Example Problem CO2-7

Viscous Fingering with Dissolution of CO_2 into Brine

Abstract: *CO_2 injected into saline reservoirs partitions into a CO_2-dominate phase (gas phase) and CO_2 dissolved in the aqueous brine. The gas phase is generally less dense than the aqueous brine yielding an upward buoyant force on the gas phase, causing it to rise with respect to the aqueous phase. When the gas phase encounters a low permeability obstruction it spreads laterally beneath the obstruction. CO_2 in the gas phase moving laterally beneath the obstruction dissolves into the aqueous brine in contact with the gas phase. When CO_2 dissolves into an aqueous brine phase, the resulting brine is up to 1% denser than the CO_2-free brine. Whereas the lesser dense gas phase is stable over the aqueous brine as is moves laterally beneath an obstruction, the resulting layer of denser CO_2-rich aqueous brine is not stable over the lesser dense CO_2-free aqueous brine {i.e., Rayleigh-Taylor instability, (Rayleigh, 1883; Taylor, 1950)}. This problem involves the development of Rayleigh-Taylor instability for two scenarios involving the dissolution of CO_2 into an aqueous phase. The first scenario involves two-phase (i.e., liquid-CO_2-aqueous) conditions and the second involves aqueous-saturated (i.e., no gas) conditions. The second scenario is one which has been compared with experiments conducted at the Masdar Institute in Abu Dhabi.*

Problem Description

This problem involves two scenarios. The first scenario considers the injection of liquid (liq-CO_2) into a laboratory-scale flow cell filled with quartz sand of uniform grain size. The second scenario considers the formation of viscous fingers from a nonuniform initial distribution of aqueous dissolved CO_2. In the first scenario, viscous finger formation is triggered without introducing initial heterogeneities and in the second scenario the initial heterogeneities trigger early-time finger formation. Exercises for this problem are only associated with the first scenario, as the second scenario requires more time to execute than reasonable for a short-course problem. Simulation results are presented and discussed for the second scenario, but the student in not expected to execute the second scenario simulation during the short course period. The first scenario will be described first, followed by the second.

Scenario 1: Pressure Cell

In this scenario, liq-CO_2 is injected into the lower left-hand corner of a rectangular flow cell [45.4 cm (w) x 14.29 cm (h) x 1.27 cm (d)] filled with 30/40 Accusand. CO_2 is injected under supercritical pressure conditions, but below supercritical temperature conditions, causing the CO_2 to be in the liquid-CO_2 state. CO_2 is injected at a rate of 8.5816 cm^3/hr for 4 hours. The injected CO_2 is then allowed to redistribute for an additional 2 hours. To maintain constant pressure conditions in the flow cell, a pressure port is implemented in the upper right-hand corner of the flow cell. The hydrologic properties of the 30/40 Accusands are listed in Table 1, where the saturation-capillary pressure function is that of Brooks and Corey (1964, 1966), the aqueous relative permeability function that of Brooks and Corey (1964, 1966) with the Burdine (1953) porosity distribution model, and the gas relative permeability that of Corey (1954).

CO_2 injected into the lower left-hand port, located at the lower left-hand node, forms a gas phase, which spreads slightly laterally, but generally vertically via the buoyancy of the gas. The constant pressure port at the upper right-hand node of the domain is specified with a Dirichlet-type boundary condition for the aqueous and gas phases. During the injection period gas continues to migrate vertically until it reaches the upper flow-cell cap; where it migrates laterally beneath the upper cap. After injection stops the gas phase forms a layer underneath the flow-cell cap. Gas saturation profiles at 1 through 6 hours are shown in Figure 1. The capillary fringe between the aqueous and gas phases in the profile at 6 hours is located approximately at the 10-cm height level. Whereas the gas saturation profiles look smooth and predictable throughout the simulation, the profiles of CO_2 dissolved in the aqueous phase, shown in Figure 2, are dominated by fingers of descending CO_2 saturated plumes. The initiation of the fingering is largely impacted by the computational grid as can be seen in the CO_2 aqueous mass fraction profile at 2 hours, in Figure 2b. This implies that for this simulation scenario the resulting fingering profiles are dependent on the grid structure. The strong development of the fingered structures over the short time period of 6 hours is a function of the small domain size of the problem. Such rapid viscous fingering structures would not be expected to form over such short time periods for field-scale geologic sequestration scenarios.

**Table 1**. Hydrologic Properties of 30/40 Accusands

| Property	30/40 Accusands
Grain Density	$\rho_g = 2650 \ kg/m^3$
Porosity	$\phi = 0.327$
Hydraulic Conductivity	$K = 6.95 \ cm/min$
Intrinsic Permeability	$k = 1.2036 \ x \ 10^{-10} \ m^2$
Sat.- Cap. Press. Func.	$\bar{s}_l = \left(\dfrac{s_l - s_{lr}}{1 - s_{lr}} \right) = \left(\dfrac{\psi}{\beta_{gl} \ h_{gl}} \right)^{\lambda}$
Gas Entry Pressure Head	$\psi = 19.06815 \ cm$
Exponent Coefficient	$\lambda = 8.476029$
Aqu. Residual Saturation	$s_{lr} = 0.052$
Aqu. Rel. Perm. Function	$k_{rl} = \left(\bar{s}_l \right)^{\left(3 + \frac{2}{\lambda} \right)}$
Exponent Coefficient	$\lambda = 8.476029$
Gas Rel. Perm. Function	$k_{rg} = \left[\left(1 - \bar{s}_l \right)^2 \right] \left[1 - \left(\bar{s}_l \right)^2 \right]$
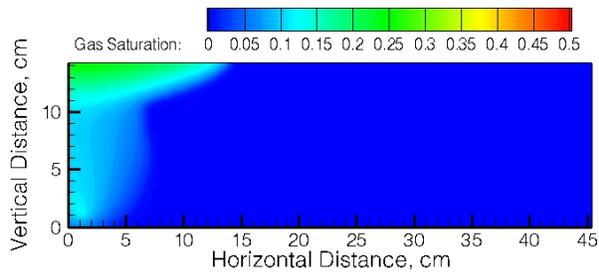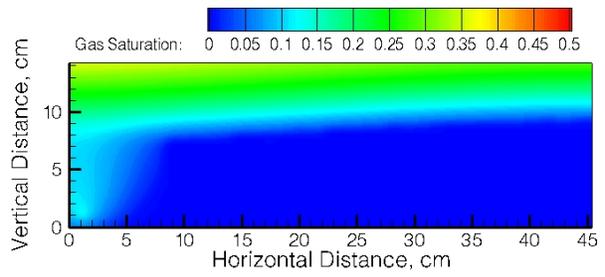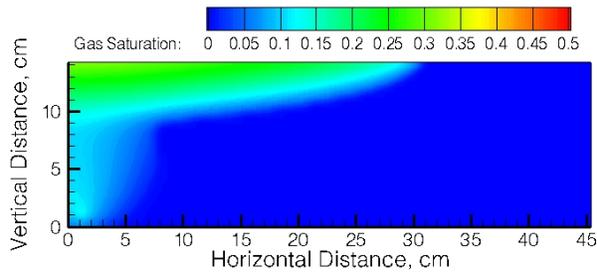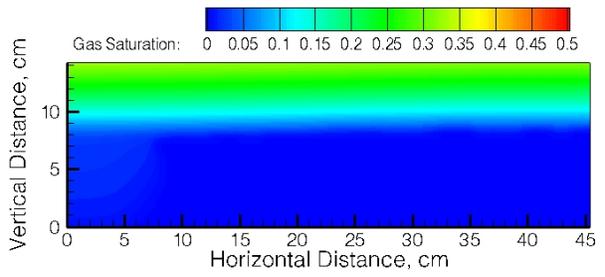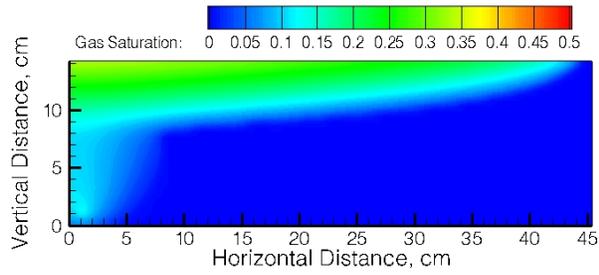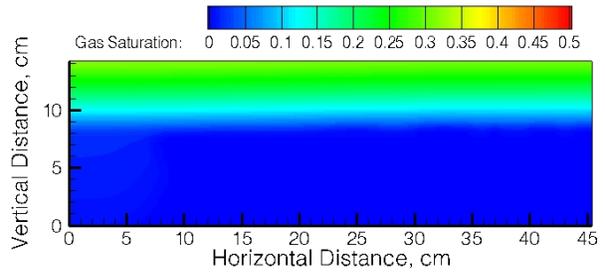
Figure 1. Scenario 1: Gas Saturation Profiles at 1, 2, 3, 4, 5, and 6 Hours in 1a, 1b, 1c, 1d, 1e, and 1f, Respectively
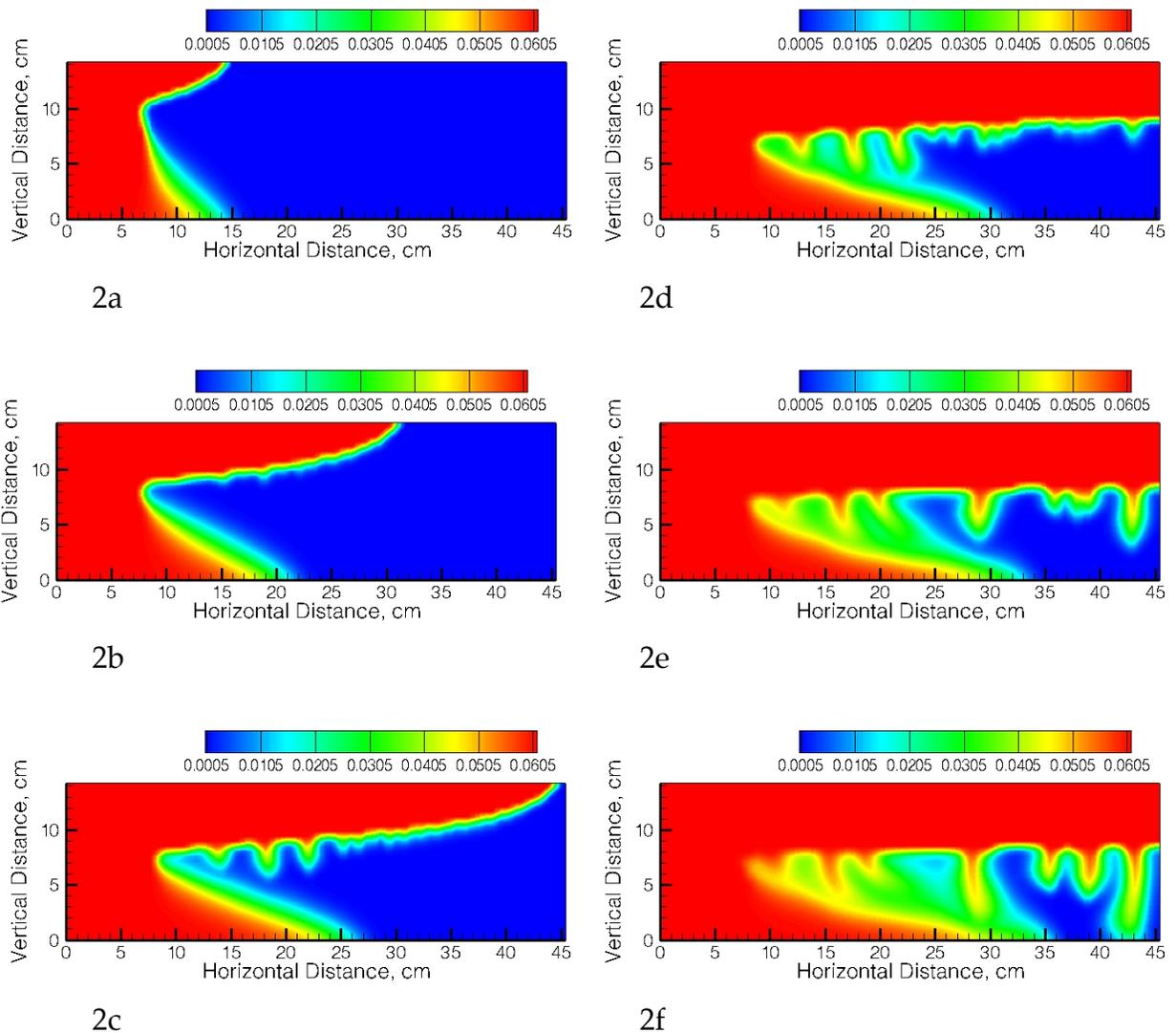
2a

2d

2b

2e

2c

2f

Figure 2. Scenario 1: CO_2 Aqueous Mass Fraction Profiles at 1, 2, 3, 4, 5, and 6 Hours in 2a, 2b, 2c, 2d, 2e, and 2f, Respectively

Scenario 2: Hele-Shaw Cell

In this scenario, a Hele-Shaw cell of 10-m (width) x 20-m (height) is modeled as a 2-dimensional flow cell filled with a porous media. The flow cell is initialized with a stepped distribution of dissolved aqueous CO_2 across the top of the flow cell. The aqueous and gas pressures are set equal to each other, creating aqueous saturated conditions throughout the domain (i.e., no gas phase). The temperature is initialized to 45°C and an initial salt concentration of 100 kg/m3 aqueous is specified. CO_2 is continually added to the top of the domain by the use of an initial condition boundary

5

condition for the aqueous phase, which includes the dissolved CO_2 concentration. The hydrologic properties of the porous media inside the domain modeling the Hele-Shaw cell are listed in Table 2, where the saturation-capillary pressure function is that of van Genuchten (1980), the aqueous relative permeability function that of van Genuchten (1980) with the Mualem porosity distribution model, and the gas relative permeability function that of van Genuchten (1980) with the Mualem porosity distribution model.

Table 2. Hydrologic Properties of Porous Media Modeling the Hele-Shaw Cell

Property	30/40 Accusands
Grain Density	$\rho_g = 2650 \; kg \, / \, m^3$
Porosity	$\phi = 0.327$
Storativity	$S = 4.5 \; x \; 10^{-6} \; 1 \, / \, m$
Intrinsic Permeability	$k_x = 1.0 \; x \; 10^{-11} \; m^2; \; k_z = 1.0 \; x \; 10^{-11} \; m^2$
Sat.- Cap. Press. Func.	$\bar{s}_l = \left[1 + \left(\alpha \, h \right)^n \right]^{-m}; \; m = 1 - \dfrac{1}{n}; \; \bar{s}_l = \dfrac{s_l - s_{lr}}{1 - s_{lr}}$
Inverse Entry Head	$\alpha = 0.2 \; cm^{-1}$
Exponent Coefficients	$n = 1.8; \; m = 0.444$
Aqu. Residual Saturation	$s_{lr} = 0.0$
Aqu. Rel. Perm. Function	$k_{rl} = \sqrt{\bar{s}_l} \left[\left(1 - \left(1 - \left(\bar{s}_l \right)^{1/m} \right)^m \right)^2 \right]$
Gas Rel. Perm. Function	$k_{rg} = \sqrt{\left(1 - \bar{s}_l \right)} \left[\left(\left(1 - \left(\bar{s}_l \right)^{1/m} \right)^m \right)^2 \right]$

The dissolved CO_2 concentration is initialized in a dental pattern at the top of the domain, which generates the initial fingering as shown in Figure 3a, after 50 days. The viscous finger migration then proceeds with the upper boundary providing a constant

source of aqueous dissolved CO_2 in the same dental pattern as used initially. The downward migration is slower than for Scenario 1, as the Hele-Shaw cell is meso-scale size (i.e., 10s of meters) and the pressure cell is laboratory-scale size (i.e., meters). As the simulation progresses the individual fingers coalesce together forming larger fingers with a faster descension rate, with the largest finger contacting the bottom of the Hele-Shaw cell around 800 days.
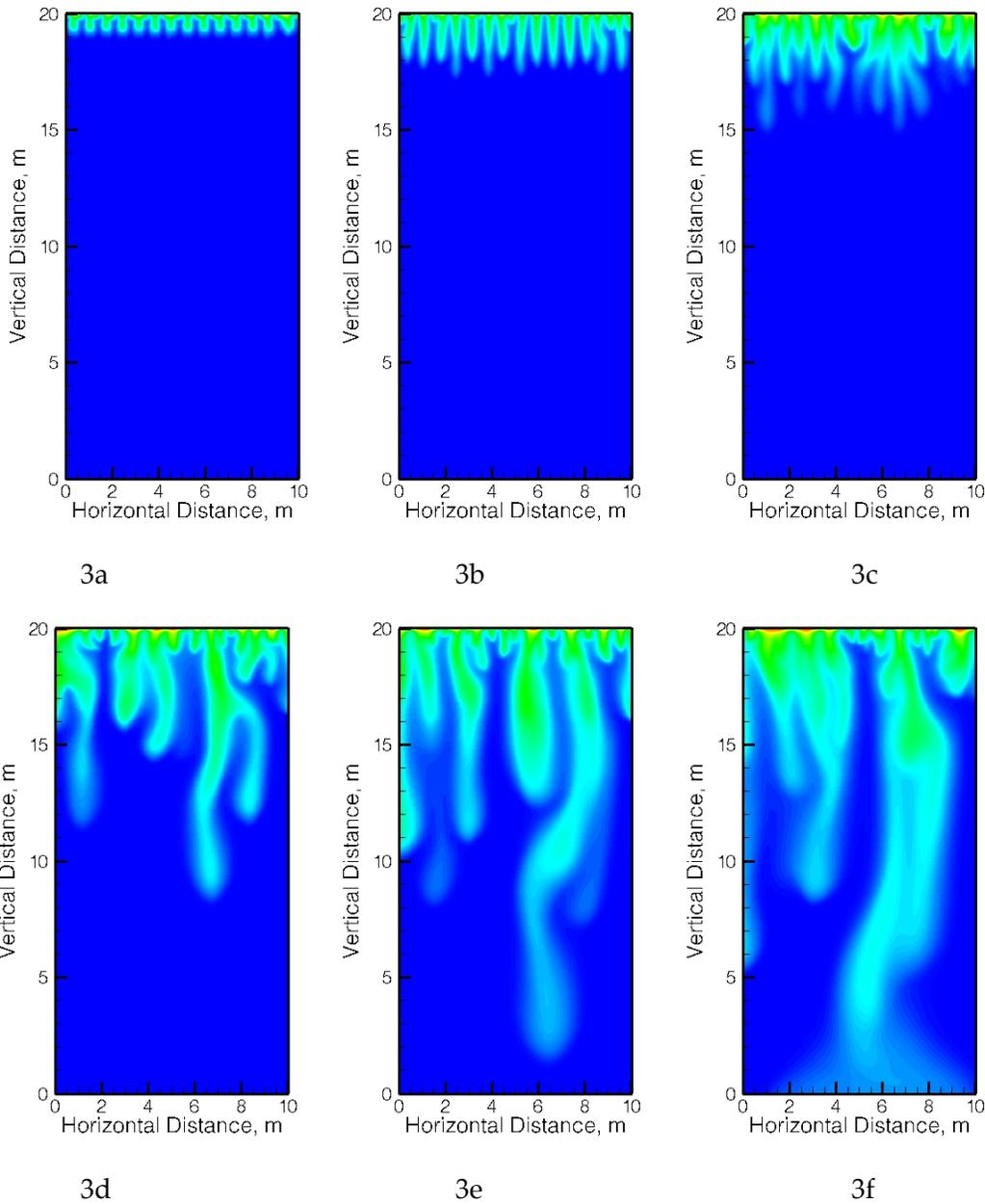
Figure 3. Scenario 2: CO_2 aqueous mass fraction profiles at 50, 100, 200, 400, 600 and 800 days in 3a, 3b, 3c, 3d, 3e, and 3f, respectively.

References

Brooks, R. H., Corey, A. T., 1964. "Hydraulic Properties of Porous Media." *Colorado State University, Hydrology Paper, No. 3*, Fort Collins, Colorado.

Brooks, R. H., and A. T. Corey. 1966. "Properties of porous media affecting fluid flow." *Journal of Irrigation and Drainage Division* 93(3):61-88.

Burdine, N.T. 1953. "Relative permeability calculations from pore-size distribution data." *Petroleum Trans.* 198:71-77.

Corey, A.T. 1954. "The Interrelation Between Gas and Oil Relative Permeabilities". *Prod. Monthly* **19** (1): 38–41.

van Genuchten, M. T. A. 1980. "A closed-form equation for predicting the hydraulic conductivity of unsaturated soils." *Soil Sci. Soc. Am. J.*, 44:892-898.

Exercises

1. (Moderate) Repeat the pressure-cell simulation, but using invariant aqueous density and viscosity. Determine an appropriate aqueous density and viscosity from a zero-time-step simulation, using the original pressure-cell simulation. Make time-history plots of gas saturation and CO_2 aqueous mass fraction and compare the results against those for the original pressure-cell simulation. Explain the observed differences.

2. (Moderate) Repeat the pressure-cell simulation, but altering the computational grid, either by altering the grid resolution (e.g., increasing the total number of nodes), or by altering the grid structure (e.g., keeping the total number of nodes constant and altering the grid spacing). Make time-history plots of gas saturation and CO_2 aqueous mass fraction and compare the results against those for the original pressure-cell simulation. Explain the observed differences.

3. (Difficult) Repeat the pressure-cell simulation using field-scale dimensions and grid resolution. Make time-history plots of gas saturation and CO_2 aqueous mass fraction and compare the results against those for the original pressure-cell simulation. Explain the observed differences.

Input Files

Scenario 1: Pressure-Cell Simulation Input File

~Simulation Title Card
1,
STOMP Example Problem CO2-7 Scenario 1,
M.D. White,
Pacific Northwest Laboratory,
10 June 2002,
11:09 AM PST,
2,
Pressure-cell simulation of supercritical CO2 injection
into pure water.

~Solution Control Card
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STOMP-CO2,
1,
0,day,6,hr,1.e-3,s,5,day,1.25,16,1.e-06,
1000,
Variable Aqueous Diffusion,
Variable Gas Diffusion,
0,

~Grid Card
Uniform Cartesian,
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0.5,in,
0.175781,in,

~Rock/Soil Zonation Card
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~Mechanical Properties Card
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~Hydraulic Properties Card
30/40 Accusand,6.95,hc:cm/min,6.95,hc:cm/min,6.95,hc:cm/min,

~Saturation Function Card
30/40 Accusand,Brooks and Corey,19.06815,cm,8.476029,0.052,,

~Aqueous Relative Permeability Card
30/40 Accusand,Burdine,,

~Gas Relative Permeability Card
30/40 Accusand,Corey,,,

~Salt Transport Card
30/40 Accusand,0.0,m,0.0,m,

~Initial Conditions Card
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Aqueous Pressure,138.0,Bar,,,,,,1,100,1,1,1,32,
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~Output Options Card
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98,1,3,
1,1,hr,cm,6,6,6,
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Gas Saturation,,
Salt Saturation,,
Salt Aqueous Mass Fraction,,
CO2 Aqueous Mass Fraction,,
Gas Pressure,Bar,
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60@0.1,hr,
5,
Gas Saturation,,
Salt Saturation,,
Salt Aqueous Mass Fraction,,
CO2 Aqueous Mass Fraction,,
Gas Pressure,Bar,

Scenario 2: Hele-Shaw Simulation Input File

~Simulation Title Card
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STOMP Example Problem CO2-7 Scenario 2,
Sylvie Chevalier,
Masdar Institute,
11 May 2012,
11:09 AM PST,
2,
Simulation of viscous finger formation in a Hele-Shaw cell
from a heterogeneous initial distribution of dissolved CO2.

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zero Gas Diffusion,
0,

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~Hydraulic Properties Card
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~Saturation Function Card
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~Aqueous Relative Permeability Card
Geologic Media,Mualem,,

~Gas Relative Permeability Card
Geologic media,Mualem,,

~Salt Transport Card
Geologic Media,0.0,m,0.0,m,

~Initial Conditions Card
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salt aqueous concentration,100.,kg/m^3,,,,,,,1,100,1,1,1,150,

~Surface flux Card
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Aqueous-Phase CO2 Mass,kg/s,kg,Bottom,1,100,1,1,150,150,
Gas-Phase CO2 Mass,kg/s,kg,Top,1,100,1,1,150,150,

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CO2 Aqueous Concentration,kg/m^3,
Aqueous saturation,,
gas saturation,,
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10,day,
50,day,
100,day,
200,day,
400,day,
600,day,
800,day,
1000,day,
1200,day,
1400,day,
1600,day,
1800,day,
8,
Salt Aqueous Concentration,kg/m^3,
CO2 Aqueous Concentration,kg/m^3,
aqueous density,,
Aqueous saturation,,
Aqueous Pressure,Pa,
gas saturation,,
gas pressure,Pa,
total CO2 mass,,

Solution to Selected Exercises

Exercise 1

The *invariant fluid density and viscosity* option in the *Solution Control Card* makes the aqueous and gas (i.e., CO_2 dominant phase) have constant density and viscosity during the simulation. When this option is invoked the aqueous and gas density and viscosity are specified in the *Solution Control Card*. To determine aqueous and gas density and viscosity, a single-node, zero-time-step simulation was executed at 138 bar and 45°C, with the aqueous and gas density and viscosity requested as output at the single reference node. The results from this simulation are shown in Table 3. The input file for this exercise is listed below.

Table 3. Invariant aqueous and gas density and viscosity determined from a single-node, zero-time-step simulation at 138 bar and 45°C

| Phase	Properties
Aqueous	$\rho_l = 1003.28 \ kg \ / \ m^3$; $\mu_l = 8.9769 \ x \ 10^{-4} \ Pa \ s$
Gas	$\rho_g = 863.142 kg \ / \ m^3$; $\mu_g = 8.2673 \ x \ 10^{-5} \ Pa \ s$

With invariant fluid properties, the aqueous density does not change with CO_2 dissolution. This does not greatly impact the gas saturation profiles, as shown in Figure 4, with the exception of the elevation of the aqueous-gas transition point at the final time step, which is lower than for the base simulation with variable density. This indicates more CO_2 remains in the gas phase. The dissolved CO_2 profiles, shown in Figure 5, are starkly different from those in Figure 2, as no viscous fingers form. This is due to the lack of a density instability, as the aqueous density is independent of dissolved CO_2 concentration. The lack of a density instability results in less mixing and a smaller fraction of the total CO_2 being dissolved in the aqueous phase.
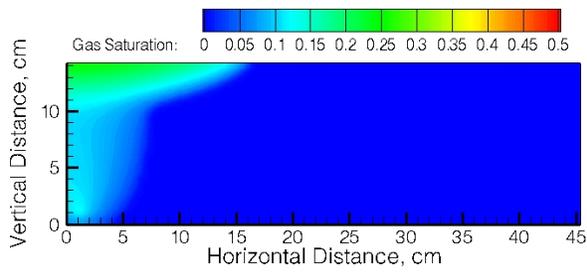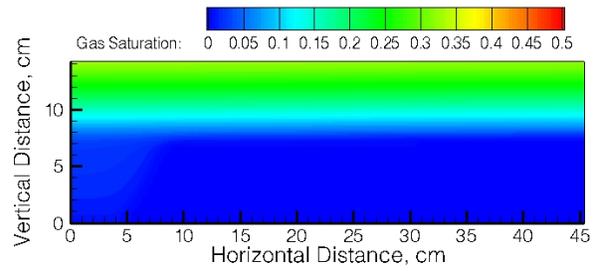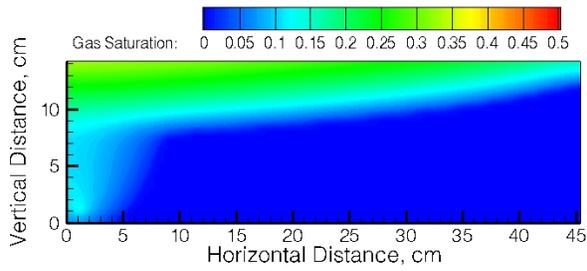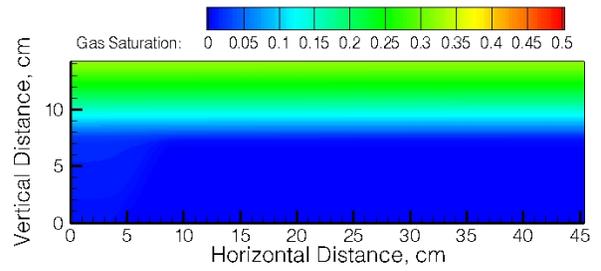
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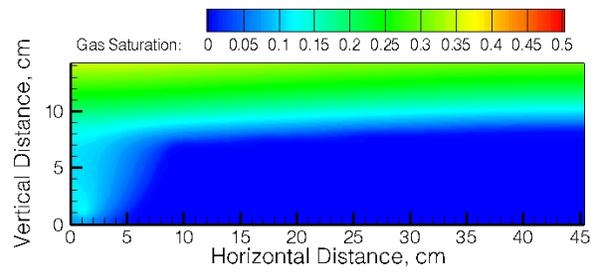
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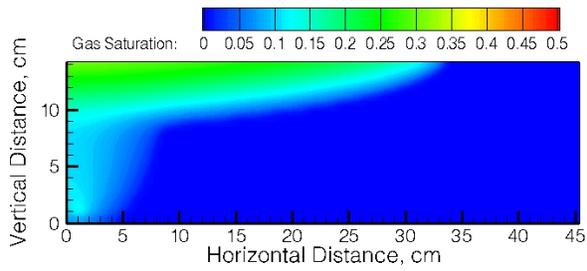
4b

4e

4c

4f

Figure 4. Exercise 1: Gas Saturation Profiles at 1, 2, 3, 4, 5, and 6 Hours in 4a, 4b, 4c, 4d, 4e, and 4f, Respectively
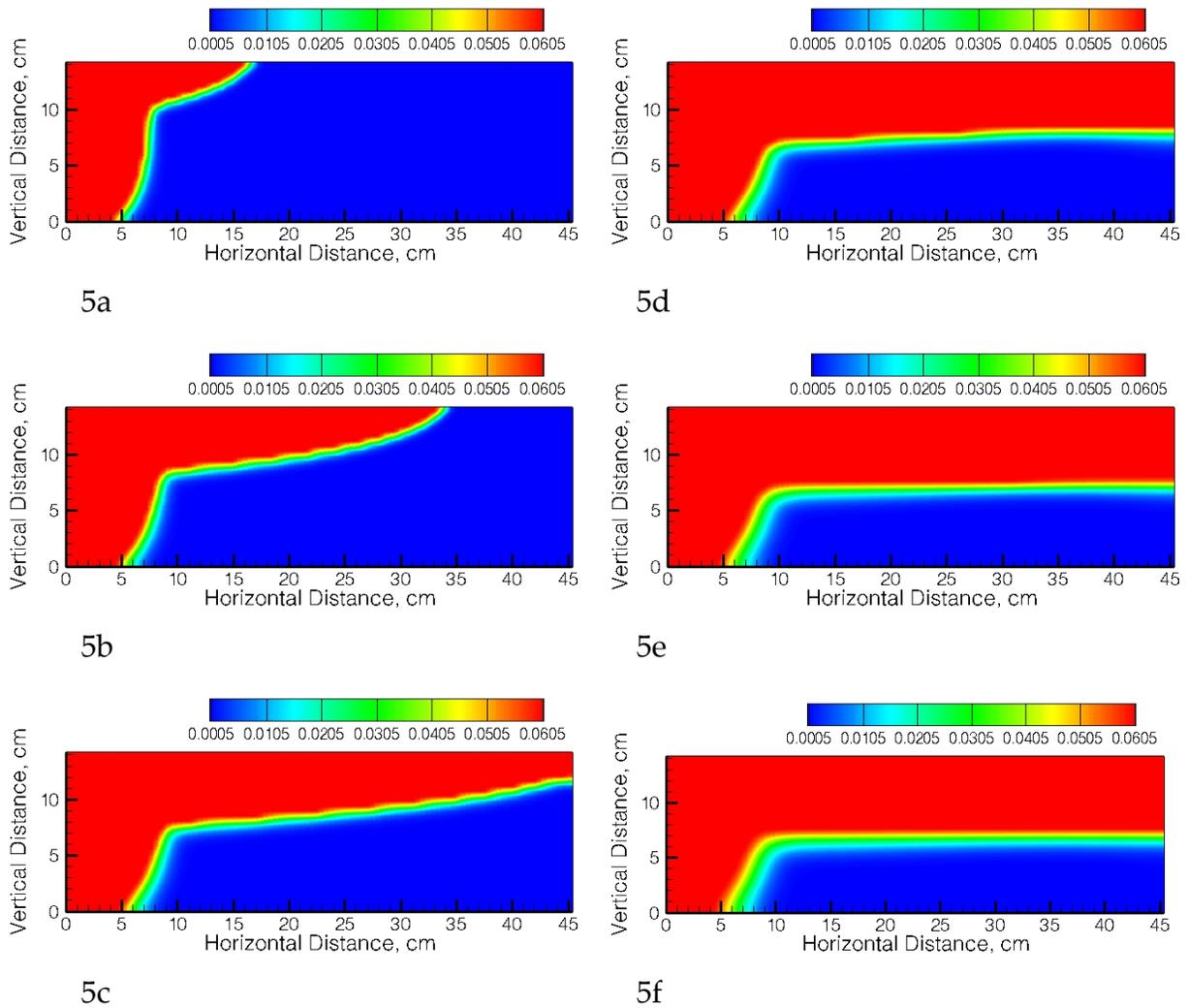
5a

5d

5b

5e

5c

5f

Figure 5. Exercise 1: CO_2 Aqueous Mass Fraction Profiles at 1, 2, 3, 4, 5, and 6 Hours in 5a, 5b, 5c, 5d, 5e, and 5f, Respectively

Input Files

Scenario 1: Exercise 1 Input File

~Simulation Title Card
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STOMP Example Problem CO2-7: Exercise 1,
M.D. White,
Pacific Northwest Laboratory,
10 June 2002,
11:09 AM PST,
2,
Pressure-cell simulation of supercritical CO2 injection
into pure water.

~Solution Control Card
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Variable Gas Diffusion,
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0.175781,in,

~Rock/Soil Zonation Card
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~Mechanical Properties Card
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~Hydraulic Properties Card
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~Saturation Function Card
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~Aqueous Relative Permeability Card
30/40 Accusand,Burdine,,

~Gas Relative Permeability Card
30/40 Accusand,Corey,,,

~Salt Transport Card
30/40 Accusand,0.0,m,0.0,m,

~Initial Conditions Card
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Aqueous Pressure,138.0,Bar,,,,,,1,100,1,1,1,32,
Temperature,25.0,C,,,,,,1,100,1,1,1,32,

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4,hr,138.0,bar,8.5816,cm^3/hr,0.0,

~Boundary Conditions Card
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98,1,3,
1,1,hr,cm,6,6,6,
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Aqueous Viscosity,,
Gas Density,,
Gas Viscosity,,
Gas Saturation,,
Salt Saturation,,
Salt Aqueous Mass Fraction,,
CO2 Aqueous Mass Fraction,,
Gas Pressure,Bar,
1,
60@0.1,hr,
9,
Aqueous Density,,
Aqueous Viscosity,,
Gas Density,,
Gas Viscosity,,
Gas Saturation,,
Salt Saturation,,
Salt Aqueous Mass Fraction,,
CO2 Aqueous Mass Fraction,,
Gas Pressure,Bar,