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A Model Comparison Initiative for a CO_2 Injection Field Test: An Introduction to Sim-SEQ

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Abstract
Because of the complex nature of subsurface flow and transport processes at geologic carbon storage (GCS) sites, modelers often need to implement a number of simplifying choices while building their conceptual models. Such simplifications may lead to a wide range in the predictions made by different modeling teams, even when they are modeling the same injection scenario at the same GCS site. Sim-SEQ is a new model comparison initiative with the objective to understand and quantify uncertainties arising from conceptual model choices. While code verification and benchmarking efforts have been undertaken in the past with regards to GCS, Sim-SEQ is different, in that it engages in model comparison in a broader and comprehensive sense, allowing modelers the choice of interpretation of site characterization data, boundary conditions, rock and fluid properties, etc., in addition to their choice of simulator. In Sim-SEQ, fifteen different modeling teams, nine of which are from outside the United States, are engaged in building their own models for one specific CO_2 injection field test site located in the southwestern part of Mississippi. The complex geology of the site, its location in the water leg of a CO_2-EOR field with a strong water drive, and the presence of methane in the reservoir brine make this a challenging task, requiring the modelers to make a large number of choices about how to model various processes and properties of the system. Each model team starts with the same characterization data provided to them but uses its own conceptual models and simulators to come up with model predictions, which can be iteratively refined with the observation data provided to them at later stages. Model predictions will be compared with one another and with the observation data, allowing us to understand and quantify the model uncertainties.

Keywords Carbon sequestration – Geological storage – Model comparison – Sim-SEQ

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Introduction

The objective of geologic carbon storage (GCS) is to prevent anthropogenic CO_2 from entering the atmosphere, thereby maintaining acceptable levels of atmospheric CO_2 (Pacala and Socolow, 2004; Gale, 2004; Bachu, 2008). In an ideal world, the CO_2 will be safely transported to sequestration sites and injected deep underground, where it will remain permanently trapped, with no negative impact on the terrestrial environment or on underground resources such as groundwater or fossil fuel deposits. In practice, however, GCS is unlikely to be perfectly effective or completely risk-free (Oldenburg et al., 2009; Birkholzer et al., 2011). This is because there are still considerable uncertainties regarding storage capacity, injectivity, caprock integrity, leakage pathways, impact on reservoir rock and formation fluids, and effectiveness of post-injection monitoring of the injected CO_2 plume (Wilson et al., 2007; Stauffer et al., 2009; Li et al., 2011; Seto et al., 2011; Dethlefsen et al., 2012). Convincing scientific research targeted at resolving and quantifying these uncertainties is needed to assure policy makers (and the public in general) that GCS is a viable technology and that it can be deployed with adequate safeguards (Kang et al., 2010).

Focusing specifically on the fate of the injected CO_2 at a GCS site, uncertainties arise from not knowing precisely how a large quantity of CO_2 injected underground will travel and behave over time. Because data from actual field test sites are limited and expensive, scientists and engineers often must rely upon conceptual and numerical models to understand and predict the subsurface movement of the injected CO_2. These models must account for multiple physicochemical processes involving interactions between the injected CO_2, the formation fluids (either brine or hydrocarbons), and the reservoir rocks (Kang et al., 2010). Depending upon the nature of the fluids already residing in the formation, these processes may include (but are not necessarily limited to) fluid flow under pressure gradients created by the injection process; buoyancy-driven flow caused by density difference between the injected and formation fluids; diffusion, dispersion and fingering (arising from formation heterogeneities and mobility contrast between the fluids); capillarity (resulting from different wetting characteristics of the fluids concerned);

dissolution into the formation fluid, mineralization, and adsorption of CO_2 (Intergovernmental Panel on Climate Change, IPCC, 2005; Mukhopadhyay et al., 2011).

Given the complexities of the underlying physical and chemical processes, building a reliable conceptual model for flow and transport of CO_2 in the subsurface is a challenging task. Modelers must take into consideration a multiplicity of length scales (from pore scale to field scale), a wide range of time scales (e.g., different trapping mechanisms playing dominant roles at different times), the coupling between processes (e.g., fluid flow, heat transfer, geochemistry, and geomechanics), different model components (e.g., fluids and their properties, caprocks, overburdens, faults and fractures, and wells), and the spatial variability of most model input parameters (and often limited knowledge about them) (Keating et al., 2010; Jahangiri and Zhang, 2011). Consequently, modelers are likely to make different choices regarding implementation of multiphase behavior of the fluids and their equations of state, approaches for coupling of processes, modeling techniques, and selection/interpretation of site characterization and monitoring data. Such model choices may cause a wide range in the predictions made by different models, even if each of these models is considering the same injection scenario at the same GCS site. In this context, the modeling activity itself is prone to uncertainty and bias associated with selecting a single set of domain-specific interpretations, processes, and mathematical systems to estimate trends in CO_2 plume. This uncertainty, referred to as model selection uncertainty, forms one of the greatest sources of uncertainty and risk for predictive modeling (Devooght, 1998).

To increase stakeholders' confidence in our ability to make reliable predictions about GCS systems, it is essential to understand the causes of model uncertainties and, if possible, quantify these uncertainties. This can be accomplished by engaging in a model comparison study involving both model-to-data and model-to-model comparison at one or more selected GCS field sites. More specifically, in such a study different modeling teams can each develop individual models for the same site, based on a single set of site characterization data, but using their respective model approaches and numerical simulators. Being able to evaluate different model results for the same site guarantees a direct comparison of models and approaches, and enables an understanding and explanation of their differences, stemming, for example, from process simplifications or parameter choices.

In this paper, we introduce Sim-SEQ, a new initiative proposed by the US Department of Energy (USDOE) on model comparison for GCS. Sim-SEQ is currently focusing on multiple modeling teams developing their own models for a single CO_2 injection field test, however, this can be extended in the future to include multiple sites. Sim-SEQ is unique in that it is not a code-comparison or benchmarking effort, a distinction we elaborate on in the next section, in which we provide a brief discussion on the differences between benchmarking and model comparison, and introduce the readers to the DECOVALEX project, the closest analog to Sim-SEQ. In the section thereafter, we briefly describe the field injection activities undertaken by the USDOE over the last few years. This is followed by a section on the specific objectives of Sim-SEQ as a coordinated effort to understand the differences among the models being developed for some of those field injection tests. We then describe the GCS field site selected for the Sim-SEQ model comparison study and the current status of the project, followed by a discussion of the future plans for the project.

Code Benchmarking vs. Model Comparison

The objective of Sim-SEQ is model comparison, which is not to be equated with code benchmarking or code verification. Benchmarking exercises related to CO_2 sequestration problems have been conducted in past efforts, for example, led by Lawrence Berkeley National Laboratory (LBNL) (Pruess et al., 2004) or by the University of Stuttgart (Class et al., 2009). Both studies involved a number of benchmark problems for which precise descriptions of model domains, boundary conditions, rock properties, etc., were given. While participants in these studies applied a variety of simulators, they all used the same set of input parameters for their model applications. Differences in model results were moderate once data interpretation issues had been resolved, and were mostly related to differences in spatial and temporal discretization (Class et al., 2009).

Model comparison, in contrast to code benchmarking, evaluates modeling studies in a much broader and comprehensive sense. Model building, according to our definition, comprises all work flow stages starting with interpretation of site characterization efforts, parameter choices based on measurements, conceptual model choices, spatial variability characteristics, decisions about domain sizes and boundary conditions, etc. We expect that these model-building choices are considerably more critical to model agreement than the question of which simulator to use. Therefore, as a model comparison study, Sim-SEQ involves all of the above-defined stages of model building; participants build their models based on various site characterization data sets and other supplemental information, rather than well defined benchmark properties.

The recent DECOVALEX project on model comparison, conducted by several international organizations involved in the geologic disposal of nuclear wastes (e.g., Rutqvist et al., 2008; Tsang, 2009; Tsang et al., 2009) can serve as an analog for Sim-SEQ. DECOVALEX (an acronym for DEvelopment of COupled models and their VALidation against EXperiments) was first established in 1992 as a cooperative effort in developing and testing models capable of simulating coupled processes. Five multi-year project stages have since been completed, each involving model comparison (not code benchmarking) for subsurface experiments conducted in underground research laboratories. The general goal of the project was to encourage multidisciplinary, interactive, and cooperative research on modeling coupled processes in geologic formations, in support of performance assessment for underground storage of radioactive waste.

Note that Sim-SEQ, which is bringing together a large number of modeling teams (from eight different countries) in an effort to understand the root causes of model uncertainty (in the context of CO_2 geologic sequestration) and the impacts of such uncertainty on our ability to predict the subsurface movement of the injected CO_2, is likely to benefit from the lessons learned during the CLEAN project (Kühn et al., 2012), which is also a collaborative effort of sixteen different partners (though all from one country, Germany) to investigate the fate of CO_2 when injected in a depleted gas field for the purposes of enhanced gas recovery. Of particular relevance to Sim-SEQ is the OpenGeoSys (OGS), initiative of the CLEAN project (Kolditz et al., 2012a). OGS is a scientific, open source scode for numerical simulation of thermo-hydro-mechanical-chemical (THMC) processes in porous media. The OGS initiative has also developed a comprehensive benchmarking book, which is valuable tool for cooperation between different developer teams. Additionally, the CLEAN project has developed a general systematic for benchmarking of CO_2 modeling (Kolditz et al., 2012b). Even though model comparison is different from benchmarking, the benchmarking tools developed in the CLEAN project provide effective guidelines for Sim-SEQ.

CO_2 Field Injection Tests in the United States

The USDOE has selected seven regional partnerships, through its Regional Carbon Sequestration Partnership (RCSP) initiative, to determine the best approaches for capturing and permanently storing CO_2 (Litynski et al., 2008; National Energy Technology Laboratory, NETL, 2011). The RCSP initiative is being implemented in three phases. The Characterization Phase (Phase I) began in September 2003 with the seven partnerships working to develop the necessary framework to validate and potentially deploy GCS technologies. In June 2005, work transitioned to the Validation Phase (Phase II), a six-year effort focused on validating promising CO_2 sequestration opportunities through a series of field tests in the seven regions. Presently, activities in the Development Phase (2008-2018+), also referred to as Phase III, are proceeding as an extension of the work completed to date. Phase III activities involve the injection of 1 million metric tons or more of CO_2 by each RCSP into regionally significant geologic formations of different depositional environments. These large-volume injection tests are designed to demonstrate that CO_2 storage sites have the potential to store regional CO_2 emissions safely, permanently, and economically for hundreds of years. Note that the first Phase III injection at a RCSP site started in April 2009, and reached the one million metric ton per year injection target in December 2009. This is the fifth project worldwide (and the first in the United States) to reach the CO_2 injection volume of 1 million metric tons. Note also that Phase III injection at a second RCSP site has begun in November 2011.

With carefully developed monitoring strategies in place, the Phase II and III field tests have either produced or are expected to provide a wealth of data on relevant site performance measures, such as the growth and migration of the CO_2 plume, local and large-scale pressure changes, injectivity, stress evolution, brine migration, and geochemical processes. These data allow (1) evaluation of the predictive modeling efforts that each partnership might have conducted prior to and during field testing, and (2) improvement of the predictive models through comparison with observation data. Note that while conceptual models for the RCSP field tests are being developed by several different research teams, using different codes and different modeling approaches, no coordinated process, prior to Sim-SEQ, has been put in place that (1) would objectively evaluate the respective models using defined and agreed-upon performance metrics, and (2) would provide a forum for discussion, interaction, cooperation, and learning among the various modeling groups.

Sim-SEQ Project Objectives

The Sim-SEQ project intends to objectively evaluate the modeling efforts of different modeling groups as they are applied to the RCSP CO_2 injection field tests. Modeling comparison efforts are initially limited to one specific RCSP field test site (see below for more details on the site), hereafter referred to as the Sim-SEQ Study site (S-3 site), but may be expanded at later stages to other sites to encompass a wider range of geologic characteristics and model challenges. The project goals are to demonstrate, in an objective manner, whether the observed system behavior at GCS sites can be predicted with confidence, and whether the remaining differences between models and measurements at GCS sites, as well as between different models, are well understood. The project will also ensure that model uncertainties are evaluated and their impact is assessed, and that lessons learned and improvements made by one specific modeling group are documented and available to all other research teams for use to improve future modeling efforts. It is expected that these goals will be realized in a project environment that fosters mutual respect, as well as multidisciplinary, interactive, and cooperative research.

The S-3 Site

The S-3 site is patterned after the Southeast Regional Carbon Sequestration Partnership (SECARB) Phase III Early Test in the southwestern part of the state of Mississippi in the United States. The Phase I and Phase II CO_2 injection tests performed by SECARB have shown that numerous formations with the potential to store significant amounts of CO_2 exist within the sedimentary wedge that underlies the Gulf Coastal Plain of southwestern Mississippi. Figure 1 shows a typical stratigraphic column of the Gulf Coast Region. A description of the geology of the site can be found in Hovorka et al. (2011).

The target formation for injection at the S-3 site is comprised of fluvial sandstones of the Cretaceous lower Tuscaloosa Formation at depths of 3300 m, which form a 4-way anticline cut by a northwest trending fault. The injection interval, which is between 6 and 26 m thick, comprises the "D" and "E" sandstones. These units were deposited as part of a coarse-grained fluvial complex, and are amalgamated to form an internally complex but relatively laterally continuous zone, with grain size overall fining upward. Mudstones of variable thickness locally isolate the "D-E" units from the overlying less areally continuous "A" through "C" sandstones and serve as the lowest regional confining system. Chlorite cement is pervasive in the "D-E" sandstones, and plays a significant role in preserving high porosity and an average permeability of 100 mD. These complex geological features present an opportunity to study the control of sedimentary architecture on fluid flow. The added complexity of a strong diagenetic imprint sometimes obscures a straightforward interpretation of depositional environments and exerts a strong overprint on hydrologic behavior.

Denbury Onshore LLC (hereafter referred to as Denbury) has hosted (since 2007) the SECARB Phase II and Phase III tests (Meckel and Hovorka, 2009; Choi et al., 2011;

Hovorka et al., 2011) in a depleted oil and gas reservoir under CO_2 flood since. The tests are managed by the Bureau of Economic Geology (BEG) at the University of Texas, Austin. To coordinate the SECARB field experiments with Denbury's commercial flood (Hovorka et al., 2011), the project was staged in several areas. Phase II test injection and monitoring started in July 2008, with CO_2 injected into the oil-bearing zone in the northern part of the site, southwest of the fault (see Figure 2). Because pressure monitoring was one of the primary objectives for the Phase II Test, a dedicated observation well in the center of the Phase II area, completed with downhole digital pressure gauges, provided continuous pressure measurements from both the injection zone and the above-zone sand. Phase II test is not the focus of Sim-SEQ but some of the data collected in this phase complement Phase III characterization and test results.

The Phase III Early Test started in April 2009 with CO_2 injection east of the Phase II area, in the eastern block of the northwest-trending fault in an area commonly known as the High Volume Injection Test (HiVIT) area (Hovorka et al., 2011) (see Figure 2). CO_2 injection rates were initially 40,000 metric tons/month but have mostly fluctuated between 50,000 and 100,000 metric tons/month, with a monthly peak of >200,000 tons. The HiVIT area reached the target injection of 1 million metric tons in July 2010 (Figure 3). The target of 1.5 million metric tons CO_2 stored was achieved in early 2011. The Sim-SEQ project focuses on one part of the HiVIT, referred to as the Detailed Area Study (DAS), located in the water leg of the reservoir, outside of but close to the reservoir under CO_2 flood. The DAS includes one CO_2 injector (Figure 4) and two observation wells. An elaborate monitoring system – including repeat 3-D seismic monitoring, geochemical monitoring of the injection interval fluids (Lu et al., 2011), groundwater quality monitoring and other monitoring approaches has been put in place for the HiVIT and DAS areas.

To correctly predict the ultimate extent of the two-phase plume, CO_2 saturation must be rigorously monitored. The DAS area has been designed to collect dense time-lapse data from an array of three closely spaced wells, i.e., F-1, F-2, and F-3, with injection occurring through well F-1 and the other two serving as observation wells, located down dip of F-1. The surface locations of the three wells are aligned approximately along an east-west direction, with F-2 positioned 70 m of F-1 to the west and 30 m of F-3 to the east. Injection in the DAS area (through well F-1) started in December 2009 with a goal to observe changes as fluids evolve from a single phase (brine) to two phase (CO_2-brine) flow system and document linkages between rock properties, pressure, gravity, and sweep efficiency (Hovorka et al., 2011). The focus of the Sim-SEQ model comparison study will be the injection and monitoring data collected in the DAS area. As mentioned before, the DAS area comprises fluvial deposits of considerable heterogeneity located in the water leg of an active CO_2-EOR field with a strong water drive. These features add significant complexity when approximating the natural system, and challenges arise in dealing with boundary conditions. In addition, presence of methane has been confirmed in the brine, which can potentially exsolve and impact pressure buildup history and CO_2 plume extent (Oldenburg and Doughty, 2011).

Current Status of Sim-SEQ

Sim-SEQ is currently (last quarter of 2011) in a phase of rapid development. A large number of researchers from not only the United States but also from other countries have embraced the value of the model comparison study envisioned in Sim-SEQ and have committed to participate in it. While the actual modeling work in Sim-SEQ has begun in the third quarter of 2011 and has not yet matured enough to perform (and report on) a meaningful model comparison study, the Sim-SEQ project management team has put in considerable effort in assembling the modeling teams, setting up a web portal for Sim-SEQ, organizing and disseminating the input data for model building to the modeling teams, and planning and organizing meetings and workshops. In the following, we briefly describe the current status of Sim-SEQ.

Modeling Teams

Sim-SEQ was initiated by a kick-off meeting on April 20, 2011, at LBNL, attended by modeling teams associated with the RCSPs. Four of these modeling teams agreed to participate in the project – these were from the Pacific Northwest National Laboratory

(PNNL), the University of Utah, BEG, and LBNL. Sim-SEQ has since been introduced at international conferences, and there has been a steady growth in the interest among modeling entities to participate in Sim-SEQ. At present, fifteen different modeling teams are involved Sim-SEQ. Out of the fifteen modeling teams, six are from the US; the rest are from other countries (two each from Japan and France,, and one each from Germany the UK, The Netherlands,, Norway, and China). In addition to the modeling teams, one team is specifically engaged in performing the model comparison studies and quantification of uncertainties. Table 1 provides a list of the organizations/institutes participating in Sim-SEQ, and the software/modeling approach that each of these teams are using or planning to use. Note that some of the participating teams have not finalized their softare/modeling approach at the time of writing this paper. From Table 1, it is clear that a wide variety of modeling approaches is being included in the Sim-SEQ model comparison study.

The Sim-SEQ Web portal

A web portal has been developed for Sim-SEQ within the framework of GS^3 (PNNL, 2011), which stands for the Geologic Sequestration Software Suite. The GS^3, developed by PNNL, is an extensible, dynamic and integrated computing environment that stewards the data, scientific software, analytical tools, and computing resources. The Sim-SEQ web portal has been developed for easy dissemination of site characterization and monitoring data among the modeling teams, and to assist modeling teams to report their model attributes and model results using standardized formats. The Sim-SEQ web portal is password-protected and is accessible only by members of the participating modeling teams. Information has already been uploaded on the web portal, with the objective to assist the participating teams with their model-building activities. It contains a general site description and relevant site characterization data for the S-3 site (see below for more information on this), which the modeling teams are using for building their models. At an appropriate time, selected monitoring data from the S-3 site will also be made available through this web portal.

Site Characterization and Available Data

Site characterization data for model building provided to the modeling teams can be broadly classified into two categories: reference information and input data. The reference information includes a number of classical papers on the Cranfield, Mississippi, site, on which the S-3 site is largely based. Of particular importance is the 1966 overview paper on the Cranfield site summarizing the site geology (Mississippi Oil and Gas Board, MOGB, 1966). This paper provides insightful information regarding the geology and fluid flow characteristics at the Cranfield site. Several other papers discuss geology, petrology, and depositional history at Cranfield.

The input data provided for modeling include both test design data and rock and fluid properties data. Most of the design data (bottom hole location, bottom hole pressure, and temperature, etc.) are provided from the three wells – F-1, F-2, and F-3. Injection and production rates are also provided for F-1 and neighboring wells. In addition to these, petrophyscial properties (e.g., porosity and permeability) are provided from a number of nearby wells. In such cases, their distances from the DAS wells are also provided. Each modeling team has been provided with secured access to all the site characterization data discussed here.

To assist modelers with model-to-data comparison and for iterative model improvements, a variety of site monitoring data will be made available to them. While the kind of monitoring data to be made available to the modelers has not yet been finalized, it is likely to include the following: daily injection rates, bottom hole pressure and bottom hole temperature at the injection well (F-1), any other operational information from the DAS relevant to model match, e.g., pump test results in observation wells prior to start of injection in F-1, flow rates during sampling, bottom hole pressure and temperature data from the observation wells (F-2 and F-3), gas breakthrough dates at the observation wells, temporal composition change of gas passing observation wells, gas saturation at selected intervals in the observation wells, and the extent of the CO_2 plume from seismic monitoring.

To develop an objective model evaluation framework for comparison of simulation results with measurements, we must define performance metrics. In the preliminary phases of modeling, performance metrics are likely to be defined for migration of the CO_2 plume as a function of time, trapping mechanisms such as solubility trapping, residual trapping, evolution of injection pressure and injectivity assessments, large-scale evolution of pressure within and above the reservoir, and brine displacement and changes in salinity.

Site parameters likely to impact modeling results and explain the spread of the metrics include handling of boundary conditions. The field has showed a strong historical water drive. Pressure was back to almost hydrostatic after a severe pressure depletion following the gas cap blow down decades ago (Hovorka et al., 2011). In addition, although the DAS area is located in a brine aquifer, the presence of an active EOR operation nearby may also impact pressure behavior because of CO_2 injection through multiple wells in the reservoir itself and production of hydrocarbons (Hosseini and Nicot, 2012). The mere presence of close-to-residual oil and gas may also impact pressure transients even without active wells (Solano et al., 2011). Another parameter of interest is the balance between run time and grid resolution - the formation is heterogeneous and how heterogeneities are incorporated will impact result metrics.

Approach

Unlike code verification or benchmarking studies, in a model comparison study like Sim-SEQ, modelers need to engage in a more comprehensive suite of model building activities, including interpretation of the data available for modeling. In a way, a modeler needs to approach the model-building activities of Sim-SEQ in exactly the same way if faced with the task of modeling a new CO_2 injection field test. Specifically, each modeling team will develop numerical models of the S-3 Site, based on the common set of characterization data discussed above, iteratively revising their models to include monitoring data as they are made available. Predictions of the system state during natural and test conditions are then used for model-to-data and model-to-model comparisons. Comparison of an individual model's predictions to data, and model-to-model cross-comparisons of selected, pre-defined outputs (e.g., performance measures) will be performed and evaluated against pre-defined acceptance limits.

Each modeling team is or will be engaged in (1) review of initial characterization data, as well as review of monitoring data as they become available, (2) conversion of the geological model into one or multiple conceptual models of site hydrogeology, (3) development of parameter sets (and their uncertainties) describing hydrogeological properties, (4) defining of scenarios and cases to be simulated, (5) developing numerical models (mesh generation, property assignment, initial and boundary conditions), (6) performing deterministic and/or probabilistic simulation runs, (7) compilation of results through calculation of predefined performance measures (e.g., plume migration, pressure buildup, etc.), and (8) participating in Sim-SEQ meetings and workshops and supporting its development, simulation, and evaluation activities.

The Sim-SEQ model comparison initiative is coordinated and managed by researchers at LBNL. Coordination activities include periodic status reviews of model plans, including model approaches, schedules, and code capabilities, as well as definition of modeling performance metrics for comparison of predictions and measurements, and timely review and evaluation of model results. The coordination team also mediates discussions about model improvement, develop lists of lessons learned, summarizes model comparison results in annual reports, organizes and facilitates conferences and workshops, and hosts the Sim-SEQ web site for sharing of data and presentations.

Strategy for Model Comparison and Uncertainty Quantification

While the exact details are yet to be finalized, a general outline has been developed for the model-to-model and model-to-data comparison strategy in Sim-SEQ. In the following, we briefly describe that strategy. While the modeling teams are allowed to use their own conceptual models (including selecting their own software, numerical grids, boundary conditions, and parameter space), they will report their model results on an analysis grid specified by the project management team. If needed, participating teams can interpolate model results from their computational grid to the analysis grid. They will also be required to submit their results at specified times (which have been developed in accordance with available observation data). Model results will be reported in terms of specified variables (for example, pressure, CO_2 saturation in the supercritical phase, dissolved CO_2 in the aqueous phase, etc.). Such pre-specified, structured reporting will assist in performing a consistent and coordinated model comparison study.

The model comparison study in Sim-SEQ will be supported by a multi-model uncertainty analysis workflow that integrates Bayesian techniques (Raftery et al., 1997; Hoeting et al., 1999; Yang et al., 2011c) for model-ensemble analysis with methods for uncertainty quantification. In the ensemble analysis, predictive performance and uncertainty are assessed and quantified for each individual model and for the ensemble as a whole. The benefit of this approach is that common design choices behind more accurate, reliable models can be identified and characterized. Ultimately, this analysis supports an iterative feedback loop to help modeling teams jointly test, refine, and verify assumptions behind their model designs.

Next Steps

The Sim-SEQ project is intended to be a multi-year effort, which is expected to last through the end of Phase III RCSP field tests. In Sim-SEQ, models are expected to be iteratively developed, evaluated, refined, and revised parallel to the field activities to meet the overall objectives. The first period of model development aims at developing models with no or minimal monitoring data. At the same time, the process of successively including monitoring data and refining the conceptual model will be examined and discussed. In later stages of the project, formal model calibration and validation exercises are likely to be undertaken, estimation and prediction uncertainties can be quantified, or specific technical challenges related to coupled-processes simulation can be addressed. Additional field RCSP tests with different model challenges may be utilized in the model comparison effort.

Summary

Sim-SEQ is a new initiative from the USDOE on model comparison for GCS. The model comparison study envisioned in Sim-SEQ, unlike benchmarking, will evaluate model building efforts in a broad and comprehensive sense. In Sim-SEQ, fifteen different modeling teams, nine of which are from outside the United States, are building their own models for one selected RCSP CO_2 injection field test site, the S-3 site. The S-3 site is patterned after the SECARB Phase III Early Test site in the southwestern parts of the state of Mississippi in the United States. The complex geological features of the S-3 site present an excellent opportunity to study the control of sedimentary architecture on fluid flow. Furthermore, the site is located in the water leg of an active CO_2-EOR field with a strong water drive. These features add significant complexity to the model and challenges arise when dealing with boundary conditions. In Sim-SEQ, it is expected that each modeling team will develop numerical models of the S-3 Site, based on the common set of characterization data provided to them, iteratively revising their models to include monitoring data as they are made available. After completing this exercise, we expect to demonstrate that differences between models and measurements at a GCS site, as well as between different models, are well understood.

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Figure Captions

Figure 1. Schematic diagram of a typical stratigraphic column in the vicinity of the S-3 site (Courtesy of Susan Hovorka, BEG)

Figure 2. Location map of High Volume Injection Test (HiVIT) and the Detailed Area Study (DAS) domains at the Cranfield site. The Sim-SEQ project focuses on the DAS. Blue dots represent historical wells.

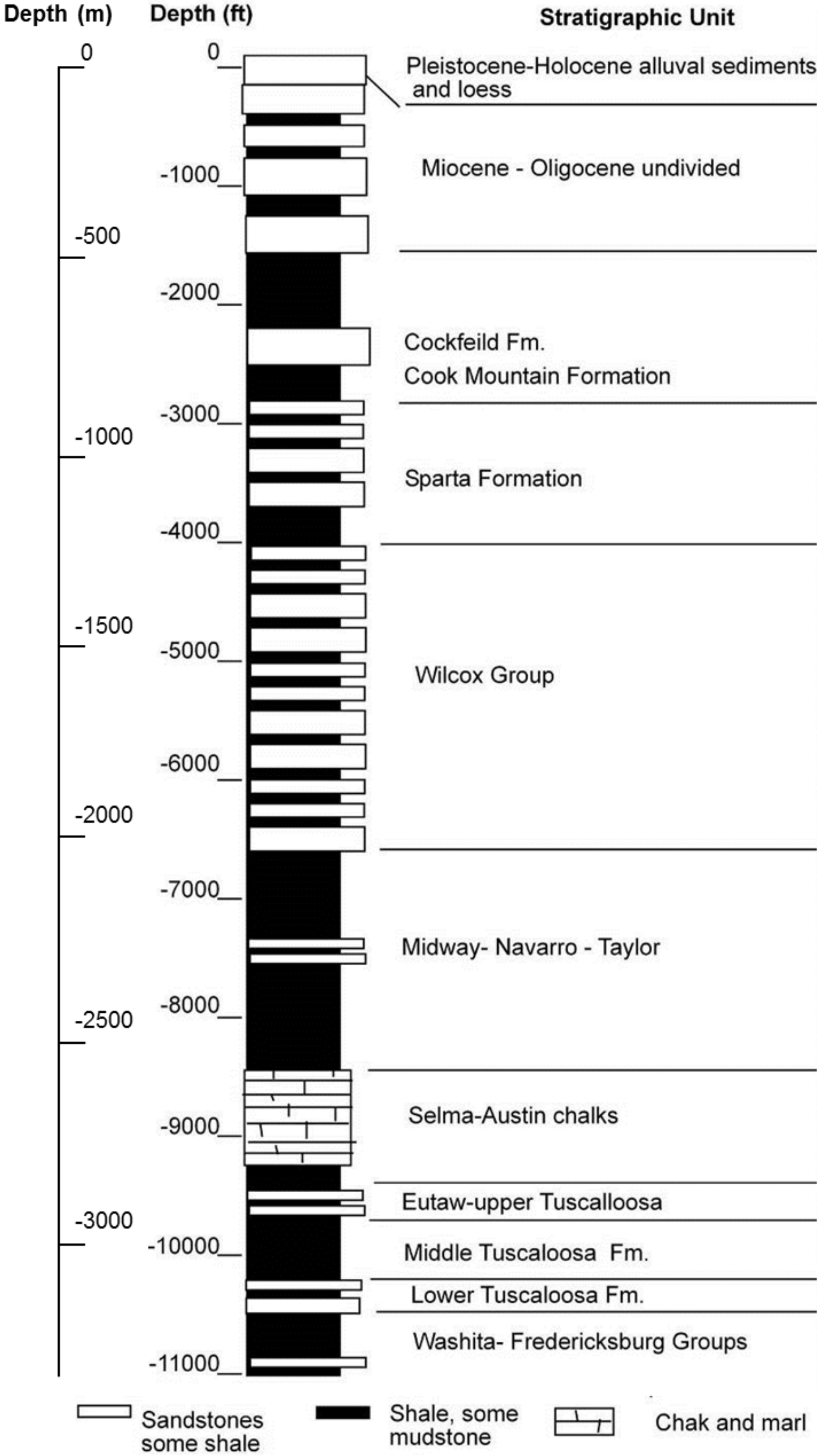
Figure 3. Cumulative CO_2 injection rate in the HiVIT area

Figure 4. Cross section showing seismic and wireline log properties projected along the dotted line shown in Figure 2. Beds are nearly flat-lying in this area, the section is vertically exaggerated ~ 6 times to show log details. Wells F-1, F-2, F-3 and surrounding

area form the DAS and are below the oil-water contact (WOC, approximate location shown on cross-section) (Courtesy of Tip Meckel, BEG)

Table Caption

Table 1. List of organizations/institutions participating in Sim-SEQ model comparison study, and the software/modeling approach each team intends to use (note that, at the time of writing this paper, the latter information is not available for a few participating teams)



Depth (m)
Depth (ft)
Stratigraphic Unit
0
-500
-1000
-1500
-2000
-2500
-3000
0
-1000
-2000
-3000
-4000
-5000
-6000
-7000
-8000
-9000
-10000
-11000
Pleistocene-Holocene alluval sediments and loess
Miocene - Oligocene undivided
Cockfeild Fm.
Cook Mountain Formation
Sparta Formation
Wilcox Group
Midway- Navarro - Taylor
Selma-Austin chalks
Eutaw-upper Tuscalloosa
Middle Tuscaloosa Fm.
Lower Tuscaloosa Fm.
Washita- Fredericksburg Groups
Sandstones some shale
Shale, some mudstone
Chak and marl

Figure 1.

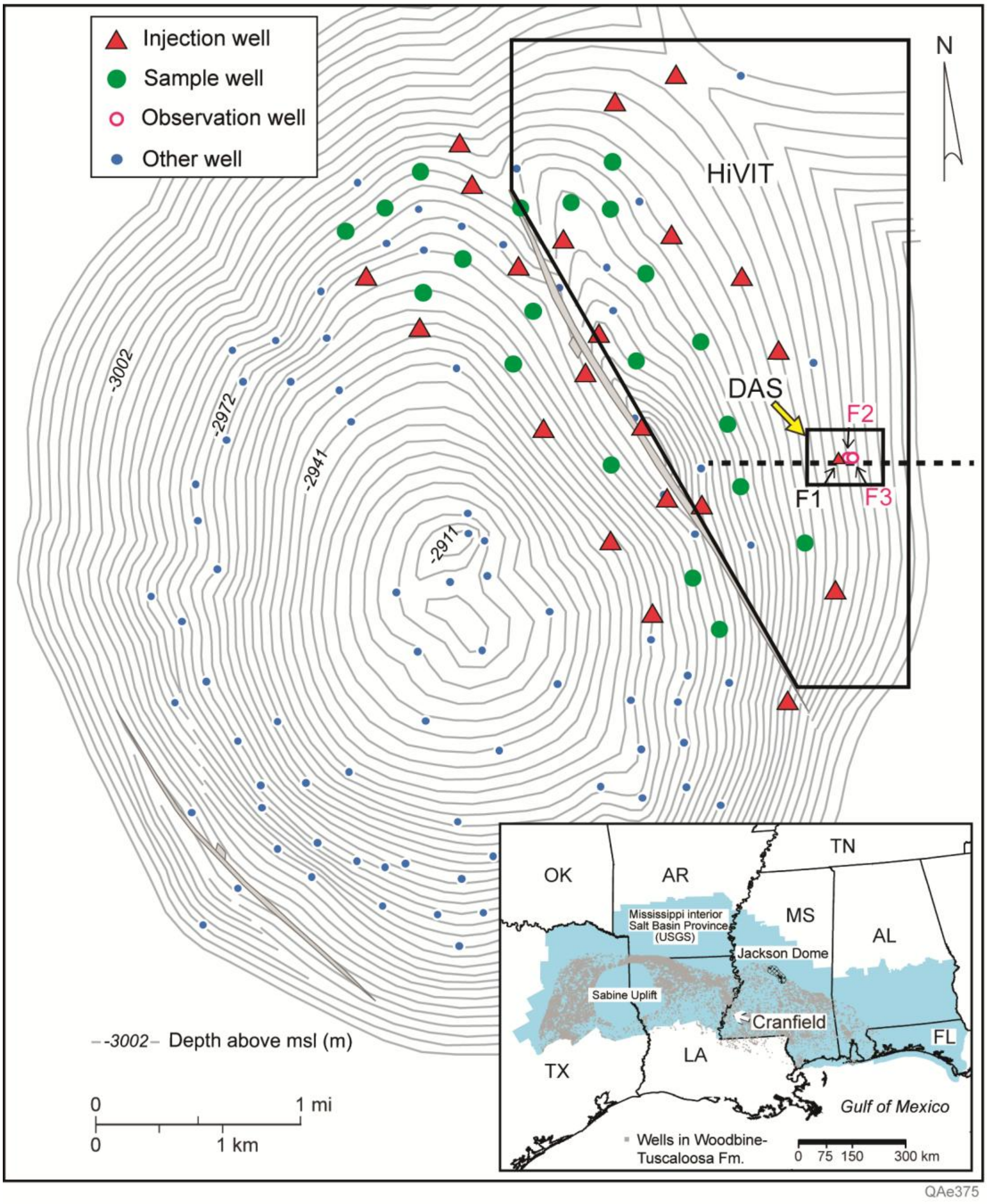
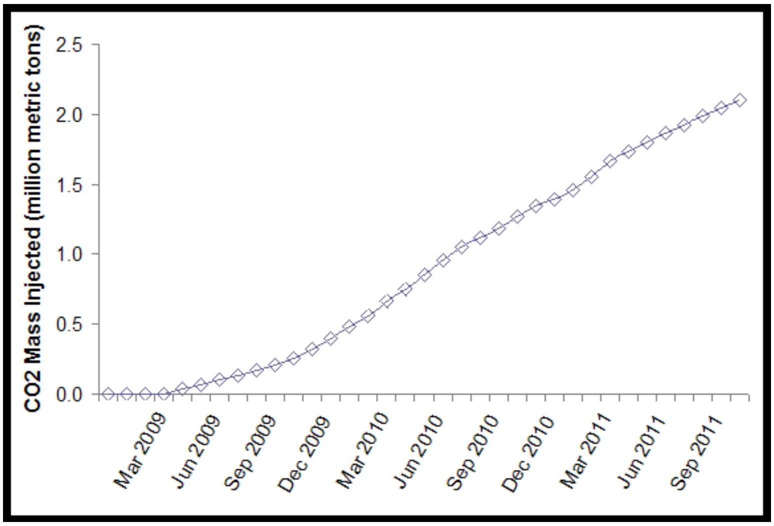

Injection well
Sample well
Observation well
Other well
N
HiVIT
DAS
F1
F2
F3
-3002
-2972
-2941
-2911
-3002 Depth above msl (m)
0
1 mi
0
1 km
OK
AR
TN
MS
AL
TX
LA
FL
Mississippi interior Salt Basin Province (USGS)
Jackson Dome
Sabine Uplift
Cranfield
Gulf of Mexico
Wells in Woodbine-Tuscaloosa Fm.
0 75 150 300 km
QAe375

Figure 2.



CO2 Mass Injected (million metric tons)
2.5
2.0
1.5
1.0
0.5
0.0
Mar 2009
Jun 2009
Sep 2009
Dec 2009
Mar 2010
Jun 2010
Sep 2010
Dec 2010
Mar 2011
Jun 2011
Sep 2011

Figure 3.

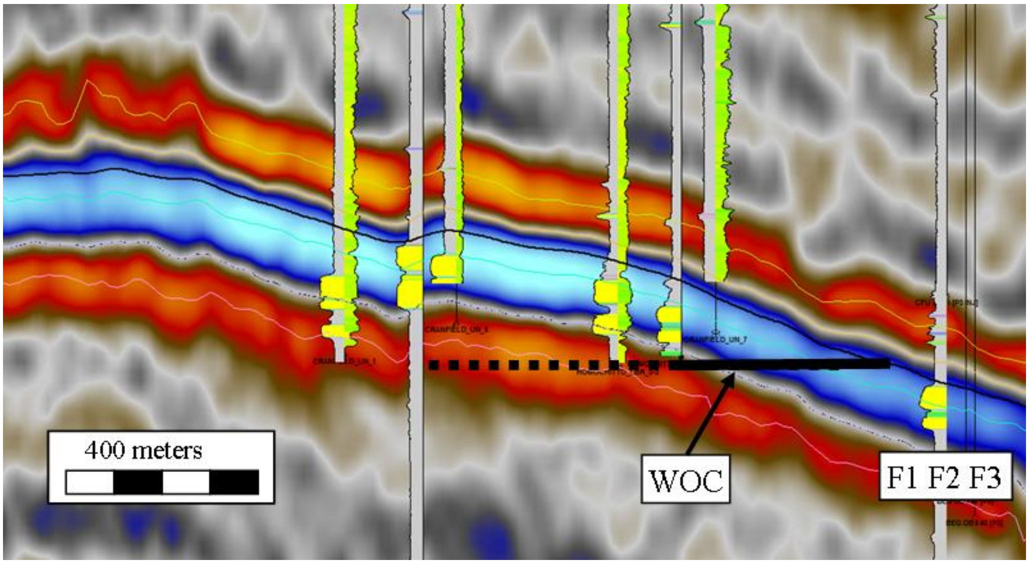


Figure 4.

Table 1.

No.	Organization/Institution	Name of Software/Model	Further Information
1.	Bureau of Economic Geology (BEG), University of Texas Austin, USA	CMG-GEM	http://www.cmgl.ca/software/gem.html
2.	Bureau de Recherches Géologiques et Minières (BRGM), France	TOUGH2/Eclipse/Petrel	http://esd.lbl.gov/research/projects/tough/software/tough2.htm; http://www.slb.com/services/software/reseng/compositional.aspx; http://www.slb.com/services/software/geo/petrel.aspx
3.	Geological Storage Consultants, Inc., USA	Not available	
4.	Imperial College, UK	Eclipse	http://www.slb.com/services/software/reseng/compositional.aspx
5.	Institute of Crustal Dynamics, China	CCS_MULTIF	Yang et al. (2011a,b), Yang et al. (2012)
6.	Lawrence Berkeley National Laboratory (LBNL), USA	TOUGH2-EOS7C/ECO2N	http://esd.lbl.gov/research/projects/tough/software/tough2.html; Pruess and Spycher (2007)
7.	Pacific Northwest National Laboratory	STOMP-CO2E	http://stomp.pnnl.gov; White and Oostrum (2006)
8.	Research Institute of Innovative Technology for the Earth (RITE), Japan	TOUGH2-ECO2N	http://esd.lbl.gov/research/projects/tough/software/tough2.html; Pruess and Spycher (2007)
9.	Sandia National Laboratory, USA	Not available	
10.	Schlumberger, France	Eclipse	http://www.slb.com/services/software/reseng/compositional.aspx
11.	Shell, The Netherlands	Not available	
12.	Taisei Corporation, Japan	TOUGH2-MP/ECO2N	http://esd.lbl.gov/research/projects/tough/
13.	Uni Research, Norway	Vertical Equilibrium With Sub-Scale Analytical	Gasda et al. (2009)

		Model (VESA)	
14.	University of Stuttgart, Germany	DUMUX	http://www.dumux.org
15.	University of Utah, USA	STOMP-CO2E	http://stomp.pnnl.gov