Example Problem CO2-3

CO_2 Injection into a 2-Dimensional Layered Brine Formation (GeoSeq #7)

Abstract: *Pressure and buoyancy driven migration of CO_2 injected into a layered formation that is representative of the Sleipner Vest field in the Norwegian sector of the North Sea is investigated. This problem is identical to Problem 7 of the code intercomparison problems developed under the GeoSeq Project (Pruess et al. 2002). A key assumption for the problem, as posed, was isothermal conditions at the formation temperature of 37˚C; therefore, STOMP-CO2 was executed for these simulations. The problem involves a constant mass rate injection of $scCO_2$ into a layered saline formation comprising sands and shales.*

Problem Description

This problem considers the injection of CO_2 under supercritical conditions ($scCO_2$) into a layered saline formation. $scCO_2$ is injected at a constant rate into the lower most sand unit of a lithologic system consisting of horizontal layers, alternating between sands and shales, as shown in Figure 1. The hydrologic system is initialized under hydrostatic conditions with a reference pressure of 110 bar at the well elevation, which are then held throughout the simulation along the right vertical boundary surface (i.e., STOMP-CO2 east boundary). Zero flux boundary surfaces are assumed for the upper horizontal shale cap (i.e., STOMP-CO2 top boundary), lower horizontal shale basement (i.e., STOMP-CO2 bottom boundary), and symmetry plane on the left vertical surface (i.e., STOMP-CO2 west boundary). The gravitational vector is assumed to be pointed vertically down. The domain is 6,000 m in length, 184 m in height, and 1 m in depth. The system was designed to simulate a unit length of a 100-m horizontal injection well where a symmetry plane was assumed in the vertical direction through the center of the well. scCO2 is injected for a 2-yr period at a rate of 0.1585 kg/s, representing a total injection rate for the 100 m injection well of 1 MMT/yr. Results to be calculated are the distribution of CO_2 mass in the sand layers at 30 days, 1 year, and 2 years, the distribution of CO_2 between the gas and aqueous phases, and the fluxes of CO_2 across the shale layers.

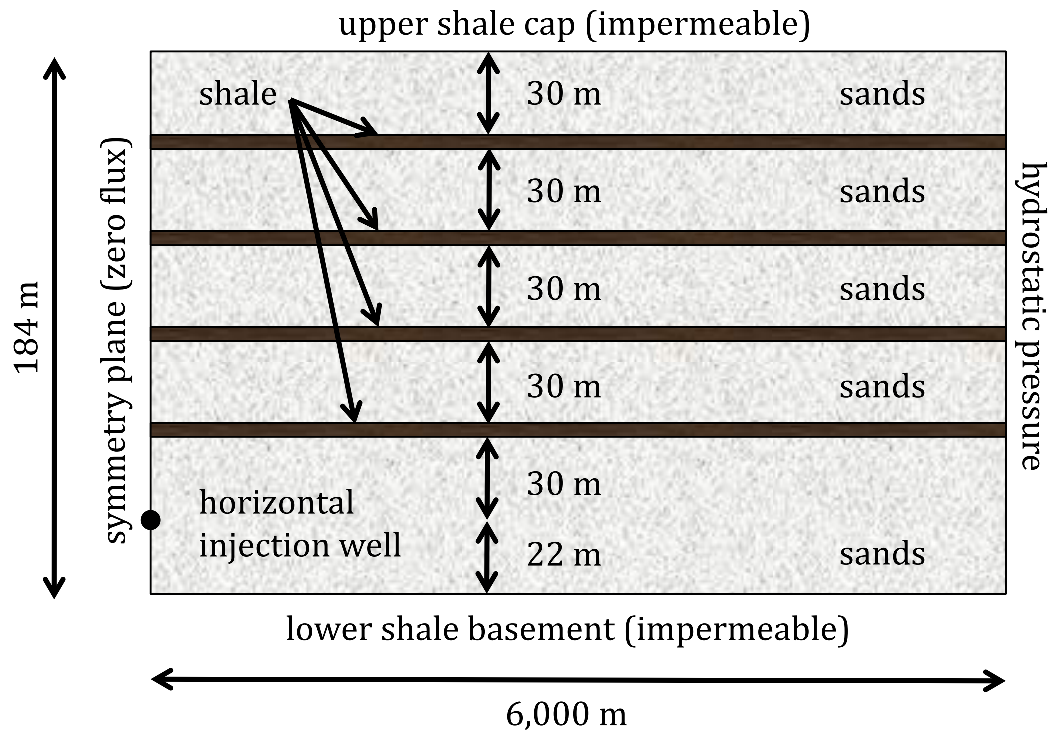

Figure 1. Schematic of the injection reservoir, showing location of the injection well and lithology

The shales differ hydrologically from the sands in that they have lower intrinsic permeability, lower porosity, and a higher entry pressure. The van Genuchten function (van Genuchten 1980) is used to describe the saturation-capillary pressure relationship and the Mualem porosity distribution function is coupled with the van Genuchten function (van Genuchten 1980) to describe the aqueous and gas relative permeability-saturation functions. The hydrologic functions, parameters, and properties are listed in Table 1. The gas relative permeability function shown in Table 1, is the corrected form of the version shown in Table G.2 of the GeoSeq documentation (Pruess et al. 2002).

Time stepping and grid spacing were not specified as part of the original GeoSeq problem description, but were left to the discretion of the modeler. For this problem two grid systems were developed: 1) 78z and 2) 193z, with the 78z grid using 78 nodes in the vertical direction and the 193z grid using 193 nodes in the vertical direction. Both grids used non-uniform spacing in the horizontal direction using a grid spacing that increases geometrically, starting with an initial spacing of 2 m. An initial time step of

1 s was used, with a time-step acceleration factor of 1.25 for the 2-year simulation period.

Table 1. Hydrology functions, parameters, and properties

Property	Sands	Shales
Intrinsic Permeability	$k = 3\ x\ 10^{-13}\ m^2$	$k = 1\ x\ 10^{-14}\ m^2$
Porosity	$\phi = 0.35$	$\phi = 0.1025$
Pore Compressibility	$\beta = 4.5\ x\ 10^{-10}\ Pa^{-1}$	
Aqu. Rel. Perm. Func.	$k_{rl} = \left(\bar{s}_l\right)^{1/2} \left[1 - \left(1 - \left(\bar{s}_l\right)^{1/m} \right)^m \right]^2 ; \bar{s}_l = \frac{s_l - s_{lr}}{1 - s_{lr}}$	
Aqu. Residual Saturation	$s_{lr} = 0.20$	$s_{lr} = 0.20$
Exponent Coefficient	$m = 0.4$	$m = 0.4$
Gas. Rel. Perm. Func.	$k_{rg} = \left(\bar{s}_g\right)^{1/2} \left[\left(1 - \left(1 - \bar{s}_g \right)^{1/m} \right)^m \right]^2 ; \bar{s}_g = \frac{s_g - s_{gr}}{1 - s_{gr}}$	
Gas Residual Saturation	$s_{gr} = 0.05$	$s_{gr} = 0.05$
Exponent Coefficient	$m = 0.4$	$m = 0.4$
Sat.- Cap. Press. Func.	$\bar{s}_l = \frac{s_l - s_{lr}}{1 - s_{lr}} = \left[1 + \left(\alpha\, \beta_{gl}\, h_{gl} \right)^n \right]^{-m} ; m = 1 - \frac{1}{n}$	
Aqu. Residual Saturation	$s_{lr} = 0.05$	$s_{lr} = 0.05$
Exponent Coefficient	$m = 0.4; n = 1.667$	$m = 0.4; n = 1.667$
Inverse Entry Head	$\alpha = 2.735\, m^{-1}$	$\alpha = 0.158\, m^{-1}$

Simulation results from other modeling groups and numerical simulators for this problem are reported in Pruess et al. (2002). $scCO_2$ injected into the system enters the domain beneath the first shale layer and then migrates both horizontally and vertically under pressure gradient and buoyancy forces. The migration pattern is controlled by both the pressure and buoyancy driving forces and the contrast in entry pressure and intrinsic permeability between the sand and shale layers. Gas saturation profiles at 30 days, 1 year and 2 years after the start of injection are shown in Figure 2. Saturation profiles reported in Pruess et al. (2002) for the same points in time are shown in Figure 3. The GeoSeq results show slightly more extended plumes beneath each of the shale layers compared with the STOMP-CO2 results. Otherwise there is good agreement between the simulations.

The pressure distribution in the domain is a function of the CO_2 injection rate, the overall resistance of the injected CO_2 to displace the formation brine, the phase relative permeabilities, and formation intrinsic permeabilities. The pressure distribution after two years is shown in Figures 4 and 5 for the STOMP-CO2 and TOUGH2/ECO2 simulations respectively. The phase distribution of CO_2 mass in the domain over time is shown in Figure 6. At the end of the simulation, 0.149 of the CO_2 mass occurs as dissolved in the aqueous phase. The TOUGH2/ECO2 simulator predicted 0.215 of the CO_2 mass to be dissolved in the aqueous phase. The higher aqueous mass in the TOUGH2/ECO2 simulation is probably due to the larger lateral spread beneath the shale layers. The amount of CO_2 mass in each of the sand layers is shown in Figures 7 and 8 for the STOMP-CO2 and GeoSeq simulations. There is good agreement between the total amounts of CO_2 in the sand levels, but the arrival times are advanced in the STOMP-CO2 simulations. The arrival times were determined to be dependent on the gas relative permeability model. The model function reported in Pruess et al. (2002) was not a standard form. When this equation was implemented in STOMP-CO2 the simulation results showed poor agreement with those for the GeoSeq simulations (Pruess et al. 2002). As a result, the more conventional form of the gas relative permeability function shown in Table 1 was implemented for the simulation results shown.

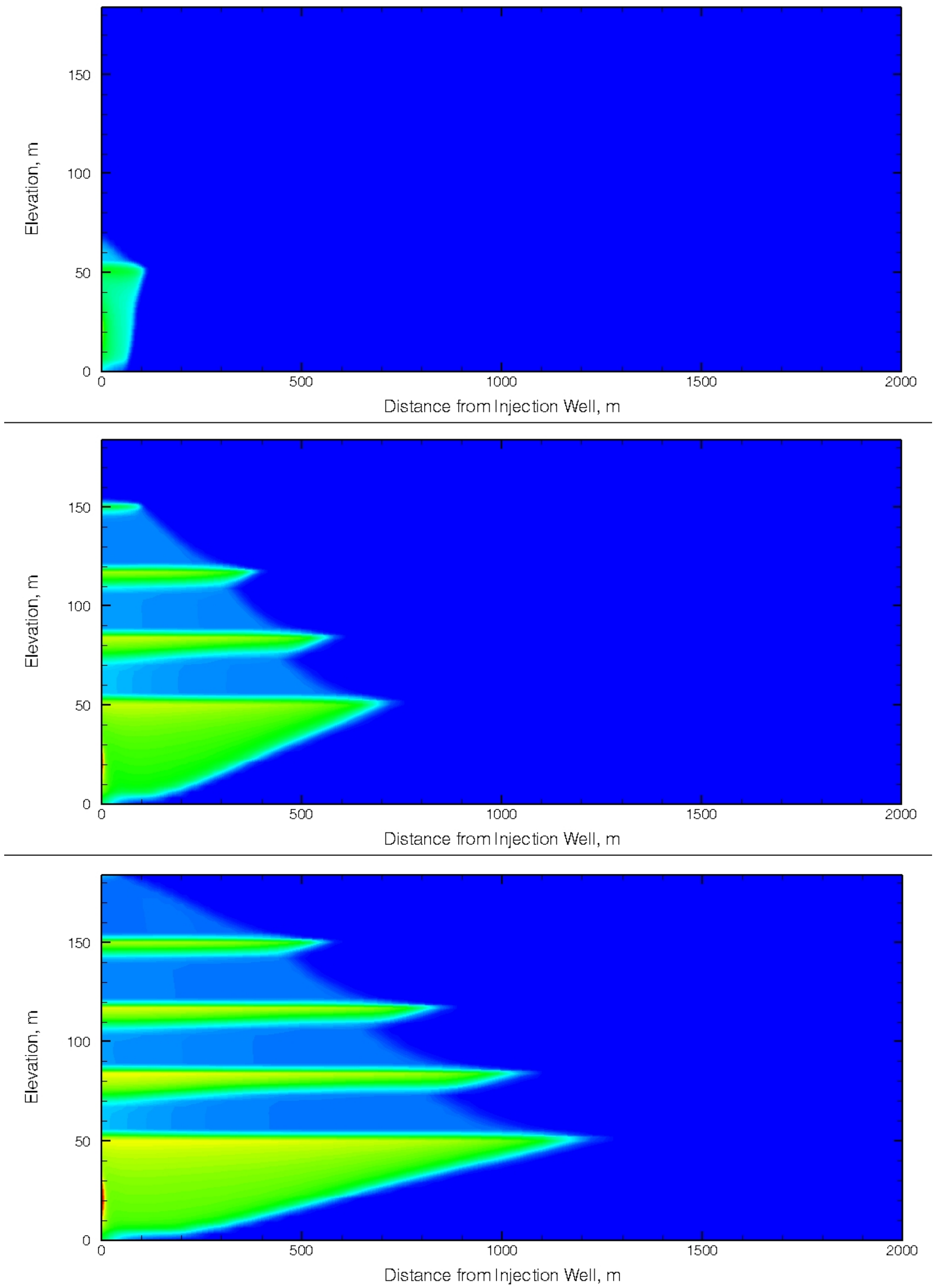

Figure 2. Gas saturation profiles from STOMP-CO2 at 30 days, 1 year, and 2 years

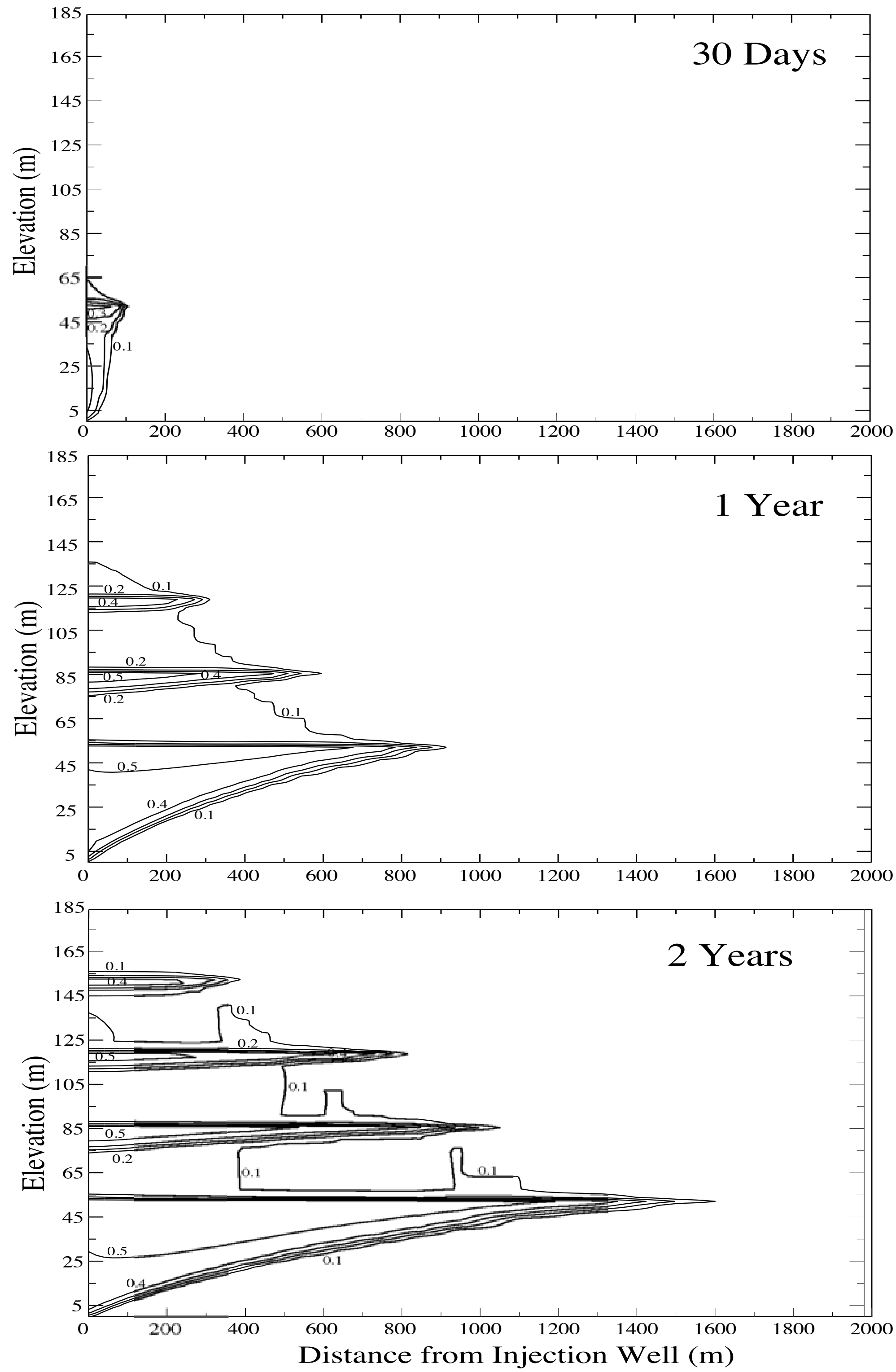

Figure 3. Gas saturation profiles from TOUGH2 at 30 days, 1 year, and 2 years from Pruess et al (2002)

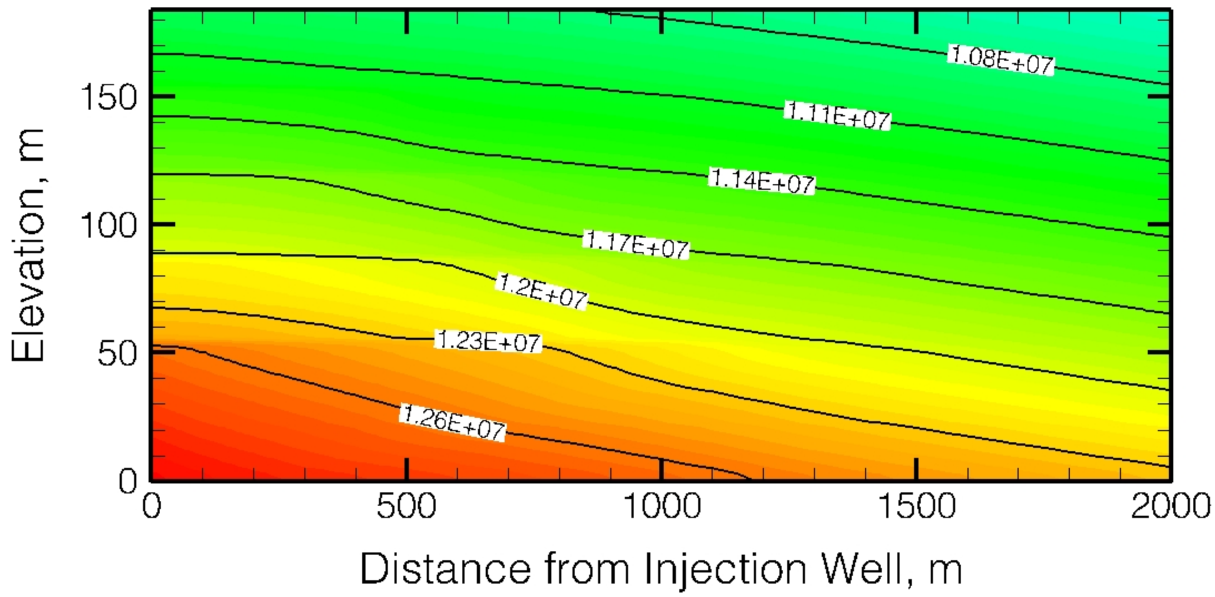

Figure 4. Pressure distribution from STOMP-CO2 after 2 years of CO_2 injection

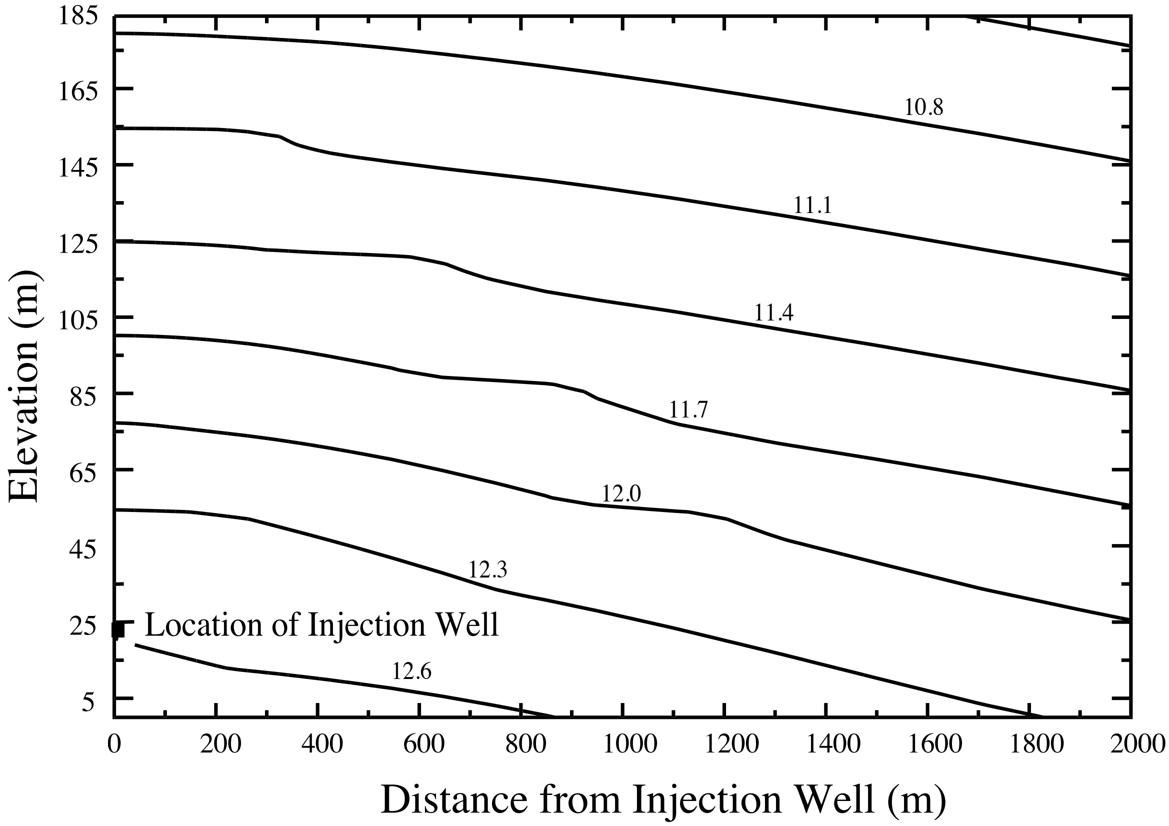

Figure 5. Pressure distribution from TOUGH2 after 2 years of CO_2 injection from Pruess et al (2002)

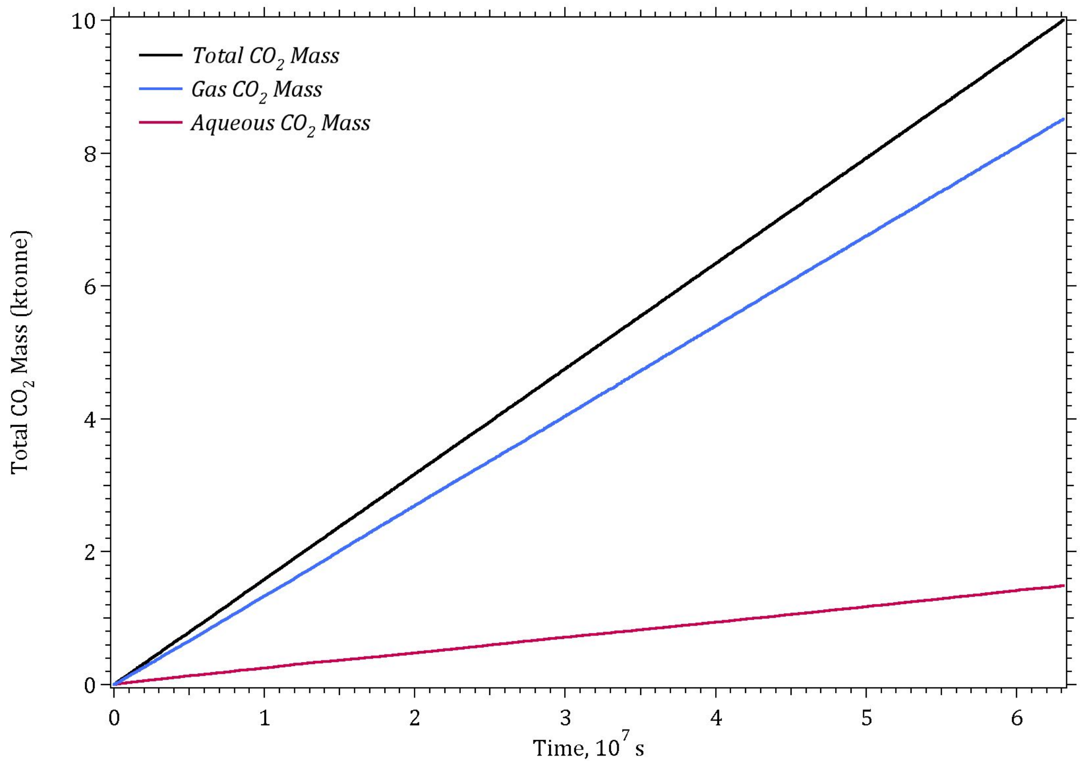

Figure 6. CO_2 phase distribution from STOMP-CO2 as a function of time

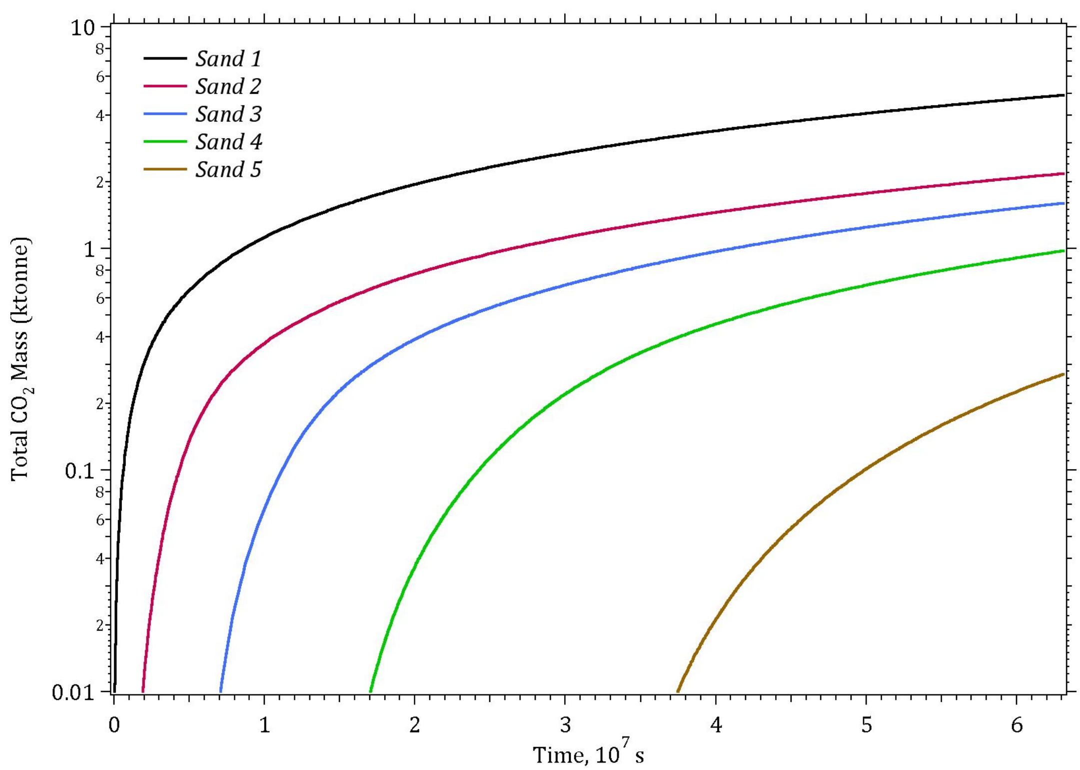

Figure 7. Total CO_2 in sand horizons from STOMP-CO2 as a function of time

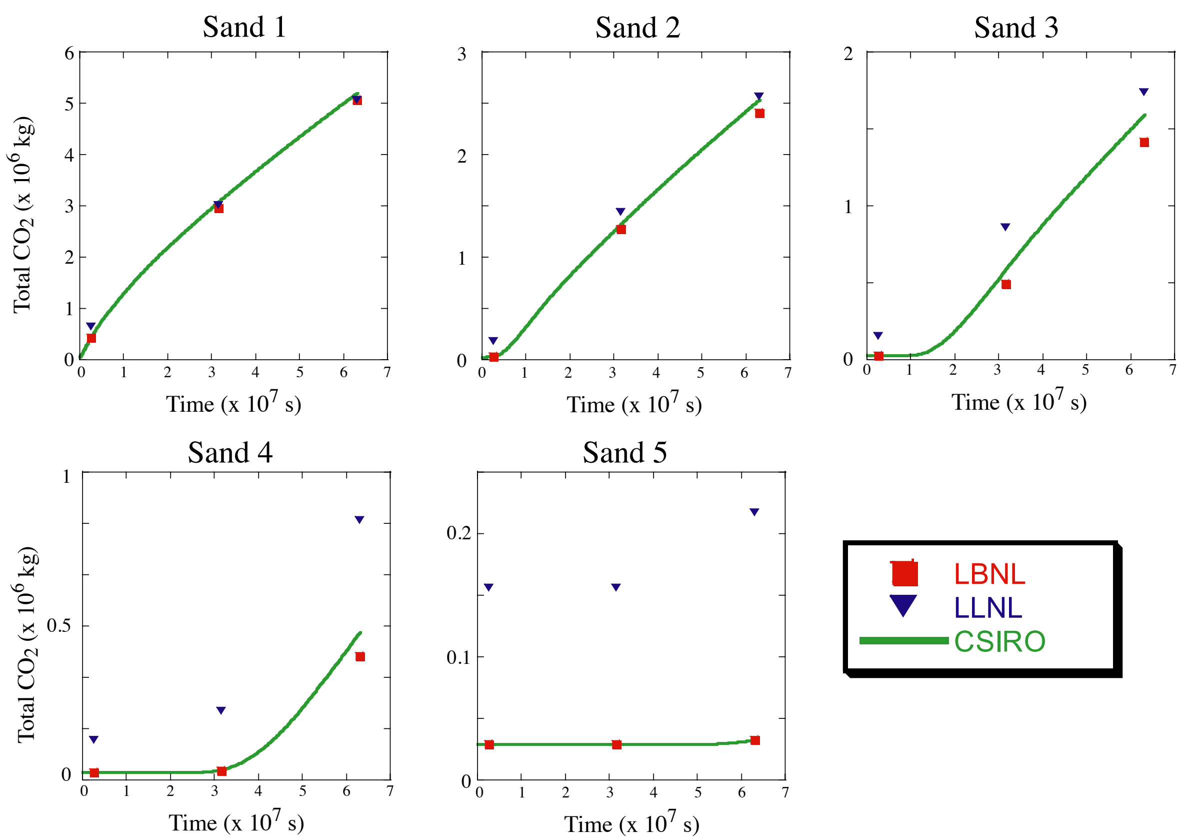

Figure 8. Total CO_2 in sand layers from from LBNL (TOUGH2/ECO2), LLNL (NUFT), and CSIRO (TOUGH2/ECO2) from Pruess et al. (2002) as a function of time

References

Pruess, K., J. Garcia, T. Kovscek, C. Oldenburg, J. Rutqvist, C. Steefel, and T. Xu. 2002. Intercomparison of Numerical Simulation Codes for Geologic Disposal of CO2, Lawrence Berkeley National Laboratory, LBNL-51813, Berkeley, California.

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

Exercises

1. (Basic) Repeat the 78z simulation, but make the permeability of the shale layers vary with depth:

   layer 4 (upper-most shale layer) $k = 1 \text{ x } 10^{-17}\ m^2$

   layer 3 (upper-middle shale layer) $k = 1 \text{ x } 10^{-16}\ m^2$

   layer 2 (lower-middle shale layer) $k = 1 \text{ x } 10^{-15}\ m^2$

   layer 1 (lower-most shale layer) $k = 1 \text{ x } 10^{-14}\ m^2$

2. (Moderate) Repeat the 78z simulation as a cylindrical problem with the injection point located at the center of the cylinder and the screened interval being the height of the lower-most sand layer. Use an injection rate of 31.7 kg/s for the entire cylinder and screened interval.
3. (Difficult) Examine whether the simulation results are dependent on the selected vertical grid spacing by developing a computational domain with a nearly uniform vertical grid spacing of 1 m, with 0.5-m grid spacings used adjacent to the sand-shale interfaces.

Input Files

78z Simulation Input File

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STOMP Example Problem CO2-3: 78z,
M.D. White,
Pacific Northwest Laboratory,
24 January 2012,
09:11 PST,
20,
Intercomparison of simulation models for CO2 disposal in
underground storage reservoirs.
Test Problem 7: CO2 Injection into a 2D Layered Brine Formation
This test problem is patterned after the CO2 injection project
at the Sleipner Vest field in the Norwegian sector of the North Sea,
and is intended to investigate the dominant physical processes
associated with the injection of supercritical CO2 into a layered
medium. Significant simplifications have been made, the most important
of which is the assumption of isothermal conditions (37 °C, the
ambient temperature of the formation). CO2 injection rates
(1,000,000 tonnes per year), system geometry, and system permeabilities
correspond approximately to those at Sleipner, although no attempt was
made to represent details of the permeability structure within the
host formation. Injection of the supercritical CO2, which is less
dense than the saline formation waters into which it is injected,
causes it to rise through the formation. Its rate of ascent, however,
is limited by the presence of four relatively low permeability shales.
The top and bottom of the formation is assumed to be impermeable.
The only reactive chemistry considered in this problem is the
dissolution of CO2 in the aqueous phase. (Pruess and Garcia, 2000).

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Shale,2650,kg/m^3,0.1025,0.1025,Compressibility,4.5e-10,1/Pa,,,Millington and Quirk,

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Shale,van Genuchten,0.158,1/m,1.667,0.20,0.4,0.0,

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Exercise 1 Input File

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STOMP Example Problem CO2-3 Exercise 1,
M.D. White,
Pacific Northwest Laboratory,
24 January 2012,
09:11 PST,
20,
Intercomparison of simulation models for CO2 disposal in
underground storage reservoirs.
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~Solution Control Card
Normal,
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Variable Gas Diffusion,
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Shale-1,van Genuchten,0.158,1/m,1.667,0.20,0.4,0.0,

~Aqueous Relative Permeability Card
Sands,Mualem Irreducible,0.4,0.20,
Shale-4,Mualem Irreducible,0.4,0.20,
Shale-3,Mualem Irreducible,0.4,0.20,
Shale-2,Mualem Irreducible,0.4,0.20,

```
Shale-1,Mualem Irreducible,0.4,0.20,

~Gas Relative Permeability Card
Sands,van Genuchten,0.4,0.05,
Shale-4,van Genuchten,0.4,0.05,
Shale-3,van Genuchten,0.4,0.05,
Shale-2,van Genuchten,0.4,0.05,
Shale-1,van Genuchten,0.4,0.05,

~Salt Transport Card
Sands,0.0,m,0.0,m,
Shale-4,0.0,m,0.0,m,
Shale-3,0.0,m,0.0,m,
Shale-2,0.0,m,0.0,m,
Shale-1,0.0,m,0.0,m,

~Initial Conditions Card
Gas Pressure,Aqueous Pressure,
4,
Gas Pressure,112.0525,Bar,,,,,-0.1001218,1/m,1,100,1,1,1,78,
Aqueous Pressure,112.0525,Bar,,,,,-0.1001218,1/m,1,100,1,1,1,78,
Temperature,37.0,C,,,,,,,1,100,1,1,1,78,
Salt Mass Fraction,0.032,,,,,,,,1,100,1,1,1,78,

~Boundary Conditions Card
1,
East,Aqueous Initial Condition,Gas Initial Condition,Aqueous Initial Condition,
100,100,1,1,1,78,1,
0,s,,,,,,,,,

~Source Card
1,
Gas Mass Rate,Water-Vapor Mass Fraction,1,1,1,1,8,8,1,
0,s,112.0525,bar,0.1585,kg/s,0.0,

~Output Options Card
4,
1,1,8,
1,1,18,
1,1,33,
1,1,48,
1,1,s,m,6,6,6,
8,
Gas Saturation,,
CO2 Gas Mass Fraction,,
CO2 Aqueous Mass Fraction,,
Gas Pressure,Pa,
Aqueous Density,kg/m^3,
Integrated CO2 Mass,kg,
Integrated Aqueous CO2 Mass,kg,
Integrated Gas CO2 Mass,kg,
2,
30,day,
1,year,
7,
Gas Saturation,,
CO2 Gas Mass Fraction,,
CO2 Aqueous Mass Fraction,,
```

```
Gas Pressure,Pa,
Diffusive Porosity,,
Gas Density,kg/m^3,
Aqueous Density,kg/m^3,

~Surface Flux Card
5,
Total CO2 Flux,kg/s,kg,Top,1,100,1,1,18,18,
Total CO2 Flux,kg/s,kg,Top,1,100,1,1,21,21,
Total CO2 Flux,kg/s,kg,Top,1,100,1,1,36,36,
Total CO2 Flux,kg/s,kg,Top,1,100,1,1,51,51,
Total CO2 Flux,kg/s,kg,Top,1,100,1,1,66,66,
```

Exercise 2 Input File

```
~Simulation Title Card
1,
STOMP Example Problem CO2-3 Exercise 2,
M.D. White,
Pacific Northwest Laboratory,
24 January 2012,
09:11 PST,
20,
Intercomparison of simulation models for CO2 disposal in
underground storage reservoirs.
Test Problem 7: CO2 Injection into a 2D Layered Brine Formation
This test problem is patterned after the CO2 injection project
at the Sleipner Vest field in the Norwegian sector of the North Sea,
and is intended to investigate the dominant physical processes
associated with the injection of supercritical CO2 into a layered
medium. Significant simplifications have been made, the most important
of which is the assumption of isothermal conditions (37 °C, the
ambient temperature of the formation). CO2 injection rates
(1,000,000 tonnes per year), system geometry, and system permeabilities
correspond approximately to those at Sleipner, although no attempt was
made to represent details of the permeability structure within the
host formation. Injection of the supercritical CO2, which is less
dense than the saline formation waters into which it is injected,
causes it to rise through the formation. Its rate of ascent, however,
is limited by the presence of four relatively low permeability shales.
The top and bottom of the formation is assumed to be impermeable.
The only reactive chemistry considered in this problem is the
dissolution of CO2 in the aqueous phase. (Pruess and Garcia, 2000).

~Solution Control Card
Normal,
STOMP-CO2,
1,
0,yr,2,yr,1.0,s,0.1,yr,1.25,16,1.e-06,
10000,
Variable Aqueous Diffusion,
Variable Gas Diffusion,
0,

~Grid Card
Cylindrical,
100,1,78,
```

```
0.0,m,2.0,m,4.1,m,6.3,m,8.6,m,11.1,m,
13.7,m,16.4,m,19.2,m,22.2,m,25.4,m,28.7,m,
32.2,m,35.8,m,39.7,m,43.8,m,48.0,m,52.5,m,
57.2,m,62.2,m,67.4,m,72.9,m,78.7,m,84.8,m,
91.2,m,97.9,m,105.0,m,112.4,m,120.2,m,128.5,m,
137.1,m,146.2,m,155.8,m,165.9,m,176.5,m,187.6,m,
199.4,m,211.7,m,224.7,m,238.3,m,252.7,m,267.8,m,
283.6,m,300.3,m,317.9,m,336.4,m,355.8,m,376.3,m,
397.8,m,420.4,m,444.2,m,469.2,m,495.5,m,523.2,m,
552.3,m,582.9,m,615.1,m,649.0,m,684.7,m,722.2,m,
761.6,m,803.1,m,846.7,m,892.6,m,940.8,m,991.6,m,
1045.0,m,1101.1,m,1160.2,m,1222.3,m,1287.7,m,1356.4,m,
1428.7,m,1504.8,m,1584.8,m,1668.9,m,1757.4,m,1850.5,m,
1948.4,m,2051.4,m,2159.7,m,2273.7,m,2393.5,m,2519.6,m,
2652.2,m,2791.6,m,2938.3,m,3092.6,m,3254.9,m,3425.6,m,
3605.2,m,3794.0,m,3992.7,m,4201.6,m,4421.4,m,4652.5,m,
4895.7,m,5151.4,m,5420.4,m,5703.4,m,6000.0,m,
0.0,deg,360.0,deg,
0.0,m,7@3.0,m,1@2.0,m,9@3.0,m,1@2.0,m,
3@1.0,m,
1@1.0,m,1@2.0,m,8@3.0,m,1@2.0,m,1@1.0,m,
3@1.0,m,
1@1.0,m,1@2.0,m,8@3.0,m,1@2.0,m,1@1.0,m,
3@1.0,m,
1@1.0,m,1@2.0,m,8@3.0,m,1@2.0,m,1@1.0,m,
3@1.0,m,
1@1.0,m,1@2.0,m,8@3.0,m,1@2.0,m,1@1.0,m,

~Rock/Soil Zonation Card
9,
Sands,1,100,1,1,1,18,
Shale,1,100,1,1,19,21,
Sands,1,100,1,1,22,33,
Shale,1,100,1,1,34,36,
Sands,1,100,1,1,37,48,
Shale,1,100,1,1,49,51,
Sands,1,100,1,1,52,63,
Shale,1,100,1,1,64,66,
Sands,1,100,1,1,67,78,

~Mechanical Properties Card
Sands,2650,kg/m^3,0.35,0.35,Compressibility,4.5e-10,1/Pa,,,Millington and Quirk,
Shale,2650,kg/m^3,0.1025,0.1025,Compressibility,4.5e-10,1/Pa,,,Millington and Quirk,

~Hydraulic Properties Card
Sands,3.e-12,m^2,3.e-12,m^2,3.e-12,m^2,
Shale,1.e-14,m^2,1.e-14,m^2,1.e-14,m^2,

~Saturation Function Card
Sands,van Genuchten,2.735,1/m,1.667,0.20,0.4,0.0,
Shale,van Genuchten,0.158,1/m,1.667,0.20,0.4,0.0,

~Aqueous Relative Permeability Card
Sands,Mualem Irreducible,0.4,0.20,
Shale,Mualem Irreducible,0.4,0.20,

~Gas Relative Permeability Card
Sands,van Genuchten,0.4,0.05,
```

```
Shale,van Genuchten,0.4,0.05,

~Salt Transport Card
Sands,0.0,m,0.0,m,
Shale,0.0,m,0.0,m,

~Initial Conditions Card
Gas Pressure,Aqueous Pressure,
4,
Gas Pressure,112.0525,Bar,,,,,-0.1001218,1/m,1,100,1,1,1,78,
Aqueous Pressure,112.0525,Bar,,,,,-0.1001218,1/m,1,100,1,1,1,78,
Temperature,37.0,C,,,,,,,1,100,1,1,1,78,
Salt Mass Fraction,0.032,,,,,,,,1,100,1,1,1,78,

~Boundary Conditions Card
1,
East,Aqueous Initial Condition,Gas Initial Condition,Aqueous Initial Condition,
100,100,1,1,1,78,1,
0,s,,,,,,,,,

~Source Card
4,
Gas Mass Rate,Water-Vapor Mass Fraction,1,1,1,1,1,7,1,
0,s,112.0525,bar,1.8288,kg/s,0.0,
Gas Mass Rate,Water-Vapor Mass Fraction,1,1,1,1,8,8,1,
0,s,112.0525,bar,1.2192,kg/s,0.0,
Gas Mass Rate,Water-Vapor Mass Fraction,1,1,1,1,9,17,1,
0,s,112.0525,bar,1.8288,kg/s,0.0,
Gas Mass Rate,Water-Vapor Mass Fraction,1,1,1,1,18,18,1,
0,s,112.0525,bar,1.2192,kg/s,0.0,

~Output Options Card
4,
1,1,8,
1,1,18,
1,1,33,
1,1,48,
1,1,s,m,deg,6,6,6,
8,
Gas Saturation,,
CO2 Gas Mass Fraction,,
CO2 Aqueous Mass Fraction,,
Gas Pressure,Pa,
Aqueous Density,kg/m^3,
Integrated CO2 Mass,kg,
Integrated Aqueous CO2 Mass,kg,
Integrated Gas CO2 Mass,kg,
2,
30,day,
1,year,
7,
Gas Saturation,,
CO2 Gas Mass Fraction,,
CO2 Aqueous Mass Fraction,,
Gas Pressure,Pa,
Diffusive Porosity,,
Gas Density,kg/m^3,
Aqueous Density,kg/m^3,
```

```
~Surface Flux Card
5,
Total CO2 Flux,kg/s,kg,Top,1,100,1,1,18,18,
Total CO2 Flux,kg/s,kg,Top,1,100,1,1,21,21,
Total CO2 Flux,kg/s,kg,Top,1,100,1,1,36,36,
Total CO2 Flux,kg/s,kg,Top,1,100,1,1,51,51,
Total CO2 Flux,kg/s,kg,Top,1,100,1,1,66,66,
```

Exercise 3 (193z) Input File

```
~Simulation Title Card
1,
STOMP Example Problem CO2-3: 193z,
M.D. White,
Pacific Northwest Laboratory,
24 January 2012,
09:11 PST,
20,
Intercomparison of simulation models for CO2 disposal in
underground storage reservoirs.
Test Problem 7: CO2 Injection into a 2D Layered Brine Formation
This test problem is patterned after the CO2 injection project
at the Sleipner Vest field in the Norwegian sector of the North Sea,
and is intended to investigate the dominant physical processes
associated with the injection of supercritical CO2 into a layered
medium. Significant simplifications have been made, the most important
of which is the assumption of isothermal conditions (37 °C, the
ambient temperature of the formation). CO2 injection rates
(1,000,000 tonnes per year), system geometry, and system permeabilities
correspond approximately to those at Sleipner, although no attempt was
made to represent details of the permeability structure within the
host formation. Injection of the supercritical CO2, which is less
dense than the saline formation waters into which it is injected,
causes it to rise through the formation. Its rate of ascent, however,
is limited by the presence of four relatively low permeability shales.
The top and bottom of the formation is assumed to be impermeable.
The only reactive chemistry considered in this problem is the
dissolution of CO2 in the aqueous phase. (Pruess and Garcia, 2000).

~Solution Control Card
Normal,
STOMP-CO2,
1,
0,yr,2,yr,1.0,s,0.1,yr,1.25,16,1.e-06,
10000,
Variable Aqueous Diffusion,
Variable Gas Diffusion,
0,

~Grid Card
Cartesian,
100,1,193,
0.0,m,2.0,m,4.1,m,6.3,m,8.6,m,11.1,m,
13.7,m,16.4,m,19.2,m,22.2,m,25.4,m,28.7,m,
32.2,m,35.8,m,39.7,m,43.8,m,48.0,m,52.5,m,
57.2,m,62.2,m,67.4,m,72.9,m,78.7,m,84.8,m,
```

```
91.2,m,97.9,m,105.0,m,112.4,m,120.2,m,128.5,m,
137.1,m,146.2,m,155.8,m,165.9,m,176.5,m,187.6,m,
199.4,m,211.7,m,224.7,m,238.3,m,252.7,m,267.8,m,
283.6,m,300.3,m,317.9,m,336.4,m,355.8,m,376.3,m,
397.8,m,420.4,m,444.2,m,469.2,m,495.5,m,523.2,m,
552.3,m,582.9,m,615.1,m,649.0,m,684.7,m,722.2,m,
761.6,m,803.1,m,846.7,m,892.6,m,940.8,m,991.6,m,
1045.0,m,1101.1,m,1160.2,m,1222.3,m,1287.7,m,1356.4,m,
1428.7,m,1504.8,m,1584.8,m,1668.9,m,1757.4,m,1850.5,m,
1948.4,m,2051.4,m,2159.7,m,2273.7,m,2393.5,m,2519.6,m,
2652.2,m,2791.6,m,2938.3,m,3092.6,m,3254.9,m,3425.6,m,
3605.2,m,3794.0,m,3992.7,m,4201.6,m,4421.4,m,4652.5,m,
4895.7,m,5151.4,m,5420.4,m,5703.4,m,6000.0,m,
0.0,m,1.0,m,
0.0,m,1@0.5,m,51@1.0,m,1@0.5,m,
1@0.5,m,2@1.0,m,1@0.5,m,
1@0.5,m,29@1.0,m,1@0.5,m,
1@0.5,m,2@1.0,m,1@0.5,m,
1@0.5,m,29@1.0,m,1@0.5,m,
1@0.5,m,2@1.0,m,1@0.5,m,
1@0.5,m,29@1.0,m,1@0.5,m,
1@0.5,m,2@1.0,m,1@0.5,m,
1@0.5,m,29@1.0,m,1@0.5,m,

~Rock/Soil Zonation Card
9,
Sands,1,100,1,1,1,53,
Shale,1,100,1,1,54,57,
Sands,1,100,1,1,58,88,
Shale,1,100,1,1,89,92,
Sands,1,100,1,1,93,123,
Shale,1,100,1,1,124,127,
Sands,1,100,1,1,128,158,
Shale,1,100,1,1,159,162,
Sands,1,100,1,1,163,193,

~Mechanical Properties Card
Sands,2650,kg/m^3,0.35,0.35,Compressibility,4.5e-10,1/Pa,,,Millington and Quirk,
Shale,2650,kg/m^3,0.1025,0.1025,Compressibility,4.5e-10,1/Pa,,,Millington and Quirk,

~Hydraulic Properties Card
Sands,3.e-12,m^2,3.e-12,m^2,3.e-12,m^2,
Shale,1.e-14,m^2,1.e-14,m^2,1.e-14,m^2,

~Saturation Function Card
Sands,van Genuchten,2.735,1/m,1.667,0.20,0.4,0.0,
Shale,van Genuchten,0.158,1/m,1.667,0.20,0.4,0.0,

~Aqueous Relative Permeability Card
Sands,Mualem Irreducible,0.4,0.20,
Shale,Mualem Irreducible,0.4,0.20,

~Gas Relative Permeability Card
Sands,van Genuchten,0.4,0.05,
Shale,van Genuchten,0.4,0.05,

~Salt Transport Card
Sands,0.0,m,0.0,m,
```

```
Shale,0.0,m,0.0,m,

~Initial Conditions Card
Gas Pressure,Aqueous Pressure,
4,
Gas Pressure,112.17765,Bar,,,,,-0.1001218,1/m,1,100,1,1,1,193,
Aqueous Pressure,112.17765,Bar,,,,,-0.1001218,1/m,1,100,1,1,1,193,
Temperature,37.0,C,,,,,,,1,100,1,1,1,193,
Salt Mass Fraction,0.032,,,,,,,,1,100,1,1,1,193,

~Boundary Conditions Card
1,
East,Aqueous Initial Condition,Gas Initial Condition,Aqueous Initial Condition,
100,100,1,1,1,193,1,
0,s,,,,,,,,,

~Source Card
1,
Gas Mass Rate,Water-Vapor Mass Fraction,1,1,1,1,23,23,1,
0,s,110,bar,0.1585,kg/s,0.0,

~Output Options Card
4,
1,1,23,
1,1,53,
1,1,54,
1,1,88,
1,1,s,m,6,6,6,
8,
Gas Saturation,,
CO2 Gas Mass Fraction,,
CO2 Aqueous Mass Fraction,,
Gas Pressure,Pa,
Aqueous Density,kg/m^3,
Integrated CO2 Mass,kg,
Integrated Aqueous CO2 Mass,kg,
Integrated Gas CO2 Mass,kg,
2,
30,day,
1,year,
7,
Gas Saturation,,
CO2 Gas Mass Fraction,,
CO2 Aqueous Mass Fraction,,
Gas Pressure,Pa,
Diffusive Porosity,,
Gas Density,kg/m^3,
Aqueous Density,kg/m^3,


~Surface Flux Card
5,
Total CO2 Flux,kg/s,kg,Top,1,100,1,1,53,53,
Total CO2 Flux,kg/s,kg,Top,1,100,1,1,57,57,
Total CO2 Flux,kg/s,kg,Top,1,100,1,1,92,92,
Total CO2 Flux,kg/s,kg,Top,1,100,1,1,127,127,
Total CO2 Flux,kg/s,kg,Top,1,100,1,1,162,162,
```

Solutions to Selected Exercises

Exercise 3

To examine whether the simulation results were dependent on the selected vertical grid spacing, a second simulation was conducted that used more nodes in the vertical direction. This domain used uniform 1-m vertical grid spacing with 0.5-m grid spacing at the sand-shale interfaces. The complete 193z input file is shown above. The gas saturation distribution at 2 years is shown in Figure 9. Comparing this profile with that from the 78z simulation reveals only slight changes in the gas saturation distribution, with more extension of the gas phase beneath the shale layers. Simulation results for the distribution of CO_2 mass between phases and sands layers also show only slight differences compared to the 78z simulation. As the differences in the simulation results between the 78z and 193z simulations are only slight, the 78z simulations are considered to have sufficient grid resolution.

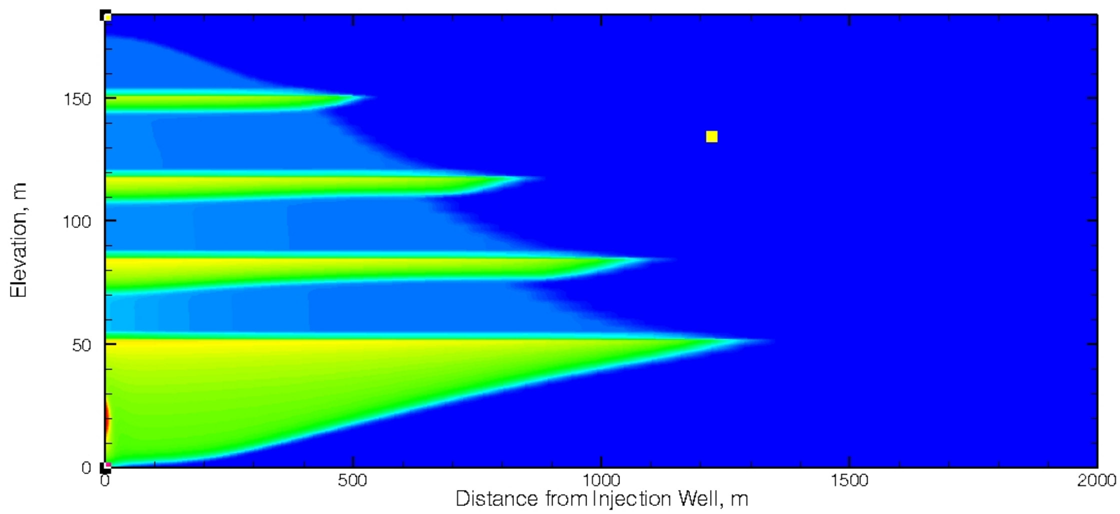

Figure 9. Gas saturation profiles from STOMP-CO2 at 2 years