

# **GCEP Progress Report for the Stanford Center for Carbon Storage**

## **Investigators**

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## **Abstract**

The primary theme of research at SCCS is related to enhanced recovery of oil and gas combined with CO<sub>2</sub> storage, mixed gas injection processes, the development of monitoring technologies for all classes of geological storage, the characterization of both near-well and distal geochemical processes during CO<sub>2</sub> injection, and computational optimization of the design and operation of large projects.

As part of the CCP3 Contingencies Project, we submitted a report (White Paper, July 2013) that summarized the state-of-the-science for monitoring & intervention technology activities based on a review of the existing literature. In some cases, quite a bit is known. For example, there are a number of monitoring approaches available for leak detection, including field demonstrations of a variety of techniques for detecting small quantities of CO<sub>2</sub> in the subsurface. We developed and quantitatively evaluated intervention options for responding to unforeseen fluid leakage or lack of project conformance in CO<sub>2</sub> storage projects as the final part of CCP3 Phase I Project. Whereas CO<sub>2</sub> storage has to date been shown to be safe and effective, the possibility for unforeseen CO<sub>2</sub> leakage up faults and fractures, leakage up active or abandoned wells, unexpected plume migration, or brine displacement into drinking water aquifer is still a possibility. Being prepared to address these residual risks, with a set of options for stopping leakage, controlling plume migration within the storage reservoir, will eliminate or minimize environmental damage to drinking water or to the near surface environment. This will provide an additional measure of confidence for regulators and the public alike, thus facilitating CCS.

We conducted our first Annual Workshop on CO<sub>2</sub>-EOR & Storage in January 2013 at Stanford University. The workshop was divided into two sessions focusing on conventional EOR & unconventional topics such as shale gas, residual oil zones & a brainstorming session for progressing university research for EOR vs Storage aspects of Carbon. The event concluded with a student poster session showcasing the current graduate research at SCCS. We showcased our research during the second Annual research review, held in May 2013, and received a very positive interest & feedback. The meeting was attended by guests & affiliates from the oil & gas industry (Apache, Chevron, ExxonMobil, Schlumberger, Shell, and USGS), faculty, research staff and students involved with SCCS. We discussed some of the major aspects of carbon storage research split into four sessions with multiple short talks on a variety of interesting problems, including:

- (i) CO<sub>2</sub>-sequestration simulation studies with emphasis on capillary pressure and permeability heterogeneity;
- (ii) Monitoring of CO<sub>2</sub> plume and reservoir diagnostics;
- (iii) Geochemical processes during CO<sub>2</sub> injection coupled with reactive transport modeling; and
- (iv) Improved process modeling for design, operation and risk assessment.

We organized group seminars every other week on campus to discuss latest student research and quarterly webinars on topics of special interest.

## Introduction

Carbon storage refers to the set of technologies developed to inject the captured carbon dioxide (CO<sub>2</sub>) gas in deep geological formations for long term storage. It is a potential means of mitigating the contribution of fossil fuel emissions to global warming. There are unanswered fundamental scientific questions that must be addressed to consider implementation of large-scale projects of geological CO<sub>2</sub> storage and sequestration within the next several decades.

A focus on the investigation and development of methods for dealing with CO<sub>2</sub> leakage is urgently needed for industry and regulators alike to be prepared for managing such events should they arise. A quick response to unforeseen events will reduce the risks and costs associated with them, and increase public confidence in CCS as a climate mitigation option. Specifically, options for managing each step in the chain of events illustrated in Figure 1, from leak detection to completion of the intervention, are needed.

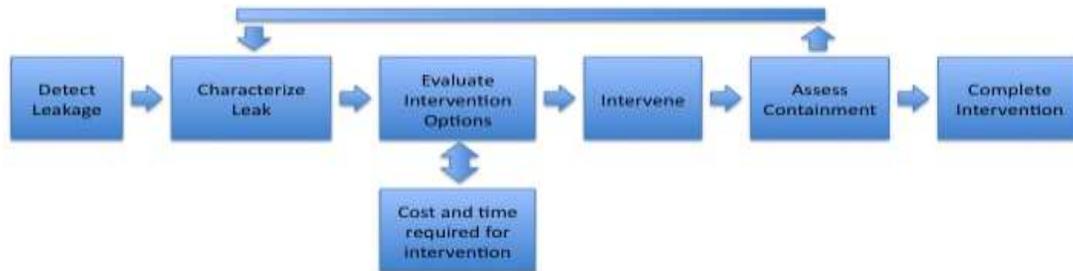


Figure 1. Work-flow for leakage intervention showing the chain of events expected over the intervention activity.

A scenario-based approach was used to carry out and integrate the results of this project. We began by simulating leakage in a typical storage project in a saline aquifer. The model was based on a deep section of the Powder River Basin in Wyoming, consisting of a thick sequence of sandstone, shale, and anhydrite. Leakage rates, pressure buildups, and saturations from this model were used for calculating seismic responses and assessing how soon after injection began would it be possible to detect leakage. Based on these simulations we concluded that the leak could be detected with a few years after the project started, when a total of about 5000 tonnes of CO<sub>2</sub> had leaked out of the storage reservoir and accumulated in an overlying aquifer above the seal. These simulations set the stage for higher resolution simulations, which addressed the following issues:

- Influence of fault and reservoir properties on leakage;
- Effectiveness of stopping injection on leak mitigation;
- Effectiveness and permanence of hydraulic controls such as fluid extraction and brine injection on leak mitigation;
- Potential for accelerated trapping of CO<sub>2</sub> in the overlying aquifer;
- Effectiveness of polymer and reactive barriers (e.g. amorphous silica) on stopping leakage;
- Barrier emplacement strategies; and

- Evolution of fault permeability due to plugging with reactive materials.

In addition to these simulation studies, we also performed laboratory experiments to test the most promising commercially available sealant, H<sub>2</sub>Zero™ by Halliburton. A barrier emplacement strategy, based on measured gel times was also developed.

Besides the CCP3 Project outlined above, SCCS also funded the following students & post-docs in 2013: Mahnaz Firouzi, Julia Reece, Sara Farshidi, Avinoam Rabinovich, Folake Ogunbanwo and Amir Salehi. The status and progress of their research is described in the Results section.

## **Background**

In previous years it was apparent that the global impetus for CCS had slowed down somewhat as economies around the world focused on other more immediate priorities, and demonstration projects tackled first-of-a-kind cost escalation. However, now, as the world's economies continue to recover and demonstration project learnings are dissected and understood for continued improvement, we expect CCS to move back and garner interest. The oil & gas industry needs to be well placed for this potential eventuality and the work of SCCS (through CCP3 Project & other research within the group) has been crucial in building the important blocks of the big puzzle.

## **Results**

Following are the projects completed/undergoing within the SCCS research groups:

1. The CCP Contingencies initiative aimed to identify anomalies that may lead to containment failure at a CO<sub>2</sub> storage site and formulate an intervention plan using existing or developing new technologies. Developing the capability to detect, characterize and intervene in unanticipated CO<sub>2</sub> or displaced brine migration adds an additional layer of stakeholder reassurance around CO<sub>2</sub> storage.
2. Adsorption and transport of CO<sub>2</sub> in carbon and clay micropores in shale: from atomistic to molecular scale models, Dawn Geatches, Mahnaz Firouzi and Beibei Wang of Prof Jen Wilcox's Research Group: Storing CO<sub>2</sub> underground is one of the proposed methods of mitigating the emission of CO<sub>2</sub> into the atmosphere. One type of underground store is depleted oil and gas reservoirs, whose estimated capacity ranges from 60-120 GT CO<sub>2</sub>, equivalent to 10-20 years of US CO<sub>2</sub> emissions. In this work we focus on the storage of CO<sub>2</sub> in exhausted gas shales, and in particular the roles that the organic matter and clay minerals play in the adsorption and transport of CO<sub>2</sub> through the micropore networks. Atomistic models of clay surfaces using quantum mechanical methods were created. These models enabled us to identify whether chemical conversion of CO<sub>2</sub> to a carbonate occurred. Using these structurally robust models, larger clay pores have been created, which will be used in non-equilibrium molecular dynamics simulations to investigate CO<sub>2</sub> transport through micropores. In addition, CO<sub>2</sub> adsorption within carbon micropores has been modeled using Grand Canonical Monte Carlo simulations. The simulation results will be compared to experimental

measurements, to gain a deeper understanding of both the merits and limitations of the modeling methods used in this study.

3. Fault permeability during shear slip and its effect on seal integrity, Julia S. Reece, Arjun H. Kohli, and Mark D. Zoback: The preliminary shear deformation and fault permeability results on sawcut shale samples with varying mineralogical composition were presented. The deformation data from a Haynesville reservoir sample containing 22% clay indicate stable sliding behavior with a coefficient of friction varying between 0.53 and 0.61. Upon shearing, fault permeability of the shale sample decreases by about 2.5 orders of magnitude within the first millimeter of shear displacement and continues to decrease up to the maximum axial displacement of 4 mm. This ongoing experimental study examines the effect of shear deformation on fault permeability in intact shales with varying clay contents, under varying stress conditions, and with different gases as pore fluids. Experiments are being carried out in a triaxial apparatus with three different types of samples: 1) shale cores with sawcuts representing faults; 2) shale cores naturally broken along faults; and 3) shale wafers between aluminum forcing blocks. After individual shear deformation increments at a constant axial displacement rate of 1mm/s, fault permeability is measured using steady state Darcy flow. Petrographic analysis of thin sections and scanning electron microscope images as well as fault roughness measurements will provide insights into the microstructure of faults in the various shale samples. Testing of the hypothesis that during stable sliding in clay-rich samples, fault permeability will decrease with increasing shear deformation due to the formation of a clay smear, whereas during unstable, stick-slip sliding in samples with low clay content, fault permeability will increase due to the accumulating damage in the gouge layer is underway. The relationship between shear deformation and fault permeability is important to understand how shear slip, induced by the injection of CO<sub>2</sub>, may affect the seal integrity of CO<sub>2</sub> repositories.
4. Modeling Coupled Flow and Reactions in Carbon Storage Problems, Sara Farshidi, Denis Voskov, Lou Durlinsky and Hamdi Tchelepi: This work addresses the numerical treatment of chemical reactions, as required for many subsurface flow applications including geological carbon storage. Chemical reaction modeling has been incorporated into an existing EOS-based compositional simulator (AD-GPRS). Both kinetic and equilibrium, as well as heterogeneous and homogeneous, chemical reactions are treated. Two numerical formulations have been implemented. One of these is based on the so-called “natural” set of variables, and the other uses overall composition. The two approaches display different computational advantages and drawbacks, though numerical solutions have been shown to be in essential agreement. Natural variables have the advantage of avoiding equation of state calculations in the two phase zone, while the use of overall composition avoids variable switching, which leads to reduced complexity. In carbon storage simulations, the overall-composition formulation displays advantages in cases where the brine phase disappears in some grid blocks. For such cases, special numerical treatments for simulations that apply natural variables had to be developed.

Numerical results (using GPRS) are presented below that illustrate our capabilities. These results were generated using the natural variable treatment. In this model, CO<sub>2</sub> is injected into the center of a three-dimensional aquifer for 40 years, and the system is then simulated for another 1960 years. The 10.9 km×10.9 km×97.5 m system is divided into 50×50×16 (total of 40,000) blocks. The heterogeneous permeability field is shown in Fig. 2. Fig. 3 displays the CO<sub>2</sub> in the supercritical ‘gas’ phase at the end of the injection period (for clarity, the model is sliced at the well block, and only the central portion is shown). We see that CO<sub>2</sub> has migrated to the top of the aquifer and has also spread laterally. The fate of the injected CO<sub>2</sub> as a function of time is shown in Fig. 4. After 2000 years, more than half of the CO<sub>2</sub> is in the gas phase and only 10% has been mineralized. It is also apparent that there is very little mineralization for the first 200 years. Simulations of this type can be used to evaluate the impact of well locations, CO<sub>2</sub> injection rates, and other parameters on the timing and amount of mineralization achieved.

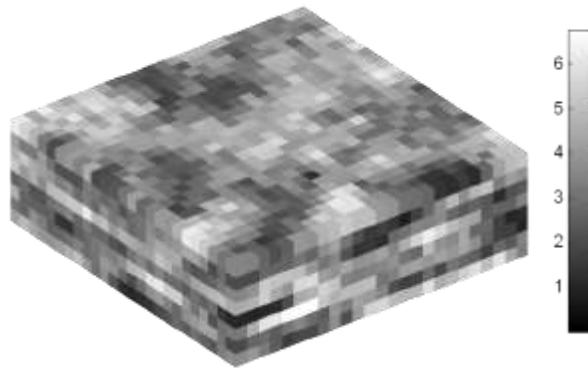


Figure 2- Heterogeneous permeability field

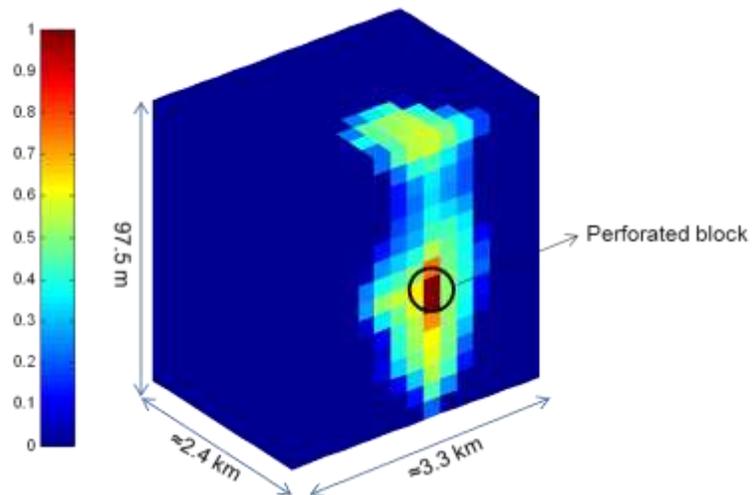


Figure 3- CO<sub>2</sub> phase saturation after 40 years of injection (central portion of the model shown)

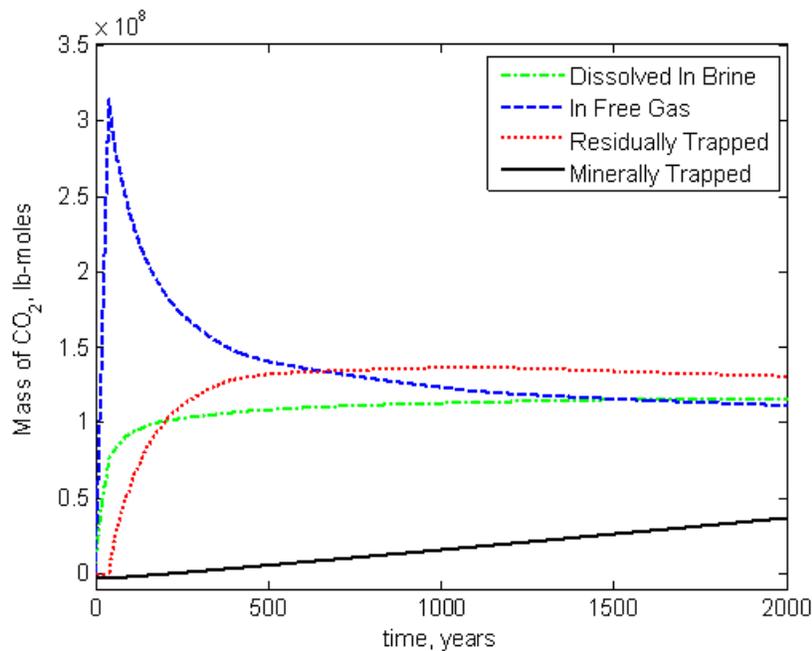


Figure 4- Distribution of the injected CO<sub>2</sub> over time

5. Upscaling of Two-Phase Flow with Capillary Heterogeneity and Gravity Effects, Avinoam Rabinovich and Lou Durlofsky: Avinoam Rabinovich joined Stanford as a post-doc in March 2014, so this work is at an early stage. Capillary pressure heterogeneity is an important effect in CO<sub>2</sub> storage simulations, but it is computationally expensive to model in fine-scale simulations. The development of accurate and efficient upscaling procedures will enable much faster simulations for problems that include these effects. In this research, we aim to incorporate capillary heterogeneity and gravity into existing upscaling techniques for two-phase flow problems. The first goal is to develop a general, high-precision global upscaling method that is robust with respect to changes in flow conditions such as flow rate. This in itself is a challenging problem, as the upscaled functions may be flow-rate dependent, and we wish to avoid computing them for many different flow regimes. Subsequently, ensemble level upscaling to account for geological uncertainty will be considered.
6. Effect of pseudocomponent selection on the simulation of a CO<sub>2</sub> gas injection process, Folake Ogunbanwo and Tony Kovscek: Enhanced oil recovery by carbon dioxide (CO<sub>2</sub>) gas injection is highly dependent on the composition of the fluid in the reservoir and the operating conditions. In the case of a multi-component mixture, the simulations of CO<sub>2</sub> EOR processes can be computationally intensive. Lumping of the components into pseudocomponents is frequently done to reduce simulation cost resulting in some loss in accuracy. A match in the phase diagram of the multicomponent mixture and the resulting lumped mixture is typically used

to validate the lumping scheme. This work focuses on matching the paths in compositional space of the descriptive fluid with that of the lumped mixture for validation of the grouping scheme. This method has been shown to work for an isothermal, isobaric, immiscible displacement using 1-D simulations in a compositional simulator. Future work involves extending this method to a miscible systems with operating conditions which vary with production.

7. Upscaling of Compositional Flow Simulation based on a Non-Equilibrium Formulation, Amir Salehi and Hamdi Tchelepi: Compositional simulation of oil reservoirs is necessary for accurate representation of the physics associated with near-miscible gas injection processes (e.g. CO<sub>2</sub> injection). Performing the simulations using the fine-scale geocellular model is computationally expensive; as a result, reliable upscaling methods for compositional flows are needed. Compared with black-oil models, the interactions between the thermodynamic phase behavior and the sub-grid heterogeneities pose significant additional challenges to upscaling. A new framework to upscale multi-component, multi-phase compositional displacements is introduced with special attention to accurate representation of the phase behavior on the coarse grid. This work uses a mass-conservative formulation and introduces an upscaled molar mobility for each phase. These upscaled flow functions account for the sub-scale absolute and relative permeability variations, as well as, compressibility effects. They also correct - somewhat - for numerical dispersion effects at the coarse-grid level.

The upscaling of the thermodynamic phase behavior is performed as follows. Instantaneous thermodynamical equilibrium is assumed to be valid at the fine-scale, and coarse-scale equations are derived, in which the thermodynamic phase behavior is not necessarily at equilibrium. Deviation from local equilibrium may be due to different bypassing mechanisms, such as fingering and channeling. As a result, the fugacity of a component in the two phases may not be equal at the coarse scale, and this deviation is quantified by the coarse-scale thermodynamic functions. It is demonstrated that these upscaled functions can be interpreted as a transformation of the equilibrium phase space on the fine scale to a modified region of similar shape, but with tilted tie-lines. Description to modify the widely used Barker-Fayers ( $\alpha$ ) factors based on the new upscaled thermodynamic functions is given. The proposed methodology is applied to various challenging gas injection problems. We compare our upscaling method with standard upscaling techniques for compositional simulation, and we show significant improvements, both in accuracy and computational efficiency, of the new approach. As future direction, the plan is to test the proposed algorithm for more realistic cases including gravity in 3-D domains and thermal three-phase compositional models.

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