Intercomparison of Simulation Models for CO2 Disposal in Underground Storage Reservoirs

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ABSTRACT

An intercomparison study between simulation codes for terrestrial sequestration of CO2 is proposed. The objectives are, on the one hand, to focus and evaluate key processes through numerical simulation and, on the other, to explore the strengths of different codes and achieve acceptance of such codes for use in the development of geologic systems for CO2 disposal. This will be carried out through the study of a series of test problems by groups using their simulation codes. A progression from simple and uncoupled to increasingly complex and coupled problems is envisioned. The proposed study will attempt to involve interested technical groups worldwide, and will proceed through an iterative process of problem definition, solution comparison, discussion and refinement. The Internet will be used as a medium for communicating and organizing activities, and for a flexible exchange of information and documentation of results. In addition, it is planned to hold a series of workshops. The present write-up includes an initial set of eight proposed test problems and represents the first step in the process. Readers are encouraged to communicate with us at the email address above to indicate their interest and to provide suggestions and input.

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 disposal 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 arising 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) and 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 in this report is shown by entering the problem numbers into appropriate positions in Table 1. Simulation capabilities for CO2 injection into coalbeds are still in an early stage of development. No coalbed-related test problems are proposed in the present report, 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	8	8	8		
gas	1, 2	1, 2	1, 2		
coalbed					

Process issues and available and needed modeling capabilities are quite different for the different types of potential CO2 storage reservoirs. For example, aquifer disposal of CO2 would most likely occur at conditions that are not too far from the critical point of CO2 (P_{crit} = 73.82 bar, T_{crit} = 31.04 ˚C; Vargaftik, 1975), requiring an accurate and robust description of the thermodynamics of near-critical CO2. Other issues for aquifer disposal include hydrodynamic instabilities (viscous, gravitational), interaction of CO2-water mixtures with heterogeneities on different scales, the kinetics of CO2 dissolution in saline aqueous fluids during unstable immiscible displacement, and chemical interactions between aqueous CO2-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 CO2 disposal (Katz and Lee, 1990). Considerable work on flow processes in water-CO2 systems has been done in geothermal reservoir engineering (e.g., O'Sullivan et al., 1985; Battistelli et al., 1997; Xu and Pruess, 2000). In geothermal applications, temperatures are higher and CO2 pressures lower than would be expected in CO2 aquifer disposal systems.

For CO2 injection into natural gas fields, the important issues involve the degree of mixing, and hydrodynamic dispersion effects in single phase flow as CO2 displaces *in situ* gas. Enhanced oil recovery (EOR) using CO2 requires an understanding of the complex phase behavior of mixtures of CO2 and crude oil. There is much practical experience with using CO2 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 CO2 injection, as well as for coupled hydrochemical effects due to interaction of CO2 with mineral assemblages. Both types of effects require rather sophisticated codes that handle couplings between physiochemical 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, 2000). 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 CO2, the experience will be relevant to CO2 also. Practical experience with large-scale injection of CO2 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. This report includes a first preliminary set of problems (see below) and is intended to initiate the study. It is being disseminated widely to groups worldwide that have relevant expertise and access to simulation tools for geologic sequestration of greenhouse gases. 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. 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 as footnotes to the problems. We have established a website (URL: http://esd.lbl.gov/GEOSEQ/) that will be used to document problem sets and post solutions and discussions. 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 the sample problems to be used in the model intercomparison study will be 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 the mechanics of 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 preliminary plan and schedule are proposed as follows:

1) Initial problem sets (this report) - Month 0
2) Receiving responses, suggestions, input and proposals of test problems from interested groups - Month 2
3) Selection of first set of benchmark problems and emailing of problem specifications to interested groups - 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

An initial set of proposed test problems is attached to this report. The titles are as follows.

Test Problem 1. Mixing of Stably Stratified Gases
Test Problem 2. Advective-Diffusive Mixing Due to Lateral Density Gradient
Test Problem 3. Radial Flow from a CO2 Injection Well
Test Problem 4. CO2 Discharge Along a Fault Zone
Test Problem 5. Mineral Trapping in a Glauconitic Sandstone Aquifer
Test Problem 6. Hydromechanical Responses During CO2 Injection into an Aquifer-Caprock System
Test Problem 7. CO_2 Injection into a 2-D Layered Brine Formation
Test Problem 8. CO_2-Oil Displacement and Phase Behavior

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

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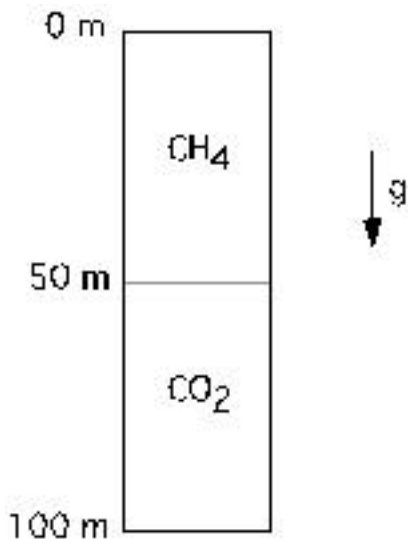
Test Problem 1. Mixing of Stably Stratified Gases[#]

1. INTRODUCTION AND GENERAL DESCRIPTION

In this problem, CO2 and CH4 gases are placed in contact one on top of the other and allowed to mix as controlled by diffusion and associated flow at 40 bars, 40 ˚C. Mixing in the system is limited because the denser gas (CO2) is on the bottom and the lighter gas (CH4) is on the top. The diffusion and flow are assumed to be one-dimensional. A residual liquid water saturation of 0.1 exists within the pores.



2. LIST OF PROCESSES BEING STUDIED

Molecular diffusion.

Density, viscosity, and solubility formulations of water, CO2, and CH4 as functions of pressure, temperature, and composition (P, T, X).

Advection in response to pressure gradients induced by equimolar diffusion of species with different molecular weights.

3. DEFINITION OF THE PROBLEM AND INPUT DATA

Boundary conditions:

No heat or mass flux through any boundaries (i.e., all boundaries are no-flow).

Initial conditions:

T = 40 ˚C (isothermal throughout)

[#] proposed by Curt Oldenburg; e-mail: CMOldenburg@lbl.gov

P (Z = 0 m) = 40 bars

X initially stratified with CO2 occupying the bottom half of the domain and CH4 occupying the top half.

Input data:

a) Porosity, tortuosity, residual liquid saturation (0.1, 1., 0.1, respectively)

b) Molecular diffusivity (1×10^{-7} m^2 s^{-1})

c) Permeability and relative permeability ($k = 10^{-14}$ m^2, linear k_{rg}, liquid immobile)

d) Density, viscosity, and solubility in water of CO2 and CH4 as functions of P, T, and X.

e) Vapor-liquid equilibrium properties of water.

4. PROBLEM VARIATIONS

a) Diffusion only with no gas-phase flow.

b) Low pressure scenario (P = 1 bar).

c) High pressure scenario (P = 100 bar)

d) Mixing by Dusty Gas Model instead of advective-diffusive Fickian model.

5. DEFINITION OF RESULTS TO BE CALCULATED

Vertical profiles at various times of :

a) CO2 and CH4 masses in liquid and gas phases per unit volume.

b) Pressure.

c) Density of the gas mixture.

6. COMPARISON CRITERIA

Profiles at the same times should match within 5%.

7. REFERENCES

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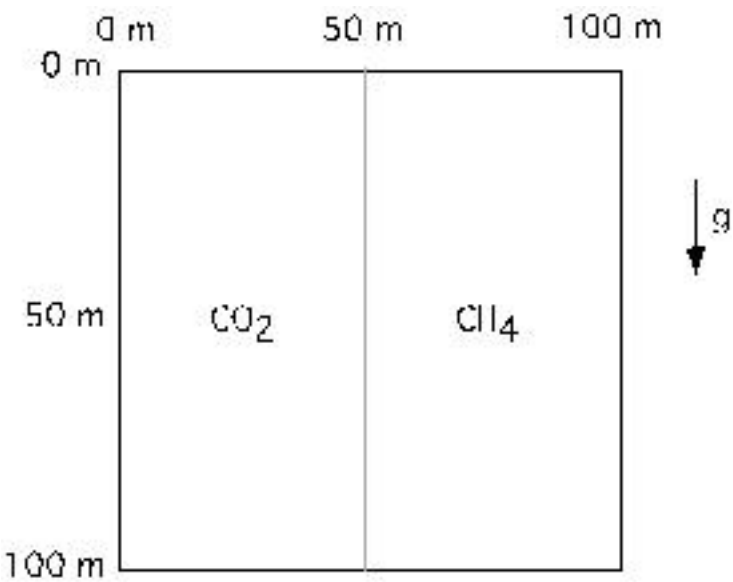
Test Problem 2. Advective-Diffusive Mixing Due to Lateral Density Gradient[#]

1. INTRODUCTION AND GENERAL DESCRIPTION

In this problem, CO2 and CH4 gases are placed side-by-side in a container and allowed to mix by advection and diffusion. The strong lateral density gradient between the dense CO2 gas and the relatively light CH4 gas causes a strong flow where CO2 tends to move downward and CH4 tends to move upward to the top of the container. The flow and diffusion are assumed to be two-dimensional. A residual liquid water saturation of 0.1 exists within the pores.



2. LIST OF PROCESSES BEING STUDIED

Gravity-driven advection in response to strong lateral density gradient.

Molecular diffusion.

Density, viscosity, and solubility formulations as functions of pressure, temperature, and composition (P, T, X).

Because of the strong advection, numerical dispersion will arise for most numerical methods.

3. DEFINITION OF THE PROBLEM AND INPUT DATA

Boundary conditions:

No heat or mass flux through any boundaries (i.e., all boundaries are no-flow).

[#] proposed by Curt Oldenburg; e-mail: CMOldenburg@lbl.gov

Initial conditions:

T = 40 ˚C (isothermal throughout)

P (Z = 0 m) = 40 bars

Initial composition field with CO2 on the left-hand half of the domain and CH4 on the right-hand half of the domain.

Input data:

a) Porosity, tortuosity, liquid saturation (0.1, 1., 0.1, respectively)

b) Molecular diffusivity (1×10^{-7} m^2 s^{-1})

c) Permeability and relative permeability ($k = 10^{-14}$ m^2, linear k_{rg}, liquid immobile)

d) Density, viscosity, and solubility in water of CO2 and CH4 as functions of P, T, and X.

e) Vapor-liquid equilibrium properties of water.

4. PROBLEM VARIATIONS

a) Low pressure scenario (P = 1 bar).

b) High pressure scenario (P = 100 bar).

c) Mixing by Dusty Gas Model instead of advective-diffusive Fickian model.

d) Substitute nitrogen (N2) or air for CO2.

5. DEFINITION OF RESULTS TO BE CALCULATED

Horizontal profiles at Z = 50 m at various times of

a) CO2 and CH4 masses in gas and liquid phases per unit volume.

b) Density of the gas mixture.

6. COMPARISON CRITERIA

Profiles at the same times should match within 5%.

7. REFERENCES

To be supplied.

Test Problem 3. Radial Flow from a CO2 Injection Well[&]

1. INTRODUCTION AND GENERAL DESCRIPTION

This problem addresses two-phase flow of CO2 and water for simplified flow geometry and medium properties. The aquifer into which injection is made is assumed infinite-acting, homogenoeus, and isotropic. Gravity and inertial effects are neglected, injection is made at a constant mass rate, and flow is assumed 1-D radial (line source). Under the conditions stated the problem has a similarity solution where dependence on radial distance R and time t occurs only through the similarity variable $\xi = R^2/t$ (O'Sullivan 1981; Doughty and Pruess 1992).

2. LIST OF PROCESSES BEING STUDIED

Two-phase flow of CO2 and water subject to relative permeability and capillary effects.
Change of fluid density, viscosity, and CO2 solubility with pressure and salinity.
Formation dry-out with precipitation of salt.

3. DEFINITION OF THE PROBLEM AND INPUT DATA

Problem parameters are summarized in Tables 3.1 and 3.2

4. PROBLEM VARIATIONS

Neglect salinity of the aqueous phase. Include non-isothermal effects. Include permeability changes due to precipitation. Inject gas that is 50 % CO2, 50 % N2.

5. DEFINITION OF RESULTS TO BE CALCULATED

Data on CO2 and brine density and viscosity, and CO2 solubility, for the range of thermodynamic conditions encountered in the problem. Gas saturation, dissolved CO2 mass fraction, fraction of void space containing precipitated salt, and fluid pressure as functions of the similarity variable $\xi = R^2/t$. (Use both profiles at constant time and time-series data at a specific location for plotting.)

6. COMPARISON CRITERIA

Results should match within +/- 5 %.

7. REFERENCES

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[&] proposed by Karsten Pruess; e-mail: K_Pruess@lbl.gov

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Table 3.1 Hydrogeologic parameters.

Permeability Porosity Pore compressibility Aquifer thickness	$k = 10^{-13}\ m^2$ $\varphi = 0.12$ $c = 4.5 \times 10^{-10}\ Pa^{-1}$ 100 m
Relative permeability	
liquid: van Genuchten function (1980) $k_{rl} = \sqrt{S^*}\left\{1-\left(1-\left[S^*\right]^{1/\lambda}\right)^{\lambda}\right\}^2$ irreducible water saturation exponent	$S^* = (S_l - S_{lr})/(1 - S_{lr})$ $S_{lr} = 0.30$ $\lambda = 0.457$
gas: Corey curve (1954) $k_{rg} = (1-\hat{S})^2(1-\hat{S}^2)$ irreducible gas saturation	$\hat{S} = \dfrac{(S_l - S_{lr})}{(1 - S_{lr} - S_{gr})}$ $S_{gr} = 0.05$
Capillary pressure	
van Genuchten function (1980) $P_{cap} = -P_0\left(\left[S^*\right]^{-1/\lambda} - 1\right)^{1-\lambda}$ irreducible water saturation exponent strength coefficient	$S^* = (S_l - S_{lr})/(1 - S_{lr})$ $S_{lr} = 0.0$ $\lambda = 0.457$ $P_0 = 19.61$ kPa

Table 3.2 Initial conditions and injection specifications

Pressure	120 bar
Temperature	45 ˚C
Salinity	15 wt.-% NaCl
CO2 injection rate	100 kg/s

Test Problem 4. CO2 Discharge Along a Fault Zone[&]

1. INTRODUCTION AND GENERAL DESCRIPTION

This problem explores CO2 loss from storage through a leaky fault, using a highly simplified 1-D linear flow geometry. It is envisioned that an aquifer into which CO2 disposal is made is intersected by a vertical fault, which establishes a connection through an otherwise impermeable caprock to another aquifer 500 m above the storage aquifer (Fig. 4.1a). This situation is idealized by assuming 1-D flow geometry and constant pressure boundary conditions as shown in Fig. 4.1b (Pruess and García, 2000).

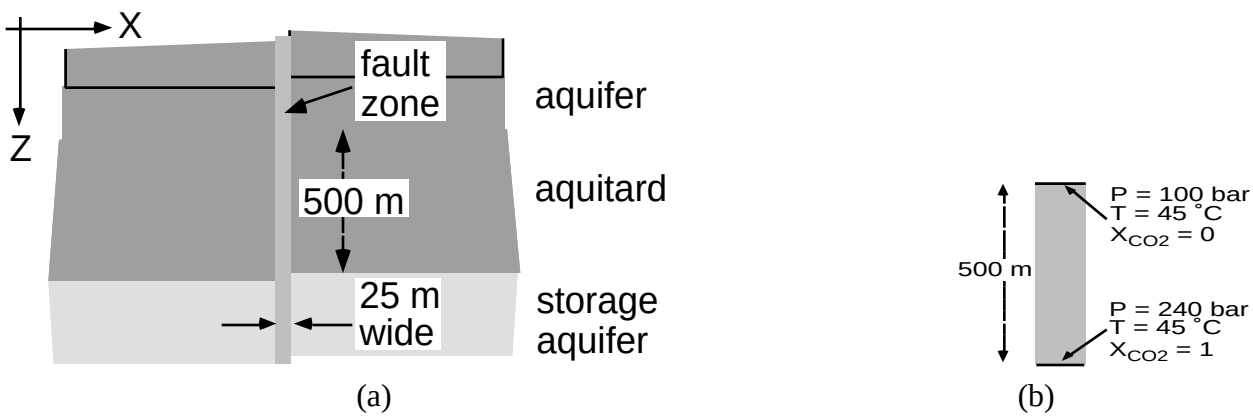

Figure 4.1 Schematic of the fault zone model (a) and applied boundary conditions (b).

2. LIST OF PROCESSES BEING STUDIED

Immiscible displacement of water by CO2 subject to pressure, gravity, and capillary pressure effects.

Change of fluid density, viscosity, and CO2 solubility with pressure.

Formation dry-out.

3. DEFINITION OF THE PROBLEM AND INPUT DATA

Hydrogeologic parameters are identical to those of problem 3 (Table 3.1), except that porosity is increased to 35 %. The fault zone is assumed to be 25 m wide and 500 m tall, with boundary conditions as given in Fig. 4.1b. The reservoir fluid is assumed to be pure water (no salinity). Initial conditions are pressures in hydrostatic equilibrium relative to P = 100 bar at the top; temperature is held constant at T = 45 ˚C throughout.

[&] proposed by Karsten Pruess; e-mail: K_Pruess@lbl.gov

4. PROBLEM VARIATIONS

Include salinity of the aqueous phase and permeability changes due to precipitation. Include non-isothermal effects. Assume gas composition is 50 % CO_2, 50 % N_2.

5. DEFINITION OF RESULTS TO BE CALCULATED

Data on CO_2 and water density and viscosity, and CO_2 solubility, for the range of thermodynamic conditions encountered in the problem. Vertical profiles of gas saturation, fluid pressure, and dissolved CO_2 mass fraction at different times. CO_2 inventory in gas and liquid phases after 10^7 seconds. Mass flow rates of CO_2 at the bottom and of water at the top vs. time (normalized for a 1 m thick section).

6. COMPARISON CRITERIA

Results should match to with +/- 5 %.

7. REFERENCES

Pruess, K. and J. García. Multiphase Flow Dynamics During CO_2 Injection into Saline Aquifers, submitted to *Environmental Geology,* September 2000.

Test Problem 5. Mineral Trapping in a Glauconitic Sandstone Aquifer*

1. INTRODUCTION AND GENERAL DESCRIPTION

This problem addresses geochemical effects of CO2 injection into a glauconitic sandstone aquifer, and analyzes the impact of CO2 immobilization through carbonate precipitation. Batch reaction modeling of the geochemical evolution of this aquifer is performed in the presence of CO2 at high pressure. The problem is based on Gunter et al. (1997), who modeled water-rock reactions when CO2 is injected into a glauconitic sandstone aquifer in the Alberta Sedimentary Basin, Canada. Additional processes are considered such as presence of organic matter and its oxidation.

2. LIST OF PROCESSES BEING STUDIED

The following processes are considered: (1) equilibrium aqueous complexation, (2) redox processes, (3) the kinetics of chemical interactions between the host rock minerals and the aqueous phase (organic matter dissolution is a non-equilibrium processes), and (4) CO2 solubility dependence on pressure, temperature and salinity of the system. In addition, changes in porosity are monitored during the simulations.

3. DEFINITION OF THE PROBLEM AND INPUT DATA

The initial condition used in the simulation is a pure 1.0 M solution of sodium chloride reacting with the primary minerals listed in Table 5.1 at a temperature of 54 ˚C, a pH of 7, and an Eh of -0.1 V. Reactant phases are those minerals initially present in the aquifer formation (Table 5.1). The reactant minerals dissolve progressively into the formation water, thus modifying the water composition and leading to precipitation of product phases. Two simulations are to be performed with the same initial conditions. The first simulation examines water-rock interaction under natural conditions without CO2 injection. The second simulation considers a CO2 injection pressure of 260 bar. The CO2 gas pressure is assumed to be maintained in equilibrium with the solution at all times. A simulation time of 100,000 years is used for both simulations.

The rate law for kinetic mineral dissolution and precipitation is taken from Lasaga (1984) and Steefel and Lasaga (1994):

$$r_m = A_m k_m \left[1 - \left(\frac{Q_m}{K_m} \right)^{\mu} \right]^{n}$$

* proposed by Tianfu Xu; e-mail: Tianfu_Xu@lbl.gov

Figure 7.1 Schematic representation of geometry for CO2 injection in Utsira Formation.

Boundary conditions:

No heat or mass flux is allowed across any of the boundaries except the vertical boundary 6,000 meters from the injection well. This boundary is fixed at hydrostatic pressure, thus allowing flow into and out of the domain so as to avoid overpressuring the formation. The 6,000 meter boundary is chosen, however, to be far enough from the injection well that the CO_2 does not reach this boundary after 2 years of injection.

Initial conditions (Table 7.1):

a) T = 37 ˚C (isothermal throughout)
b) P = hydrostatic (approximately 110 bars at injection point, approximately 90 bars at top of formation).
c) CO_2 in the aqueous phase in equilibrium with a P_{CO2} of 0.5 bars, a typical value for sedimentary formation waters at the temperature we are considering.

Table 7.1 Initial conditions and injection specifications

Pressure at well	110 bar
Temperature	37 ˚C
Salinity	3.2 wt.-% NaCl
CO2 injection rate	0.1585 kg/s in half space

Injection specifications (Table 7.1):

a) Temperature = 37 ˚C
b) Injection rate: 31.7 kg/s over entire screen length (100 meters), corresponding to 0.317 kg/s for the 1 meter thick section considered. Because of symmetry, injection rate in half space is therefore 0.1585 kg/s.
c) Height of well cell: 1 meter.
d) Injection time scale: 2 years

Input data (Table 7.2):

a) Capillary pressure and relative permeability described with van Genuchten parameters (both liquid and gas mobile). Porosity is 35% for sands, 10.25 % for shales.
b) Fully saturated permeability ($k = 3 \times 10^{-12}$ m^2 in sand layers, $10^{-14} m^2$ in shales)
c) Density, viscosity, and solubility in water of CO_2 as functions of P and T (Span and Wagner, 1996).
d) Vapor-liquid equilibrium properties of water.

4. PROBLEM VARIATIONS

Include non-isothermal effects by making the CO_2 injection temperature equal to 65 ˚C.

5. RESULTS TO BE CALCULATED

Liquid and gas saturations as a function of space and time. CO_2 concentration in the aqueous phase as a function of space. Gas and liquid fluxes.

6. COMPARISON CRITERIA

Results should match within +/- 5%.

Table 7.2 Hydrogeologic parameters

Permeability Porosity Aquifer thickness	Sands: 3×10^{-12} m^2; Shales: $10^{-14} m^2$ Sands: $\varphi = 0.35$; Shales: $\varphi = 0.1025$ 184 m
Relative permeability	
liquid: van Genuchten function (1980) $k_{rl} = \sqrt{S^*}\left\{1-\left(1-\left[S^*\right]^{1/\lambda}\right)^{\lambda}\right\}^2$ irreducible water saturation exponent	$S^* = (S_l - S_{lr})/(1 - S_{lr})$ $S_{lr} = 0.20$ $\lambda = 0.400$
gas: van Genuchten function (1980) $k_{rg} = \sqrt{S_g^*}\left\{1-\left(1-\left[S_g^*\right]^{1/\lambda}\right)^{\lambda}\right\}^2$ irreducible gas saturation exponent	$S_g^* = (S_g - S_{gr})/(1 - S_{gr})$ $S_{gr} = 0.05$ $\lambda = 0.400$
Capillary pressure	
van Genuchten function (1980) $P_{cap} = -P_0\,([S^*]^{-1/\lambda} - 1)^{1-\lambda}$ irreducible water saturation exponent strength coefficient	$S^* = (S_l - S_{lr})/(1 - S_{lr})$ $S_{lr} = 0.20$ $\lambda = 0.400$ Sand: $P_0 = 3.58$ kPa; Shale: $P_0 = 62.0$ kPa

7. REFERENCES

van Genuchten, M.Th. A Closed-Form Equation for Predicting the Hydraulic Conductivity of Unsaturated Soils, *Soil Sci. Soc. Am. J.*, Vol. 44, pp. 892 - 898, 1980.

Span, R. and W. Wagner. A New Equation of State for Carbon Dioxide Covering the Fluid Region from the Triple-Point Temperature to 100 K at Pressures up to 800 MPa, *J. Phys. Chem. Ref. Data*, Vol. 25, No. 6, pp. 1509 - 1596, 1996.

Test Problem 8. CO_2-Oil Displacement and Phase Behavior[1]

1. INTRODUCTION AND GENERAL DESCRIPTION

This problem probes our ability to predict accurately the interplay of CO_2-oil phase behavior and multiphase flow. CO_2 is injected into an oil-containing medium under two different conditions leading to miscible and immiscible displacement. This initial problem is posed in a one-dimensional geometry so that direct comparison can be made to available analytical solutions that have been derived for the CO_2-oil flow problem (Monroe *et al.* 1990, Orr *et al.* 1993). These solutions do not include the effects of capillary and hydrodynamic dispersion, but the effect of volume change on mixing will be computed.

2. LIST OF PROCESSES BEING STUDIED

Multiphase flow of CO_2 and oil subject to relative permeability and phase behavior effects.
Development of miscibility in CO_2-oil systems.
Numerical formulations for density, viscosity, and CO_2 solubility in oil.
Degree of numerical dispersion in numerical solutions.

3. DEFINITION OF THE PROBLEM AND INPUT DATA

- Oil composition: 10% CH_4, 20% C_4, and 70% C_{10}.
- Injected gas composition: 100% CO_2
- Injection P: case (a) P= 11.0 MPa and case (b) P= 12.0 MPa.
- Injection condition: constant volumetric rate
- Temperature: T = 71.1 °C and isothermal throughout.
- Geometry: one dimensional.
- Permeability and porosity: comparisons will be made in nondimensional form and so need not be specified.
- Relative permeability: $k_{rg} = \left(\frac{S_g}{1 - S_{or}}\right)^2$; $k_{ro} = \left(\frac{1 - S_g - S_{or}}{1 - S_{or}}\right)^2$ where $S_{or} = 0.2$
- Phase behavior: Reference results will be computed from the Peng-Robinson equation of state (Peng and Robinson, 1976) with the critical properties, volume corrections, and interaction coefficients tabulated by Orr *et al.* (1993). For comparison purposes, any phase behavior package can be employed.

4. PROBLEM VARIATIONS

Extend to more than 4 components to examine degree of chromatographic separation of various components. Include other combustion gases and N_2 in the injection gas. Examine the accuracy of prediction of the minimum miscibility pressure.

5. DEFINITION OF RESULTS TO BE CALCULATED

Saturation and composition profiles along the one-dimensional medium. For consistency the abscissa should be x_D/t_D where the dimensionless distance, x_D, is defined as x/L, the dimensionless time, t_D, is $q_{inj}t/\varphi AL$, and A is the cross-sectional area of the medium.

6. COMPARISON CRITERIA

Profiles should reproduce the location of saturation and composition shocks within ± 5%.

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[1] proposed by Tony Kovscek; email: kovscek@pangea.stanford.edu

7. REFERENCES

Monroe, W.W., M.K. Silva, L.L. Larson, and F. M. Orr, Jr., 1990, Composition Paths in Four Component Systems: Effect of Dissolved Methane on 1D CO_2 Flood Performance, *SPE Res. Eng.*, Aug, 423-432.

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