and $k$ is the core absolute permeability (measured with water). Total volumetric flow rates (CO$_2$ + water) are kept constant at 15 ml/min for the Berea, Paaratte, and Tuscaloosa, and 10 ml/min for the Mt. Simon throughout the experiment. This corresponds to capillary numbers ranging between $10^{-8}$ and $10^{-7}$. CO$_2$ saturation is incrementally increased from zero (drainage, CO$_2$ displacing water) by simultaneously increasing the relative volumetric flux of CO$_2$ and decreasing the relative flow of water. At each stage that the CO$_2$ flow is increased, at least 5 pore-volumes of total fluid move through the core before observations are made.

**Maximum CO$_2$ saturation:** The final stage of the drainage experiment involves flooding 100% CO$_2$ through the core. While it was generally found that constant saturation profiles could be obtained throughout the core while flowing both phases, saturation gradients existed when flowing 100% CO$_2$. As under these conditions Eq. 1 does not apply, a separate technique was required to obtain the relative permeability of CO$_2$ at the highest saturations achieved [7].
Residual CO₂ saturation: After obtaining maximal CO₂ saturations and relative permeabilities with 100% CO₂ flooding, the cores were flooded with 100% water at the experimental flow rates (15 ml/min for the Berea, Paaratte, and Tuscaloosa; 10 ml/min for the Mt. Simon). At least 10 pore volumes of water were flooded through the core and saturation was observed after the pressure drop across the core had stabilized. Because there was a gradient in the CO₂ saturation across the core during 100% CO₂ flooding, there is a corresponding gradient in the trapped CO₂ saturation after 100% water flooding. This is advantageous because it allows for the observation of the residually gas trapped saturation for a wide range of initial saturations.

Figure 3: Slice averaged CO₂ saturation during core flooding experiments.

Results

The slice-average saturation of CO₂ at various fractional flows of CO₂ and water are shown in Figure 3. CO₂ saturation in the cores ranged from less than 5% and up to 30% depending on the CO₂:H₂O flow ratio. When 100% CO₂ was injected, CO₂ saturations at the inlet face of the core ranged from 30-60%. The high permeability Berea and Paaratte showed large ranges in CO₂ saturation during two-phase flow compared with the lower permeability Mt. Simon and Tuscaloosa. From the capillary pressure-saturation curves for the four rocks (Fig. 4 and parameters in Table II) it can be seen that generally higher ranges in capillary pressure are required for the Mt. Simon and Tuscaloosa to achieve equivalent ranges in saturation as the Berea and Paaratte sandstones.
Both steady-state and maximum relative permeability values derived at each saturation are shown in Figure 5. Both best-fit Brooks-Corey curves and those derived from the mercury porosimetry are plotted with the measured data in the figure. In all cases the CO$_2$ relative permeability at irreducible water saturation was assumed to be 0.95. The capillary pressure based prediction fits the Berea very closely, but is not a good predictor for the Paaratte and Mt. Simon. In the Mt. Simon, the water relative permeability drops and the CO$_2$ relative permeability rises more steeply than in the Berea and Paaratte sandstones. In the case of the Tuscaloosa, the Purcell-Burdine relationships predict from the MICP data that the water relative permeability will drop steeply at low CO$_2$ saturation relative to the other sandstones, and that the crossover point of the two curves will be at higher water saturation than the other rocks. It is clear that the poor sorting of the Tuscaloosa plays a dominant role in determining the shape of the relative permeability curve.

### Table II: Best-fit Brooks-Corey capillary pressure parameters.

<table>
<thead>
<tr>
<th>Name</th>
<th>$P_e$ [psi]</th>
<th>$S_{wi}$ [-]</th>
<th>$\lambda$ [-]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Berea</td>
<td>.37</td>
<td>.11</td>
<td>.67</td>
</tr>
<tr>
<td>Paaratte</td>
<td>.3</td>
<td>.05</td>
<td>.9</td>
</tr>
<tr>
<td>Mt. Simon</td>
<td>.67</td>
<td>.18</td>
<td>.55</td>
</tr>
<tr>
<td>Tuscaloosa</td>
<td>0</td>
<td>.05</td>
<td>N/A</td>
</tr>
</tbody>
</table>

Graphs plotting the residual CO$_2$ saturation vs. the initial CO$_2$ saturation prior to imbibition are shown in Figure 6. Absolute values for the residual saturation observed in this study (dependent on the maximal CO$_2$ saturation that was obtained) range between 10-25% gas saturation. In the case of the Mt. Simon the initial vs. residual curve appears to be non-monotonic, suggestive of a rock with mixed wetting behavior. This is in agreement with a study showing that the CO$_2$-water system is mixed wet on mica surfaces, a mineral that is taken to be an analogue to the illite found in abundance in the Mt. Simon [8]. In general, residual gas trapping is similar to what has been observed with
analogous fluids in Berea and other rocks [9], and simulations using normal values of the Land trapping coefficient or Spiteri parameters seem justified.

**Figure 5:** Drainage relative permeability curves. Dotted lines: Brooks-Corey predictions from the MICP data; Solid lines: best-fit Brooks-Corey curves through the data.

**Figure 6:** Residual CO$_2$ saturation plotted as a function of initial CO$_2$ saturation. Solid line shows best fit Spiteri model, dotted line shows Land model with a core-averaged Land trapping coefficient.
Conclusions

Steady-state CO₂-water multiphase flow experiments have been performed on sandstone rocks representing a range of rock types and flow parameters. In three of the four cores, relative permeability and residual gas trapping observed at representative reservoir pressures and temperatures appears to be consistent with a two-phase system which is strongly water-wetting. In one core that contains a substantial fraction of illite clay, there is indication that the system is closer to mixed wet. A defining characteristic of the CO₂-water system is the low viscosity of the CO₂ which results in low CO₂ saturations during multiphase flow conditions and poor displacement efficiency during conditions of single phase flow through a partially saturated medium. This may adversely affect the results of relative permeability experiments using the non-steady state method, could contribute to low injectivities in commercial scale projects, and lead to poor predictive capabilities for reservoir simulators ignoring capillarity.

Publications and Presentations

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5. S. Krevor, R. Pini, L. Zuo, S.M. Benson, Multiphase flow of CO₂ and water in reservoir rocks at reservoir conditions. European Geosciences Union General Assembly 2011, April 3-8, Vienna, Austria
8. S. Krevor and S.M. Benson, Measuring 13CO₂ for surface monitoring in the geologic storage of CO₂, International Conference on Environmentally Preferred Advanced Power Generation, Feb 8-10, Costa Mesa, CA USA

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3. Permeability Models for Numerical Simulation of Core Flooding Experiments

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Background
Previous reports have already discussed one of the main objectives of this research group’s goals, which is to demonstrate the ability to replicate laboratory experiments using numerical simulation. In the context of this work, this is defined as simulating the experimentally measured sub-core scale CO₂ saturation distribution within a rock core, the average pressure drop across the core under different fluid injection scenarios, and finally, the core-average CO₂ saturation in the core. The workflow for this is procedure is to conduct a core flooding relative permeability experiment, as described in the 2007 and 2008 annual reports, then to use the exact same conditions in a multiphase flow numerical simulator to predict the spatial distribution of CO₂ as measured by medical CT scanning during the core flooding experiment. The results in the 2009 report showed that a promising workflow could be established for running these simulations, particularly with respect to calculating a sub-core scale permeability distribution, which is required to run sub-core scale simulations of the experiment. Details of this method are included in the 2009 report for reference, and this report will focus on three main aspects that aim at (1) demonstrating the ability to simulate the experiments performed in the laboratory, (2) at showing that these simulations can be done with an acceptable degree of accuracy, and (3) at showing that the permeability grid that our procedure calculates is accurate and unique.

Methodology

Experiments: Two different rock cores were used to demonstrate the ability to replicate experimental measurements, namely a Berea sandstone and a rock core from the Otway Basin Pilot Project in Australia, called the Waare C core, after the rock formation from which it was cut. The porosity maps of these two cores are shown below in Figure 1. The gravity and injection directions for the experiment shown in the figure are typical of all figures in this presentation.

![Porosity distributions for the Berea (left) and Waare C (right) cores.](image)

**Figure 1:** Porosity distributions for the Berea (left) and Waare C (right) cores.
The Berea core is relatively homogeneous, however there is a distinct bedding plane, which is difficult to distinguish in the figure, but will be more evident later. On the contrary, the Waare C core is highly heterogeneous with several bedding planes characterized by low porosity and perpendicular to the direction of flow.

The multiphase flow experimental system is described in Section 2 of this report and it is briefly summarized here for the sake of clarity. A rock core is placed in a sealed container at reservoir conditions, and brine is injected at a constant flow rate. The outlet pressure is kept constant with a back-pressure pump and the pressure drop is measured by pressure transducers on each end of the core, thus allowing to measure the absolute permeability of the core by applying Darcy’s law. Next, CO$_2$ is introduced to the injection stream at a given fractional flow; once the pressure and saturation in the core are stable, the saturation distribution within the core is measured with a CT scanner. The fractional flow of CO$_2$ is then increased and the process is repeated until 100 percent CO$_2$ is being injected into the core. At each step the pressure drop is recorded, and the relative permeability can be calculated using Darcy’s Law extended to multiphase flow.

The fractional flows that will be used in this study are 90% CO$_2$ for the Berea core, and 95% for the Waare C core. The measured saturation distributions at these fractional flows are shown in Figure 2. It can be seen that the saturation distribution of the Berea core is uniform with exception of a distinct plane of low saturation that crosses the core. For the Waare C core, the saturation distribution reflects the characteristic features described above for the porosity, with marked planes of low saturation that are perpendicular to the direction of flow.

![Figure 2: Steady-state saturation distributions for the Berea (90% CO$_2$ Injection) and the Waare C (95% CO$_2$ Injection) cores.](image)

The history matched relative permeability curves used in the simulation are shown in Figure 3.
Figure 3: Relative permeability curves for the Berea (solid blue lines) and Waare C (dashed red lines) cores.

In addition to this data, capillary pressure is also measured experimentally, and each measured dataset is fitted to the following equation

$$P_c = \sigma \cos \theta \frac{1}{k} J(S_w)$$

(1)

where $\sigma$ is the interfacial tension between brine and CO$_2$, $\theta$ is the contact angle of CO$_2$, $\Phi$ is the porosity and $k$ is permeability. The equation uses the following $J$-Function:

$$J(S_w) = A \left( \frac{1}{S_\lambda^{\lambda_1}} - 1 \right) + B \left( 1 - S_\lambda^{\lambda_2} \right)^{1/\lambda_2}$$

(2)

where $A$, $B$, $\lambda_1$, and $\lambda_2$ are fitting parameters and $S_\ast$ is a normalized saturation defined by,

$$S_\ast = \frac{S_w - S_{wr}}{1 - S_{wr}}$$

(3)

with brine saturation $S_w$ and residual liquid phase saturation $S_{wr}$. The obtained fitted curves are shown in Figure 4 along with the measured data for both cores. The corresponding fitting parameters are given in Table I. The figure shows that a satisfactory fit could be obtained for the Berea core, whereas this is not the case for the Waare C core, especially at low brine saturations. With the given $J$-Function, a better fit is not attainable due to the irregular shape of the experimentally measured curve.
Figure 4: Capillary pressure data for the Berea (blue symbols, left) and Waare C (green symbols) cores together with best fit curves (Eq.1). Fitting parameters are given in Table I.

Table I: Parameters fitted to the capillary pressure equation, Eq. 1, for the two cores investigated in this study.

<table>
<thead>
<tr>
<th>Core</th>
<th>k [md]</th>
<th>$\phi$</th>
<th>$S_w$</th>
<th>A</th>
<th>B</th>
<th>$\lambda_1$</th>
<th>$\lambda_2$</th>
<th>$\sigma$ [N/m]</th>
<th>$\theta$ [deg]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Berea</td>
<td>941</td>
<td>24.09</td>
<td>0.13</td>
<td>0.012</td>
<td>0.3</td>
<td>2.8</td>
<td>2.8</td>
<td>0.0338</td>
<td>0</td>
</tr>
<tr>
<td>Waare C</td>
<td>62.3</td>
<td>18.11</td>
<td>0.03</td>
<td>0.01</td>
<td>0.04</td>
<td>2</td>
<td>1.9</td>
<td>0.0285</td>
<td>0</td>
</tr>
</tbody>
</table>

Simulations: To conduct the simulations, sub-core scale permeability grids must also be calculated to complement the laboratory measurements. These are calculated as given by Eq. 4 and explained in the 2009 report.

$$k_i = c_o \frac{1}{P_c} \phi_i \left( S_w,i \right) \left( \sigma \cos(\theta) \right)^2$$

Input to this equation are the measured sub-core scale saturation distribution $S_w,i$ and the measured average capillary pressure, $P_c$. As saturation gradients exist within the core during the core flooding experiments $P_c$ is calculated individually for each slice, rather than as a simple core-average. The obtained permeability distributions for the two rock cores are shown in Figure 5. It can be seen from the figure, that the characteristic bedding plane of the Berea core observed in Figure 2 is also present in Figure 5; as this was not the case for the porosity distribution (Figure 1), we can presume that permeability is not necessarily a strong function of porosity in this core. The Waare C core has a permeability field which is qualitatively similar to the porosity distribution, and is quite heterogeneous.
Figure 5: Permeability distributions for the Berea (left) and Waare C (right) cores.

The simulations are conducted using TOUGH2-MP and by applying the conditions given in Table II. Up-scaling factors refer to CT measured values at the core scale and are applied by volume averaging measured CT values. The porosity and permeability distributions as well as relative permeability curves are known from the experiments. In addition, Eq. 1 is used for the capillary pressure and to each simulation grid is assigned a unique capillary pressure curve by scaling the equation with the corresponding porosity and permeability values.

### Table II: Simulation Conditions and Gridding Data.

<table>
<thead>
<tr>
<th></th>
<th>Berea Core</th>
<th>Waare C Core</th>
</tr>
</thead>
<tbody>
<tr>
<td>T (°C)</td>
<td>50</td>
<td>3</td>
</tr>
<tr>
<td>P (MPa)</td>
<td>12.411</td>
<td>63</td>
</tr>
<tr>
<td>xNaCl (ppm)</td>
<td>0</td>
<td>12.411</td>
</tr>
<tr>
<td>Diam. (cm)</td>
<td>5.08</td>
<td>5.08</td>
</tr>
<tr>
<td>Length (cm)</td>
<td>10.2</td>
<td>8.33</td>
</tr>
<tr>
<td>Q&lt;sub&gt;e&lt;/sub&gt; (ml/min)</td>
<td>3</td>
<td>3</td>
</tr>
<tr>
<td>Y-Z Upscaling</td>
<td>Y-Z Cell Size (mm)</td>
<td>Y-Z Upscaling</td>
</tr>
<tr>
<td>X Upscaling</td>
<td>X Upscaling</td>
<td>X Upscaling</td>
</tr>
<tr>
<td>X Slices</td>
<td>X Slices</td>
<td>X Slices</td>
</tr>
<tr>
<td>X Voxel Size (mm)</td>
<td>2</td>
<td>3</td>
</tr>
</tbody>
</table>

Results

Experiments vs. Simulations: The simulation results are shown in Figure 6. For the sake of better comparison between experimental and simulated results, a slice from each core has been selected. The standard deviation (σ) representative for the saturation distribution within the whole core is also shown. The visualization allows appreciating the good agreement between simulation and experiments, both in terms of spatial distribution and saturation values. The results of these slices are representative of the entire core results.

In order to quantitatively determine the accuracy of the method, Figure 7 shows the simulated saturations as a function of the corresponding measured experimental saturation for the two slices shown above. For a better comparison the line representing a perfect correlation is shown along with the data. The Berea core shows very little deviation from the measured values is observed, and follows the perfect correlation line very well. The Waare C results do have significantly more scatter, which may be
expected due to the strong heterogeneity of the core, but they generally agree with the correlation line.

Figure 5: Comparison between simulation and experimental results (saturations) for Berea (Slice 16) and Waare C (Slice 12) cores.

Figure 6: Comparison between predicted and measured saturations for the Berea (blue symbols) and the Waare C (red symbols) cores.
Table III reports values for the parameters used to determine the accuracy of the simulations, namely the $R^2$ fit (saturation), and the deviations with respect to the experimental results for the core average saturations and pressure drop. The table shows that the core average $R^2$ fit of the saturation prediction to the experimental measurement is very good for the Berea, over 0.90, and quite good for the Waare C, over 0.72. In addition, the core average saturation and pressure drop are predicted with good accuracy, which could be improved by conducting a better relative permeability history match.

**Table III:** Accuracy of the simulations with respect to the experimental results.

<table>
<thead>
<tr>
<th></th>
<th>$R^2$</th>
<th>$S_{CO2}$ Error (%)</th>
<th>$\Delta P$ Error (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Berea</td>
<td>0.909</td>
<td>0.5</td>
<td>3.1</td>
</tr>
<tr>
<td>Waare C</td>
<td>0.727</td>
<td>7.9</td>
<td>7.8</td>
</tr>
</tbody>
</table>

Proof of correctness: One important facet of this work is to show that the permeability distribution is both accurate and unique. It has been shown that the simulations using the permeability distributions generated from Eq. 4 are indeed accurate, however their uniqueness has not been proved. Saturation is an input to the equation, and since the former is measured at different fractional flows, there are multiple possible inputs into the equation. If the permeability distributions calculated using Eq. 4 are correct, then each measured saturation distribution input should yield the same permeability grid output.

Up to this point, one major limitation to this is the experimental error, which depends on the experimental conditions, but can exceed 25 percent saturation points. Therefore, in order to compare different permeability grids using different saturation distribution measurements as input, experimental conditions were adjusted to reduce the error to below 6 percentage points for the Berea core shown previously.

For the Berea core, saturation measurements were performed at 70% and 90% CO$_2$ fractional flow, the latter being the experiment shown in Figure 2. Figure 7 shows permeability distributions obtained by using the experimental data as input to Eq. 4. From a qualitative point of view, the distributions look very similar. The quantitative comparison between the two sets of data is shown in Figure 8 with the help of the density distribution functions. It can be seen that the two permeability maps have different distribution characteristics, which can only partially be attributed to experimental error. The calculated experimental error in each grid to one standard deviation is reported in Table IV, and is on the order of 1-10 millidarcies. The error in the difference between the two distributions is on the order of 45 millidarcies, or about a factor of 5 larger than experimental error, with a standard deviation of 460 millidarcies, or about a factor of two larger than the permeability distributions themselves.
Figure 7: Permeability distributions of the Berea core created with 70% CO₂ injection (left) and 90% CO₂ injection (Right).

Figure 8: Density distribution functions for the computed permeability at 70% CO₂ injection (red) and 90% CO₂ injection (blue).

Table IV: Error estimation associated to the permeability distribution.

<table>
<thead>
<tr>
<th>Grid</th>
<th>S_{CO2} Ave</th>
<th>Perm Error [md]</th>
<th>Perm Std. Dev. [md]</th>
</tr>
</thead>
<tbody>
<tr>
<td>70</td>
<td>0.2063</td>
<td>1.4</td>
<td>254</td>
</tr>
<tr>
<td>90</td>
<td>0.2654</td>
<td>9.5</td>
<td>256</td>
</tr>
</tbody>
</table>

In addition, the first bin of the 70 percent distribution has many more instances than the 90 percent distribution. We attribute this to the inability of CO₂ to penetrate as much pore space at 70% fractional flow as compared to the 90% case: as the CO₂ injection fraction increases, saturation of CO₂ increases, and so does capillary pressure. The capillary pressure controls the radius of pore throats, which can be penetrated by CO₂, as given by

\[ P_c = \frac{2\sigma \cos \theta}{r} \]  

(5)
In other words, high fractional flows result in more pores being invaded by CO$_2$. Since saturation is an input into the permeability equation, if CO$_2$ cannot penetrate into a pore, there is essentially no information about the permeability of that pore throat, except that it is below some threshold value at which CO$_2$ could penetrate the pore throat. As a result, the first bin of the permeability distribution at 70% fractional flow has many more instances than the 90% case. As CO$_2$ invades more pores, they have measured saturation greater than zero, and permeability can be calculated. In the measurements, minimum permeability values are assigned to zero saturation values; as the capillary pressure increases, an increasing number of these minimum values switch to actual permeability values and the characteristic shape of the distribution changes.

**Conclusion and future work**

This uniqueness and error analysis is recent work and future development will take place to more accurately quantify this methods ability to create accurate permeability distributions. In addition, the propagation of experimental saturation measurement error into permeability calculation errors will be studied in further detail. In addition, upscaling work will be conducted to study effective methods for upscaling core scale geological heterogeneity into larger scale models.

**Publications and Presentations**

4. Krause, M., Perrin J.-C. and Benson, S.M., Recent Progress in Predicting Permeability Distributions for History Matching Core Flooding Experiments, GCEP Symposium - Creating a Sustainable Energy System for the 21st Century and Beyond, September 28 - 29, 2010, Stanford University, USA

**Contact**

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Sally Benson: smbenson@stanford.edu
4. Simulation studies of effect of flow rate and small scale heterogeneity on multiphase flow of CO$_2$ and brine

Investigators
Chia-Wei Kuo, Graduate Researcher, Sally M. Benson, Professor, Department of Energy Resources Engineering, Stanford University.

Background
Figure 1 shows a typical core-flooding laboratory experiment conducted by Perrin et al. (2009) [1]. The experiment show large variations in CO$_2$ saturation and bypass of portions of the core that cannot be explained by buoyancy. This experiment and others motivated our research related to the combined influence of heterogeneity, gravity and capillarity on multi-phase flow of CO$_2$ and brine over a wide range of flow rates.

![Figure 1: CO$_2$ saturation for 100% CO$_2$ injection at 1.7 ml/min flow rate by Perrin and Benson, 2009.](image)

Methodology
The sensitivity studies of the steady-state multiphase flow simulation presented in the previous report (GCEP2010) are being further investigated here. The experimental data (core characterization), initial and boundary conditions, and the methodology of numerical simulation are the same: a Berea sandstone core is used with a 20.3% mean porosity and a mixture of 95%vol. CO$_2$ and 5%vol. brine is injected into a brine saturated core at reservoir condition (T=50°C and P=12.4 MPa). The main input parameters assigned to each grid element are porosity, permeability, capillary pressure curve and relative permeabilities. In particular, relative permeability- and capillary pressure-saturation functions used in the simulations are defined as follows:

$$k_{r,CO_2}(S_w) = \left( \frac{1-S_w}{1-S_{wr}} \right)^3$$

$$k_{r,w}(S_w) = \left( \frac{S_w-S_{wr}}{1-S_{wr}} \right)^7$$

$$P_{c,i}\left(S_w\right) = \sqrt{\frac{\phi_i}{k_i}} \left( S_w \right)$$

(1)

(2)
where $S_w$ is the average brine saturation, $S_{wr} = 0.15$ is the residual brine saturation, $P_{c,i}$ is calculated by scaling the J-function with the square root of the element’s porosity ($\phi_i$) to permeability ($k_i$) ratio multiplied by the CO$_2$-brine interfacial tension $\sigma = 22.47$ mN/m.

One homogeneous and two heterogeneous cores were used to investigate the effect of heterogeneity on the multiphase flow dynamics of the CO$_2$/brine system. For the homogeneous core, mean porosity and permeability values are used; heterogeneity is introduced using measured porosity values and by generating the corresponding permeability values based on a given porosity-permeability relation. In one case, the well-known Kozeny-Carman equation is used, whereas in the second case an exponential function is used to get a high contrast in the permeability distribution. According to capillary pressure curve Eq.2 and for a homogeneous core, only one uniform capillary pressure curve is required, the latter being based on mean porosity and mean permeability values. On the contrary, each grid element in the heterogeneous core has a unique pair of porosity and permeability values; hence a unique capillary pressure curve, whose consistency is maintained by using the same J-function. Simulation shows that to replicate the spatial variations in CO$_2$ saturation observed in the experiments, the capillary pressure characteristic curve must be different in each grid element.

To determine the effect of flow rate, heterogeneity and gravity on brine displacement, homogeneous and heterogeneous cores are simulated with identical parameters of relative permeability and capillary pressure. The flow rate is chosen so as to cover the range of conditions expected in the near-well region (6 ml/min) as well as at the leading edge of the plume (0.001 ml/min), which may be as far as 5 km or more from the injection well.

**Results**

**Saturation Profiles:** Figure 2 shows the steady-state average CO$_2$ saturation as a function of the distance from the inlet at various injection flow rates (1 slice $\equiv$ 3mm) and for a homogeneous core.

![Figure 2: Saturation profile along the core for a homogeneous core at various flow rates.](image-url)
A clear dependency is observed between flow rate and average CO₂ saturation, the latter being related to the brine displacement efficiency. The average saturation increases with increasing flow rates and it stabilizes once the flow rate is larger than 0.6 ml/min. Moreover, the saturation gradient that is present at low injection flow rates disappears as the latter increases. In Figures 3 and 4, these saturation profiles are compared to those obtained for the two heterogeneous cores (Kozeny-Carman and high contrast) at flow rates larger than 0.6 ml/min. Several observations can be made with respect to the high flow rates regime (or viscous dominated regime, Figure 3). At a given flow rate, the saturation profile is strongly affected by the heterogeneity of the core. As the injection flow rate decreases, the variation of saturation within the core increases; in other words, a greater flow rate is needed to reach relative constant saturation for the heterogeneous core as compared to the homogeneous core.

![Saturation profile](image)

**Figure 3:** Saturation profile along the core for four different high flow rates.

If the flow rates are further decreased (Figure 4), the saturation gradient increases and becomes smoother, with the two heterogeneous cases that eventually approach the homogeneous case. In other words, below a given threshold flow rate, the degree of heterogeneity becomes less important. In the high flow rate regime, the system is dominated by viscous forces, while the effect of gravity becomes more important as the injection rates are lowered. To isolate the gravity effect, the two heterogeneous cases are compared with and without gravity upon a change of flow rates of about two orders of magnitude.
Figure 4: Saturation profiles along the core at four different low flow rates.

Figure 5 shows that gravity is less significant in the viscous dominated regime and when a large saturation gradient occurs. At 0.05 ml/min, high contrast model already has a large saturation gradient; therefore cases with and without gravity are identical. The same apply when the flow rate is 0.005 ml/min

Different fractional flows of CO$_2$: The experimentally obtained CO$_2$ saturation distribution in the core at fractional flow of 100% CO$_2$ and at a total flow injection rate of 1.7 ml/min is compared to the simulations results for fractional flow of 95%, 79%, 61%, 34% and 26% cases at 1.2 ml/min injection rate (Figure 6). For the simulations, the Kozeny-Carman model is used to relate porosity and permeability. A similar pattern is observed between experiments and simulations: the large saturation variations along the core observed in the experiments are preserved in the simulation results. Moreover, Figure 6 indicates that average CO$_2$ saturation and the CO$_2$ distribution within the core
depends on the fractional flow of CO₂. A lower proportion of CO₂ leads to a lower saturation since the viscous pressure is not able to overcome the capillary barrier.

<table>
<thead>
<tr>
<th>Fractional Flow</th>
<th>Saturation Map</th>
<th>Average Saturation</th>
</tr>
</thead>
<tbody>
<tr>
<td>75%</td>
<td></td>
<td>24.05%</td>
</tr>
<tr>
<td>61%</td>
<td></td>
<td>20.43%</td>
</tr>
<tr>
<td>34%</td>
<td></td>
<td>16.25%</td>
</tr>
<tr>
<td>20%</td>
<td></td>
<td>14.99%</td>
</tr>
</tbody>
</table>

**Figure 6:** Saturation distribution map for four different fractional flow of CO₂ for Kozeny-Carman model (Kuo et al., 2010).

In addition, the steady-state sliced average CO₂ saturations along the core at different fractional flow of CO₂ by using Kozeny-Carman model have almost identical trends of saturation (Figure 7). The same conclusion can apply to homogeneous and high contrast models as long as flow rate is in the viscous dominated regime. The uniform saturations indicate the calculated relative permeability based on the simple Darcy’s equations is reliable.

**Figure 7:** Saturation distribution map for five different fractional flow of CO₂ for Kozeny-Carman model at 1.2 ml/min.
Conclusions

A number of simulations are presented to show the dependence of saturation on flow rates and CO$_2$ fractional flow. The effect of gravity is only important when flow rate is lower than the viscous-dominated regime. The heterogeneity effect has a big impact to saturation distribution when saturation gradient is not so strong. Low flow rates and low fractional flow of CO$_2$ always lead to low displacement efficiencies with any kind of heterogeneities.

Publications and Presentations

1. Kuo, C-W, Perrin, J-C., and Benson, S., Effect of gravity, flow Rate, and small scale heterogeneity on multiphase flow of CO$_2$ and brine, SPE132607, SPE Western Regional Meeting, 27-29 May 2010, Anaheim, California, USA.
2. Kuo, C-W, Perrin, J-C., and Benson, S., Effect of gravity, flow Rate, and small scale heterogeneity on multiphase flow of CO$_2$ and brine, Flow & Transport in Permeable Media Gordon Research Conference (GRC), 10-11 July 2010, Lewiston (ME), United States.

References

3. Kuo, C-W, Perrin, J-C., and Benson, S., 2010, Effect of gravity, flow Rate, and small scale heterogeneity on multiphase flow of CO$_2$ and brine, SPE132607, SPE Western Regional Meeting, 27-29 May 2010, Anaheim, California, USA

Contacts

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5. Including Fine-scale Capillary Heterogeneity in Modeling Multiphase Flow in Porous Media

Investigators
Boxiao Li, Graduate Researcher, Sally M. Benson, Professor, Hamdi Tchelepi, Associate Professor, Department of Energy Resources Engineering, Stanford University.

Introduction
The transport of the injected CO₂ into a geological formation, e.g., a deep saline aquifer, is influenced by the counteraction between viscous forces, gravity, and capillarity. During the injection period, the CO₂ velocity in the near well region is high, and hence viscous forces dominate the flow. As the plume extends, the CO₂ velocity at the displacement front is greatly reduced. As a result, buoyancy and capillary forces begin to compete with viscous forces. After the injection stops, also known as the post-injection period, the only driving forces of the CO₂ are gravity and capillarity, and the CO₂ plume will migrate at a very low speed. To model the long term CO₂ storage process, the simulator should demonstrate the ability in handling the counteraction between viscous, buoyancy, and capillary forces.

Computed Tomography (CT) scans after a CO₂ flood experiment on a Berea core sample initially saturated with water show a patchy distribution of CO₂ in the core after CO₂ flooding. Some regions in the core have high CO₂ saturation, while some other regions are never reached by CO₂ during the flood [1]. This experiment indicates that the distribution and transport dynamics of CO₂-brine systems in natural porous media can be dominated by spatial variations in the capillary-pressure-saturation relationship, which is caused by heterogeneity in rock properties. The importance of such small-scale capillarity heterogeneity depends strongly on the local balance of viscous, buoyancy and capillary forces. Our objective is to develop a rigorous mathematical and numerical modeling framework that models capillary heterogeneity and the counteractions between different driving forces in the CO₂-brine systems with high fidelity, which can then be used to study the behavior of large-scale systems of practical interest.

Background
Lab experiments have been conducted on core samples to examine CO₂ distribution after a CO₂ flood. To study the flow transport dynamics, numerical simulations are employed to history match the experiment results. The simulator used in previous works is TOUGH2-MP. As the research grows more complicated, the simulator is not fast enough to conduct inverse modeling, history matching or carry out larger scale simulations. Therefore, the Stanford General Purpose Research Simulator (GPRS) is explored as a new option.

GPRS aims at incorporating state-of-the-art modeling technologies in general purpose research simulation problems with high efficiency and accuracy. Equipped with robust solvers, GPRS is much faster than TOUGH2 in solving common reservoir simulation problems. More importantly, students and faculties in the development team at Stanford University are able to modify the source code whenever necessary. This means that GPRS is flexible for Benson Lab members to incorporate new physics should it be
necessary. Being a testing ground for future Benson Lab researches, GPRS will benefit the Lab in the long run. To simulate capillary heterogeneity, modifications have been made in GPRS, and its ability in tackling complicated multiphase flow dynamics is demonstrated in this report.

Methodology

Implementation in GPRS: The keyword JFUNC has been implemented in GPRS. It relies on the assumption that the capillary pressure functions of the rocks with the same lithology can be scaled by a single Leverett J-function using the permeability and porosity [2], as shown in Eq. (1).

\[
P_i(S_w) = \sigma \cos \theta J(S_w) \sqrt[3]{\frac{\phi}{k}}
\]  

(1)

The implementation enables simulation of complicated capillary heterogeneity problems, i.e., large number of capillary pressure functions in the flow domain. It allows each grid block in the simulation to have its own capillary pressure function. Besides spatial variation of saturation distribution in core flooding experiments, capillary end effect is also caused by capillary heterogeneity. It is observed in a large number of experiments that the wetting phase fluid can accumulate at the outlet of core if the core is short or the flow rate is not sufficiently high [3]. Discontinuity in capillary pressure occurs at the outlet face of the core. At one side of this interface is the porous medium, which has a capillary pressure of a certain number, while at the other side no porous medium exists, and hence capillary pressure is zero. It is the sudden loss of capillary pressure that retains water inside the core, because water as a wetting fluid prefers to attach on solid surfaces. Capillary end effect can significantly affect laboratory measurement, causing overestimation of the wetting fluid saturation. To serve the purpose of simulating the core flooding experiment, capillary end effect is implemented in GPRS as a boundary condition.

Numerical scheme: The governing partial differential equations of multiphase flow in porous media are flow and transport equations. The flow equation solves the pressure field, while the transport equation solves saturation distribution. Capillary pressure appears in the pressure field, and help determines the phase flow directions. On the other hand, it is also a function of the saturation. Therefore, capillary pressure physically ties the flow and transport equations in a highly nonlinear manner. This means that the flow and transport equations should be coupled and solved together when simulating capillary heterogeneity problems. Hence, the Fully Implicit Method (FIM), assisted by single point phase-based upstream weighting, is used as the numerical scheme in solving the governing partial differential equations, so that flux continuity is honored and the correct upstream directions of all the phases are found.

Results

Example 1: 1-D capillary equilibrium: The example considers incompressible two-phase flow in a 1-D horizontal domain, which is composed of two regions of a porous medium with identical length but different rock properties. The rock properties and relative permeability curves used in this example are listed in Table I. The left region
(region I) and right region (region II) are initially fully saturated by the wetting fluid and the non-wetting fluid, respectively, as shown in Figure 1(a). Using the Leverett J-function, the capillary pressure curves of the two regions are expressed, as shown in Figure 1(b). The domain has no source and sink, and therefore the flow is completely driven by capillary forces.

**Table 1:** Relative data for Example 1

| Rock properties | \( \phi^{(I)} = \phi^{(II)} = 0.25 \), \( k^{(I)} / k^{(II)} = 100 / 25 \text{ (md / md)} \) |
| Fluid properties | \( \mu_w = \mu_{nw} = 1 \text{ cP} \), \( \rho_w = \rho_{nw} = 1000 \text{ kg / m}^3 \) |
| Relative permeabilities | \( k_{nw} = S_w^2 \), \( k_{nw} = (1 - S_w)^2 \) |
| Capillary pressure | \( J = S_w^{-0.5} \), \( P_c = 20\sqrt{\phi / k} \cdot J \) |

\[
\begin{align*}
S_w^{(I)} & = 1 \\
S_w^{(II)} & = 0 \\
k^{(I)} / k^{(II)} & = 4
\end{align*}
\]

**Figure 1:** Initial condition and capillary pressure functions in region I and II.

Van Duijn and de Neef (1995) derived a semi-analytical solution for this example [4]. Because the capillary-pressure function abruptly changes across the region interface, saturation values at the left and right side of the interface should be different so as to guarantee the continuity of fluxes. The semi-analytical solution is able to find the correct saturation pair that honors flux continuity across the interface, and describes the evolution of saturation distribution over the entire domain. As a result, this example can be used to verify the ability of the numerical simulators in honoring flux continuity and in finding the correct flow directions.

**Figure 2:** Simulation results compared to semi-analytical solution. The blue, red and green curves show the evolution of saturation profile with time.
This problem is simulated by GPRS using a fine discretization. The results, shown in Figure 2, are in good agreement with the semi-analytical solutions, indicating that flux continuity is honored and the correct flow directions are found in the simulation. A coarse grid simulation is also conducted. Although numerical diffusion occurs, as expected in all coarse grid simulations, the result demonstrates the ability of the simulator in capturing the saturation jump across the interface, as shown in Figure 3.

**Example 2: 1-D capillarity vs. viscous forces:** This example investigates the counteraction between capillary and viscous forces. 80% fractional flow of the non-wetting phase fluid is injected from the left to the right. The rock and fluid properties, relative permeability and capillary pressure curves are the same as those in Table I, except that the viscosity of the non-wetting fluid is 0.5 cP. Two cases are studied. In the first case, the injection rate is such that the pressure drop of region II (the one with small permeability) has the same order of magnitude of its capillary entry pressure. The GPRS simulation result is illustrated by the blue curve in Figure 4. It can be seen that the injected non-wetting phase is blocked outside region II until its pressure is high enough to overcome the capillary entry pressure. Due to its low viscosity, a significant bank of the injected non-wetting fluid is observed, such that its saturation is higher than that near the inlet boundary. If the injection rate is 10 times higher, shown by the red curve, the entry pressure of region II is much easier to overcome. Hence, the shape of the displacement front is close to standard looking, and only a slight bank of the non-wetting fluid is observed.
Example 3: 2-D capillarity vs. viscous forces: In this example, the region with small permeability (region II) locates at the center of region I, see Figure 5. A bypass route exists, such that the injected non-wetting fluid can avoid the region with high capillary entry pressure. All the properties and curves used in the simulation are the same as those in Example 2. Three cases are simulated, each with a different injection rate. In the first case, the pressure drop across region II is two orders of magnitude lower than its capillary entry pressure. The simulation result shows that no non-wetting fluid is able to enter region II, as illustrated in Figure 6 (a). This is in good agreement with the experimental observations [5]. They conducted slow injection of the non-wetting phase fluid in a domain which had mostly large pores, but with some small pore regions. Their experimental result indicates the inability of the non-wetting phase to overcome the capillary entry pressure of the small pore regions.

![Figure 5: The sketch of the flow domain of Example 3.](image)

If the non-wetting phase is injected in a higher flow rate, it is able to overcome the entry pressure and enter region II, see Figure 6 (b) and (c). Figure 6 (d) shows that the higher the flow rate, the less the impact of capillary heterogeneity.

![Figure 6: GPRS simulation results of Example 3. (a), (b) and (c) are results of Case 1, 2 and 3. (d) The non-wetting phase saturation along line y = 0.5.](image)

Example 4: 3-D capillarity vs. viscous forces and gravity: In core scale and sub-core scale level, capillary, gravity and viscous forces may counteract with each other in a 3-D system. The ability of the simulator in modeling such complicated problems must be
demonstrated in order to simulate long term CO$_2$ geological storage. This example is a CO$_2$ core flooding experiment conducted by Benson Lab. The experimental conditions and related data are listed in Table II. Relative permeability and J-function curves are measured using steady state method and mercury injection, respectively. The porosity field is measured by CT scan, from which the permeability field is generated using the method proposed by Krause, M. et al. (2009) [6].

**Table II:** Experimental conditions of the core flooding experiment

<table>
<thead>
<tr>
<th>Experimental conditions</th>
<th>Rock properties</th>
</tr>
</thead>
<tbody>
<tr>
<td>T (°C)</td>
<td>Diameter (cm)</td>
</tr>
<tr>
<td>50</td>
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<tr>
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<td>Length (cm)</td>
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<tr>
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<td>10.2</td>
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</tr>
<tr>
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<tr>
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</tr>
<tr>
<td>µ$_{CO2}$ (Pa*s)</td>
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<tr>
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<td>µ$_{Brine}$ (Pa*s)</td>
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<tr>
<td></td>
<td>993.33</td>
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<tr>
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<td>Qt = 3 ml/min</td>
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<tr>
<td></td>
<td>80 % CO$_2$ fractional flow</td>
</tr>
<tr>
<td>outlet</td>
<td>Constant pressure = 1800 psi</td>
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<tr>
<td></td>
<td>Capillary end effect</td>
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The core flooding experiment is simulated using GPRS. Since capillary end effect may occur, it is also accounted for in the simulation. Figure 7 compares the cross-sectional average CO$_2$ saturation along the core measured from the experiment with that simulated by GPRS. The data were taken at 5 PVI of injection, approximately at steady state. Since the length of the core is only 10 cm, significant boundary effects are observed. GPRS is able to capture the rough shape of the boundary effect at the outlet, but fails to simulate the inlet boundary effect. In fact, what exactly caused the boundary effects is not clear, and it is unsafe to simply attribute them to capillary end effect or thermodynamic processes, etc. Nevertheless, in the center of the core, the cross-sectional average CO$_2$ saturation does not show a strong gradient, unlike what is observed near the boundaries, and the simulation result is in good agreement with experimental measurements.

**Figure 7:** Cross-sectional average CO$_2$ saturation at 5 PVI.
Slice $x = 17$ is selected for close inspection of the pixel by pixel $\text{CO}_2$ distribution over this cross section. The result, seen in Figure 8, exhibits an excellent agreement between the experimental measurement and GPRS simulation. Figure 9 shows the correlation between the simulation result and experimental measurement. The data points gather around the 100 % match line (the red line), indicating a nice match between the two sets of data.

**Figure 8:** $\text{CO}_2$ saturation on cross-sectional slice No. 17 (from experiment and simulation)

With respect to simulation speed, such simulation will take TOUGH2-MP five days in a cluster [7]. However, it only takes GPRS five hours in a personal two-core computer. This demonstrates that GPRS greatly outperforms TOUGH2 in terms of speed, and can be used in future research to simulate complicated multiphase flow dynamics in 3-D system.

**Figure 9:** $\text{CO}_2$ saturation from experiment vs. simulation (Slice No.17)

**Progress and future work**

Since GPRS outperforms TOUGH2 in terms of speed, it can be used in inverse modeling problems to study the factors that affect fluid distributions in core scale level. This will provide insights of the relationship between scales and the parameter space of the unknowns, which then can be used to study large scale problems of practical interest. Other interesting phenomena related to capillary heterogeneity can also be investigated. Examples are capillary hysteresis and boundary effects in core flooding experiments.
In terms of numeric techniques, a study can be done to improve the convergence of Newton iterations at the presence of strong capillary forces. The second order diffusion term introduced by capillary forces poses strong challenges in the convergence of Newton iteration, even for FIM approach. Although FIM is theoretically unconditionally stable, the nonlinearity of the problem may cause the iteration to diverge, forcing the simulator to cut the time step. Hence, a lot of Newton iterations are wasted. A simulator is desirable if it regulates this divergence and allows the selection of time step sizes to be totally based on accuracy instead of stability.

Publications and Presentations
1. B. Li, H. Tchelepi, S.M. Benson, Fine-scale Capillary Heterogeneity in Modeling CO\textsubscript{2} Core Flooding Experiments, GCEP Symposium - Creating a Sustainable Energy System for the 21st Century and Beyond, September 28 - 29, 2010, Stanford University, USA

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7. Personal communication with Krause, M.H.

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Hamdi Tchelepi: tchelepi@stanford.edu
6. On the distribution of CO$_2$ and water in reservoir rocks

**Investigators**
Ronny Pini, Postdoctoral Researcher, Sam Krevor, Postdoctoral Researcher, Sally Benson, Professor, Department of Energy Resources Engineering, Stanford University

**Introduction**
Predicting the long-term fate of the injected CO$_2$ into deep saline aquifers requires a thorough understanding of the multiphase properties of CO$_2$ and water in these formations. Continuum-scale rock properties such as relative permeability and capillary pressure represent essential information for reservoir simulators that are used to history match and to design field-scale injection tests. These properties depend on the fluid saturations, which in turn are influenced by rock heterogeneities observed at the sub-core scale [1]. Understanding the role of these heterogeneities on the fluid distribution in a reservoir rock provides a first step towards the development of appropriate methods for up-scaling laboratory data to predict multiphase flow behaviour throughout a reservoir.

X-ray Computed Tomography (CT) is being increasingly applied to visualize fluid flow phenomena within the pore space of a reservoir rock, due to its non-destructive nature [2-4]. Of particular interest are studies that aim at providing quantitative information on the distribution of physical properties such as porosity and fluid saturations. Medical scanners are often used for such studies as they provide a good compromise between a relatively high resolution (around 600µm × 600µm × 1mm) and sample size (2 inches in diameter and 10 cm in length in the present study) as compared to synchrotron-based microtomography, which provides micronscale resolution for samples of only a few millimetres in size [5].

One of the limits of X-ray CT is the significant noise associated to the reconstructed images. In the case of two-phase (CO$_2$ and water) flow in a porous reservoir rock, this is mainly due to relatively small density contrast between the two fluid phases as compared to the contrast between any one of the fluids and the rock. One of the strategies suggested to circumvent this problem consists of adding so-called dopants (e.g. iodinated medium) to one or the other fluid phase [2].

In this work, a methodology is described to assess the error on a pixel-by-pixel level of the CT measurement. The method is further applied to a CO$_2$/water core-flooding experiment in a Berea sandstone and three approaches are investigated aimed at reducing the uncertainty associated to the porosity and saturation values at a pixel level that are obtained by X-ray CT methods, namely the averaging over multiple scans taken at identical positions, the averaging over neighboring pixels (coarsening) and the utilization of iodine solutions. The comparison among these three approaches provides guidelines for designing experiments aimed at the quantitative estimation of the distribution of CO$_2$ and water at the sub-core scale.

**Theory**
Computed Tomography (CT). This technique creates cross-sectional images of a core that consist of a matrix with a given number of volume elements (voxels). To each voxel
is assigned a linear attenuation coefficient, $\mu$, which relates the intensity decrease of an X-ray beam with a particular effective energy to the material properties in a given voxel. Water is typically chosen as a reference material and the results are provided in terms of the so-called CT number $CT$, which is defined as the change in the linear attenuation coefficient normalized to the coefficient for water $\mu_w$, i.e.

$$CT_i = 1000 \frac{\mu_i - \mu_w}{\mu_w} \quad i = 1, \ldots, N_{\text{pix}}$$  \hspace{1cm} (1)$$

where $N_{\text{pix}}$ represents the number of voxels in one image. The typical spatial resolution of a medical CT scan is around 1 mm [4], a value which is much larger than the characteristic pore size of reservoir rocks (around 10-100\mu m). The CT numbers assigned to each voxel include therefore contributions from each pure component materials in the system (fluid phases and rock). By assuming a linear dependence with composition, porosity $\varepsilon$ and saturation $S$ in each voxel $i$ can be computed from the following relationships [1,4]:

$$\varepsilon_i = \frac{CT_{2r,i} - CT_{1r,i}}{CT_2 - CT_1} \quad i = 1, \ldots, N_{\text{pix}}$$  \hspace{1cm} (2a)$$

$$S_i = \frac{CT_{2r,i} - CT_{12r,i}}{CT_{2r,i} - CT_{1r,i}} \quad i = 1, \ldots, N_{\text{pix}}$$  \hspace{1cm} (2b)$$

with the subscripts 1r and 2r referring to the voxel CT numbers measured when the core is saturated with phase 1 ($S = 1$) and 2 ($S = 0$), respectively, whereas the subscript 12r is associated to a two-phase flow experiment. $CT_1$ and $CT_2$ are the CT numbers of the pure fluids. The procedure just described is based on the estimation of porosity and saturation values by combining the raw CT numbers obtained during different experiments at the voxel level. To this aim it is therefore of primary importance that the core remains perfectly stationary from the start to the end of the whole experimental campaign. Moreover, an assessment is needed of the measurement error propagation, if quantitative information about the porosity and the saturation are required.

Measurement error and error propagation: As a first appraisal of the error associated to the CT measurement, the repeatability on a pixel-by-pixel level of CT scans taken at identical conditions has been investigated. As an example of general validity, Figure 1 shows a histogram of the observed difference in CT number obtained by subtracting two independent scans taken at identical position during a steady-state 100\% water imbibition experiment. As it can be seen, the data create a Normal distribution $N(m, \sigma^2)$ characterized by a mean centered at zero ($m = -0.09$) and a variance ($\sigma^2 = 24.8$), the latter describing the dispersion from the average. For the sake of comparison, a normal density distribution curve estimated from these values is shown by the solid line in the same figure.
Figure 1 – Difference in CT number obtained by subtracting two independent scans taken at identical position during a steady-state 100% water imbibition experiment. The solid line represents a normal distribution curve with mean and standard deviation estimated from the experimental data.

The behavior just described is typical for measurements that are mainly affected by random errors. In such cases, a given transformation applied to the raw data (such as a subtraction or the calculation of porosity and saturation) leads to a propagation of the measurement error that can be directly estimated from the variances. In particular, the variance of a variable \( c = f(a, b) \) can be estimated as follows:

\[
\sigma_c^2 = \sigma_a^2 \left( \frac{\partial c}{\partial a} \right)^2 + \sigma_b^2 \left( \frac{\partial c}{\partial b} \right)^2 + 2\sigma_{ab} \left( \frac{\partial c}{\partial a} \right) \left( \frac{\partial c}{\partial b} \right)
\]

where \( \sigma_{ab} \) represents the covariance, which can be set to 0 when \( a \) and \( b \) are uncorrelated (i.e. randomly scattering around the average), a condition which is satisfied for the measurements reported in this study.

Methodology

In the present work, the theory just described is applied to a two-phase flow core flooding experiment performed on a Berea sandstone core. Sample dimensions are 2 inches in diameter and 10 cm in length, whereas porosity and permeability take a value of 22.1 % and 914 mD, respectively. The reader should refer to Section 3 for additional details regarding the experimental setup and the measurement procedure. The fluid distribution inside the core is determined by X-ray CT scanning. For imaging, the voxel dimension is 0.5 × 0.5 × 1mm, the tube current is 200 mA, the energy level of the radiation is 120 keV and the display field of view (DFOV) is 25 cm.

The analysis is carried out on a set of 14 scans that have been taken at a fixed position within the core once the system has reached steady state. The difference in CT number \( \Delta_{n,i} \) obtained for each pixel by subtracting two independent set of scans that have been averaged \( n \) times is defined as follows:

\[
\Delta_{n,i} = \frac{1}{n} \left( \sum_{j=1}^{n} CT_{j,i} - \sum_{k=n+1}^{2n} CT_{k,i} \right) \quad i = 1, \ldots, N_{\text{pix}} \quad \text{and} \quad n = 1, \ldots, 7
\]
Note that in Eq.5, the phase subscript has been omitted from the CT number for the sake of simpler notation. By assuming that the CT numbers obtained during each experiment are characterized by the same standard deviation $\sigma_{\text{pix}}$, an expression for the uncertainty associated to the quantity $\Delta_n$ can thus be estimated from Eq.4:

$$\sigma_{\Delta_n} = \sqrt{2} \sigma_{\text{pix},n} = \sqrt{2} \frac{\sigma_{\text{pix}}}{\sqrt{n}} \quad n = 1, \ldots, 7$$

(6)

where $\sigma_{\text{pix},n}$ is the standard deviation associated to a $n$ times-averaged scan. Eq.6 provides therefore a way of relating the uncertainty associated to the CT number on a pixel-by-pixel level ($\sigma_{\text{pix}}$ or $\sigma_{\text{pix},n}$) to the experimentally observed standard deviation obtained upon subtracting 2 independent sets of scans. Similarly, estimates for the uncertainty in the porosity and saturation can be readily obtained by applying Eq.4 to Eqs.2a and 2b, i.e.

$$\sigma_e = \frac{\sqrt{2} \sigma_{\text{pix}}}{1000}$$

(7a)

$$\sigma_S = \frac{\sqrt{2} \sigma_{\text{pix}}}{CT_{\text{wr}} - CT_{\text{gr}}} \sqrt{\frac{CT_{\text{wr}}}{CT_{\text{wr}} - CT_{\text{gr}}} \left(\frac{CT_{\text{wr}} - CT_{\text{gr}}}{CT_{\text{wr}} - CT_{\text{wsr}}}\right)^2} \approx \frac{\sqrt{2} \sigma_{\text{pix}}}{CT_{\text{wr}} - CT_{\text{gr}}}$$

(7b)

where the subscripts have now been named according to the actual phases present in the experiment, namely the water phase (saturated with gas) “ws” and the gas phase “g”. The porosity (Eq.2a) is estimated from a measurement with air ($CT_1 = -1000$) and water ($CT_2 = 0$), whereas the term in the square root (Eq.7b) is very close to 1 due to relatively low gas saturations that are typically achieved in the two-phase flow experiments, i.e. $(CT_{\text{wr}} - CT_{\text{gr}})^2 \gg (CT_{\text{wr}} - CT_{\text{wsr}})^2$. As shown in the Result section, values for $\sigma_{\text{pix}}$ are found by fitting Eq.6 to the experimental data, whereas in Eq.7b experimental slice-averaged values are used for $CT_{\text{wr}}$ (1381 H) and $CT_{\text{gr}}$ (1215 H).

It is evident from Eqs. 7a and 7b that there are two main approaches that can be followed to improve the precision of the porosity and the saturation estimates, namely by reducing the value of $\sigma_{\text{pix}}$, and/or by increasing the contrast between water and gas phase, i.e. by increasing $CT_2$ in Eq.7a and $CT_{\text{wsr}}$ in Eq. 7b. In the former case, both the averaging of the same pixel over multiple scans and the averaging over neighboring pixels (coarsening) have been investigated. In the latter case, the effect of a water phase doped with an X-ray attenuating agent (NaI, sodium iodide) has been studied. Addition of the salt to the water solution results in a change of the measured CT number and Eqs. 7a and 7b can be rearranged as

$$\sigma_S = \frac{\sqrt{2} \sigma_{\text{pix}}}{CT_{\text{wr}} - CT_{\text{gr}} + \epsilon (CT_{\text{wr}} - CT_{\text{wsr}})}$$

(8a)
\[
\sigma_t = \frac{\sqrt{2} \sigma_{\text{pix}}}{CT_{\text{ws}} + 1000}
\]  

(8b)

where \(CT^*_{\text{ws}}\) refers to the CT number of the iodinated water phase.

Results

Figure 2 shows 2D maps (3cm × 3cm) of the CT number for a slice taken at about 4.5 cm from the inlet during the core-flooding experiment: higher values (red color) correspond to regions with low porosity, whereas lower values (blue) are associated to the presence of fluid. The raw scan is compared to the images obtained by averaging over 2 and 10 consecutive scans that have been taken at the same exact position. The smoothing of the picture upon averaging is rather evident and features becomes more delineated such as a larger concentration of moderate to high CT values (yellow color) at the NW and SE corners of the image as well as the two red spots that likely due to the presence of iron oxide.

![Figure 2](image)

**Figure 2** – 2D maps (3cm × 3cm) of the CT number for a cross-section of a Berea core obtained upon averaging multiple scans on a pixel-by-pixel level.

The same 2D maps are shown in Figure 3, but this time one single scan is used, to which an averaging has been applied over neighboring pixels (coarsening), namely 2×2 and 3×3. It can be seen that although the image looses information upon coarsening as a results of a reduction of the number of pixels, it preserves the main features just described.

![Figure 3](image)

**Figure 3** – 2D maps (3cm × 3cm) of the CT number for a cross-section of a Berea core obtained upon coarsening of one single scan.
From a quantitative point of view, these two averaging schemes are compared in Figure 4, which shows $\sigma_{\Delta n}$ as a function of the number of averaged scans $n$. Three sets of data (symbols) are shown that correspond to three different degrees of coarsening $1 \times 1$ (black), $2 \times 2$ (blue) and $3 \times 3$ (red), respectively, together with the behavior predicted by Eq.6 upon fitting the parameter $\sigma_{\text{pix}}$ to each set of data. A very good agreement is observed between experiment and theoretical predictions, thus confirming the random nature of the error associated to the CT scan measurements as well as the achievement of steady-state during the experiment. Values of the fitted parameters are reported in Table 1. It can be seen from the picture that averaging over repeated scans leads to a significant decrease of the uncertainty associated to each pixel ($\sigma_{\text{pix},n} = \sigma_{\Delta n}/\sqrt{2}$). Coarsening is also effective, though to a lower extent: as given in Table 1, when compared to the pixel-uncertainty of the raw data ($\sigma_{\text{pix}} = 18$), values of 6.8 and 11 are obtained upon averaging over 7 (multiple scans) or 9 pixels ($3 \times 3$, coarsening), respectively.

![Figure 4](image)

**Figure 4** – Experimental standard deviation obtained upon subtracting two sets of independent scans that have been averaged $n$ times as a function of the number of averaged scans $n$. Solid lines represent the prediction from Eq.6. Three coarsening schemes are shown, $1 \times 1$ (black), $2 \times 2$ (blue) and $3 \times 3$ (red).

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<th>Averaged scans</th>
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<th>$n = 7$</th>
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<td>$\sigma_{\epsilon}$</td>
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<td>0.025</td>
</tr>
<tr>
<td>$2 \times 2$</td>
<td>14</td>
<td>0.021</td>
</tr>
<tr>
<td>$3 \times 3$</td>
<td>11</td>
<td>0.016</td>
</tr>
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</table>

Table 1: Uncertainty (standard deviation) on a pixel-by-pixel level associated to the CT number, porosity and saturation as obtained for different averaging schemes.

In terms of porosity and saturation, the most precise measurement clearly results from the combination of both methods and leads to $\sigma_\epsilon = 0.0059$ and $\sigma_S = 0.035$. In that case, porosity and saturation should therefore be reported with a precision of $\pm 2\sigma$. For the sake of comparison, a coarsening of $60 \times 60$ (i.e. averaging over the whole cross-section) leads
to an absolute precision of $\pm 8.5 \times 10^{-4}$ and $\pm 5 \times 10^{-3}$ for porosity and saturation, respectively.

The third approach that has been tested is the use of an X-ray attenuating agent, such as sodium iodide, to increase the contrast between the water and the gas phase. To this aim, the increase in CT number of the doped water solution has to be known. Withjack [2] reports experimentally obtained CT numbers for a range of NaI concentrations in water. For instance, by neglecting the effect of the dissolved CO$_2$ on the reported values, $CT^\nu_{ws}$ takes a value of 733 and 2267 H for a doping agent concentration of 3.7 and 15 %wt, respectively. For the sake of comparison and according to the total amount of dissolved solids (TDS), seawater contains between 10-100 g/L (~1-10%wt.) of dissolved salts, whereas for brine TDS > 100 g/L. Figure 5 shows the standard deviation associated to the saturation as a function of the number of averaged scans (Eq.8); the procedure described above for a “clean” water phase (gray curves) is now repeated for two different concentration of NaI (3.7 and 15 %wt). The addition of a doping agent significantly increases the precision of the saturation measurement: for a 15 wt% solution, the $\sigma_S$ associated to the raw data (single scan) takes a value of about 0.038, i.e. similar to the best case described above ($\sigma_S = 0.035$, with 7 repeated scans and 3x3 coarsening). Moreover, combination of the iodine solution with one or the other averaging scheme allow to reduce $\sigma_S$ below 1%abs.

![Figure 5: Standard deviation associated to the saturation as a function of the number of averaged scans (Eq.8) for three different NaI concentrations (0, 3.7 and 15 %wt.) and coarsening schemes (1x1, 2x2 and 3x3).](image)

**Conclusion**

In this work a methodology has been presented to assess the error associated to the X-ray CT measurement. Three different approaches have been investigated aimed at decreasing the uncertainty associated to estimated porosity and saturation values at the voxel level, namely the averaging over multiple scans taken at identical positions, the averaging over neighboring pixels (coarsening) and the utilization of iodine solutions. The comparison among these three approaches provides guidelines for designing experiments aimed at the quantitative estimation of the distribution of CO$_2$ and water at
the sub-core scale. Most likely, the optimal approach is a combination of the three methods presented. In the future, we plan to carry out experiments to validate the methodology presented in this work. Efforts in this direction are justified by the ultimate goal of improving our understanding on the dynamics of multiphase flow at the sub-core scale and on the role of heterogeneities on the distribution of CO$_2$ and water in the pore space of a reservoir rock.

References

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