An Intercomparison Study of Simulation Models for Geologic Sequestration of CO2

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ABSTRACT

Mathematical models and numerical simulation tools will play an important role in evaluating the feasibility of CO2 storage in subsurface reservoirs, such as brine aquifers, producing or depleted oil and gas reservoirs, and coalbeds. We have proposed and initiated a code intercomparison study that aims to explore the capabilities of numerical simulators to accurately and reliably model the important physical and chemical processes that would be taking place in CO2 disposal systems. A first set of simulation problems has been specified with input from several other organizations. These are considered prototypical for different potential storage systems and have been posted on the Internet at `http://esd.lbl.gov/GEOSEQ/`. Issues being addressed include mixing of carbon dioxide and methane (for CO2 sequestration in natural gas fields with enhanced gas recovery), displacement of water by CO2 (for CO2 disposal in saline aquifers), potential loss of CO2 through leaky faults, hydro-mechanically coupled processes such as stress-induced caprock deformation and permeability enhancement, mineral alteration as a consequence of CO2 injection, and CO2 injection into an oil reservoir. The intercomparison study is open to interested technical groups worldwide who are invited to model and study the test problems using their own codes and funding. Simulation results will be collected through the Internet and will be compared, discussed and documented through a series of workshops. It is anticipated that through interactions with other interested groups additional problem sets will be developed, proceeding from simple to complex, and from hypothetical test cases to actual laboratory and field problems.

This paper presents the approach used for the code intercomparison study and briefly summarizes specifications of the first problem set.

INTRODUCTION

Geologic sequestration of CO2 can be accomplished by separating CO2 from flue gases and subsequently injecting it into a variety of storage reservoirs, including brine aquifers, producing or depleted oil and gas reservoirs, and coalbeds. Mathematical models and numerical simulation tools will play an important role in evaluating the feasibility of CO2 storage in subsurface reservoirs, in designing and analyzing field tests, and in designing and operating geologic CO2 disposal systems. In order to establish credibility for numerical simulators as practical engineering tools, it is necessary to demonstrate that they can model accurately and reliably the important physical and chemical processes that are taking place in the system of interest.

The purpose of the code intercomparison study outlined here is to evaluate key processes in CO2 geologic sequestration, and to contribute to the acceptance of numerical simulators as viable tools for modeling CO2 disposal. To initiate the study we propose a preliminary set of simulation problems that are intended to cover some of the important phenomena and mechanisms that would arise in geologic sequestration of CO2. We envision an interactive process through which different technical groups with interests and capabilities relevant to geologic disposal of CO2 will participate in defining, solving, refining, and augmenting simulation problems. Code intercomparison studies have been successfully used as a means for establishing confidence in simulation tools in related technical fields such as petroleum engineering (Firoozabadi and Thomas, 1989), geothermal reservoir engineering (Stanford, 1980), and in nuclear waste management (Larsson, 1992; Chapman et al., 1994; Jing et al., 1995; Stephansson et al., 1996).

Depending on the storage reservoir of interest and the composition of the waste gas stream (pure CO2 vs. mixtures of CO2 with other gases), injection of CO2 in geologic formations may give rise to a number of physical and chemical phenomena, such as miscible or immiscible displacement of native fluids, dissolution of injected fluids into reservoir fluids, changes in effective stress with associated porosity and permeability change and the possibility of inducing seismic activity, chemical interactions between fluids and solids, and nonisothermal effects. Key issues arising in process simulation include (1) thermodynamics of sub- and supercritical CO2, and PVT properties of mixtures of CO2 with other fluids, including (saline) water, oil, and natural gas; (2) fluid mechanics of single and multi-phase flow when CO2 is injected into aquifers, oil reservoirs, and natural gas reservoirs; (3) coupled hydro-chemical effects due to interactions between CO2, reservoir fluids, and primary mineral assemblages; and (4) coupled hydro-mechanical effects, such as porosity and permeability change due to increased fluid pressures from CO2 injection. These issues can be tracked through a matrix of property and process issues for different CO2 storage reservoirs as shown in Table 1.

Additional topics that need to be addressed include space and time discretization and their impacts on the solution of the underlying mathematical model, and the dependence of processes and parameters on space and time scale. The code intercomparison study should progress from relatively simple, uncoupled problems that address specific issues to increasingly complex problems in which several effects would occur simultaneously. Ultimately it would be desirable to achieve a comprehensive coverage of all process aspects and couplings. The coverage of issues achieved through the eight simulation problems proposed here is shown by entering the problem numbers into appropriate positions in Table 1. Simulation capabilities for CO_2 injection into coalbeds are still in an early stage of development. No coalbed-related test problems are proposed at the present time, but they may be included in future problem sets.

Table 1. Matrix of Code Intercomparison Problems and Issues

property/process storage reservoir	PVT data	fluid flow	transport (diffusion, dispersion)	chemical reactions	mechanical couplings
brine aquifer	3, 4, 7	3, 4, 6, 7		5	6
oil reservoir	8	8	8		
gas reservoir	1, 2	1, 2	1, 2		
coalbed					

Process issues and available and needed modeling capabilities are quite different for the different types of potential CO_2 storage reservoirs. For example, aquifer disposal of CO_2 would most likely occur at conditions that are not too far from the critical point of CO_2 (P_{crit} = 73.82 bar, T_{crit} = 31.04 ˚C; Vargaftik, 1975), requiring an accurate and robust description of the thermodynamics of near-critical CO_2. Other issues for aquifer disposal include hydrodynamic instabilities (viscous, gravitational), interaction of CO_2-water mixtures with heterogeneities on different scales, the kinetics of CO_2 dissolution in saline aqueous fluids during unstable immiscible displacement, and chemical interactions between aqueous CO_2-rich fluids and primary aquifer minerals. Non-isothermal effects may also come into play. There is much experience with storage of natural gas in aquifers which is relevant to the problem of CO_2 disposal (Katz and Lee, 1990). Considerable work on flow processes in water-CO_2 systems has been done in geothermal reservoir engineering (e.g., O'Sullivan et al., 1985; Battistelli et al., 1997; Xu and Pruess, 2001). In geothermal applications, temperatures are generally higher and CO_2 pressures lower than would be expected in CO_2 aquifer disposal systems.

For CO_2 injection into natural gas fields, the important issues involve the degree of mixing, and hydrodynamic dispersion effects in single phase flow as CO_2 displaces *in situ* gas (Oldenburg et al., 2001). Enhanced oil recovery (EOR) using CO_2 requires an understanding of the complex phase behavior of mixtures of CO_2 and crude oil. There is much practical experience with using CO_2 for EOR projects (SPE, 1999), and sophisticated numerical simulation capabilities are available (Chang et al., 1994). Some numerical simulation capabilities are also available for coupled hydromechanical effects due to pressure buildup from CO_2 injection, as well as for coupled hydrochemical effects due to interaction of CO_2 with mineral assemblages. Both types of effects require rather sophisticated codes that handle couplings between physical and chemical processes of different time constants and non-linearities. Some testing of these kinds of codes has been done in related problems (Jing et al., 1998; Xu and Pruess, 2001). There is some practical as well as modeling experience with using "cushion gas" to enhance the efficiency of aquifer gas storage (Modine and Bashbush, 1987). Although this employs gases other than CO_2, the experience will be relevant to CO_2 also. Practical experience with large-scale injection of CO_2 in aquifers is limited to the single case of the Sleipner Vest field in the Norwegian sector of the North Sea (Korbol and Kaddour, 1995; Kongsjorden et al., 1997).

APPROACH

The present authors propose to organize and manage the model intercomparison study, facilitate the development and selection of appropriate test problems, distribute them to interested groups of scientists and engineers who want to participate in this exercise, and solicit, collect, reconcile, and document solutions. A first set of test problems has been assembled to initiate the study. It has been posted on the web to be accessible to groups worldwide that have relevant expertise and access to simulation tools for geologic sequestration of greenhouse gases (URL: `http://esd.lbl.gov/GEOSEQ/`). We encourage such groups to participate in the study through their own funding by making suggestions for enhancing (refining) problems and proposing additional ones, and by submitting solutions to existing simulation problems. Complete solutions of all test problems are not required; participating groups may choose to work on any subset of problems that suits their interests and capabilities. All communication should proceed electronically by e-mail to CO2sim@lbl.gov; for discussing issues related to specific test problems we encourage interested parties to communicate directly with the proposers of the test problems, whose e-mail addresses are given in the problem summaries below. Solutions and discussions will be documented and posted on our website. We plan to hold workshops at regular intervals to compare and discuss results and to refine problem definitions and develop new problems. Announcements will be posted on the web.

Development and selection of sample problems for the model intercomparison study is made on the basis of key processes expected to occur in potential CO2 storage reservoirs, taking into account existing simulation capabilities and future needs. We anticipate that several problem sets will be developed to address the variety of issues encountered in the different potential disposal reservoirs. In addition, a phased approach will be used in which problems will proceed from simple to complex. The initial test problems emphasize PVT properties at thermodynamic conditions of interest, and explore the interaction of CO2 with native reservoir fluids in simplified systems. At a later stage simulation problems will be developed that address more complex and realistic systems, where mixtures of CO2 with other gases may be injected into heterogeneous reservoirs and may be subject to coupled chemical, mechanical, and thermal interactions with the host rocks.

Benchmark problems will not be limited to hypothetical modeling exercises, but will use to the extent possible the main features and parameters of real case histories or practical field projects currently underway. For example, experience and data from the Sleipner Vest case may be used to address fluid dynamics issues, while data on mineral assemblages in natural CO2 fields such as Bravo Dome, New Mexico, and Pisgah Anticline, Mississippi, may be used for chemical speciation and reaction path modeling (Studlick et al., 1990; Pearce et al., 1996).

GUIDELINES FOR TEST PROBLEMS

1. Problems should be practical and of wide interest and applicability.
2. Contributors of problems must affirm that they have actually solved the problem to some level of correctness.
3. Problem descriptions should follow the general outline below.
4. Among the various convenient units used in any given problem specification, there must also be specifications in MKS (SI).

5. The contributor of a problem will act as coordinator and referee to answer questions and assist in judging results.
6. If there is not sufficient interest in a problem, it will be placed in an inactive category where potential testers can view it for future inclusion in the active study.

OUTLINE OF PROBLEM SPECIFICATIONS

Problems should be described using the following headings:

1. Introduction and general description
2. List of processes being studied
3. Definition of the problem and input data
4. Problem variations
5. Definition of results to be calculated
6. Comparison criteria
7. References

The section on "problem variations" lists optional modifications that may make the problem more useful for an intercomparison study. In some cases these entail simplifications that remove features deemed nonessential; other variations enhance the scope of the problem by varying parameters or by introducing additional processes.

PRELIMINARY PLAN AND SCHEDULE

The code intercomparison study was officially launched in January 2001. The preliminary plan and schedule are proposed as follows:

1. Initial problem sets - Month 0
2. Receiving responses, suggestions, input and proposals of test problems from interested groups - Month 2
3. Finalizing a first set of benchmark problems - Month 3
4. Simulation studies by interested groups - Month 3-9
5. Working meeting to discuss results, refine problem definitions, develop new test problems, and agree on future plan and schedule - Month 10

DESCRIPTIONS OF INITIAL TEST PROBLEMS

Here we give a brief summary of the initial set of proposed test problems. The first two problems address issues arising in CO2-enhanced gas recovery. Problems 3 and 4 deal with CO2 disposal in saline aquifers. Problem 5 involves a batch chemical speciation calculation, while problem 6 explores a coupled hydro-mechanical process. Problem 7 involves a 2-D field scale aquifer disposal problem, and problem 8 addresses CO2 injection into an oil reservoir. As mentioned before, full problem specifications are available on the web, at

`http://esd.lbl.gov/GEOSEQ/`.

Test Problem 1. Mixing of Stably Stratified Gases (proposed by Curt Oldenburg, CMOldenburg@lbl.gov); examines PVT properties and molecular diffusion of mixtures of CO2 and CH4 at thermodynamic conditions of T = 40 ˚C, P = 40 bars.

Test Problem 2. Advective-Diffusive Mixing Due to Lateral Density Gradient (proposed by Curt Oldenburg, CMOldenburg@lbl.gov). This problem addresses the interplay of gravity-driven advection and molecular diffusion in the system CO2-CH4.

Test Problem 3. Radial Flow from a CO2 Injection Well (proposed by Karsten Pruess, K_Pruess@lbl.gov). This is a basic two-phase line source problem for CO2 injection into a saline aquifer.

Test Problem 4. CO2 Discharge Along a Fault Zone (proposed by Karsten Pruess, K_Pruess@lbl.gov); provides a simplified representation of CO2 loss from storage along a leaky fault that intersects a storage aquifer.

Test Problem 5. Mineral Trapping in a Glauconitic Sandstone Aquifer (proposed by Tianfu Xu, Tianfu_Xu@lbl.gov). This problem performs batch reaction modeling of mineral alteration due to the presence of CO2 at high pressure in a glauconitic sandstone aquifer. Specifications are based on earlier work by Gunter et al. (1997) and include presence of organic matter and redox processes.

Test Problem 6. Hydromechanical Responses During CO2 Injection into an Aquifer-Caprock System (proposed by Chin-Fu Tsang and Jonny Rutqvist, CFTsang@lbl.gov). This problem addresses consequences of rock deformation, including potential change in permeability and porosity, during injection of CO2 into a porous aquifer beneath a low permeable caprock.

Test Problem 7. CO2 Injection into a 2-D Layered Brine Formation (proposed by Carl Steefel, Steefel1@llnl.gov). Patterned after the CO2 injection project at the Sleipner Vest field in the Norwegian sector of the North Sea, this problem is intended to investigate the dominant physical processes associated with the injection of supercritical CO2 into a layered medium.

Test Problem 8. CO2-Oil Displacement and Phase Behavior (proposed by Tony Kovscek, Kovscek@pangea.stanford.edu). This problem examines the interplay of CO2-oil phase behavior and multiphase flow, as CO2 is injected into an oil-containing medium under two different conditions that lead to miscible and immiscible displacement, respectively.

Readers are encouraged to submit comments, suggestions, and solutions to us via e-mail at CO2sim@lbl.gov. We are also interested in proposals for additional problems.

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