# Example Problem CO2E-1

# Non-Isothermal Effects on $CO_2$ Plume Evolution and Leakage through an Abandoned Well (Stuttgart #1)

**Abstract**: *Non-isothermal effects on $CO_2$ plume evolution and leakage through an abandoned well are investigated. This problem is based on Problem 1 of the benchmark study first presented at the Workshop on Numerical Models for $CO_2$ Storage in Geological Formations in Stuttgart, Germany, and focuses on injection scenarios in deep geologic formations (Class, et al., 2009). $CO_2$ is injected into a reservoir where it spreads, and upon reaching a leaky well, rises up to a shallower aquifer.*

## Problem Description

This benchmark problem is developed using (Nordbotten and Celia, 2004; Nordbotten et al., 2004; and Nordbotten et al., 2005) as references. A description and discussion of the problem have been published in (Ebigo et al., 2007). It addresses the simulation of the advective spreading of $CO_2$ injected into an aquifer, which is obviously an important process since it determines the distribution of $CO_2$ in the aquifer over time. A second topic addressed by the problem set-up is the leakage of $CO_2$ from the aquifer through an abandoned and leaky well. The reference problems developed at the Stuttgart workshop are posed as three-dimensional domains. To reduce the execution time required to complete the simulations, the problems have been recast using a two dimensional domain; which results in the radial flow impacts being lost. This yields much higher leakage rates for the two dimensional domain, but the processes observed and modeled are very similar between the two- and three-dimensional domains.

$CO_2$ is injected into an aquifer; spreads within the aquifer and, upon reaching a leaky well, rises up to a shallower aquifer. The goal of the simulation is quantification of the leakage rate which depends on the pressure build-up in the aquifer due to injection and on the plume evolution. This scenario is shown in Figure 1. The reference simulation domain had a lateral extent of 1,000 × 1,000 m. The recast simulation domain has a lateral extent of 1400 m x 1 m. At the lateral boundaries, constant boundary conditions are imposed on the system. The cross boundaries are assumed to be zero flux and adiabatic. The leaky well is at the center of the domain and the injection well is 100 m away. Both aquifers are 30-m thick and the aquitard has a thickness of 100 m. The leaky well is modeled as a porous medium with a higher permeability than the formation.

Two cases in the benchmark study are of interest (problem 1.1 and problem 1.2). In problem 1.1, the aquifer is very deep (2,840-3,000 m), which allows a number of simplifying assumptions to be made as the $CO_2$ remains in a supercritical state. The principal assumption is the use of fixed aqueous and $scCO_2$ density and viscosity. The first exercise in problem 1.1 involves relaxing this assumption and using variable fluid densities and viscosities, which are calculated internally by STOMP-CO2e. Because heat transfer is not important in this problem, STOMP-CO2e is used with the isothermal option. This saves on computational time, and requires less input parameters. In problem 1.2, the aquifer is much shallower (640-800 m) and the $CO_2$ can change state while rising to the top aquifer. Therefore, heat transfer becomes important in the solution of this problem, and STOMP-CO2e is used in full nonisothermal mode. The reference problem 1.2 creates conditions in the domain that include supercritical $CO_2$, liquid $CO_2$, and gaseous $CO_2$. In recasting the problem, the bottom temperature was elevated 2˚C to eliminate the possibility of liquid $CO_2$ conditions.

The reference problem 1.1 used constant properties for $scCO_2$ density (479 kg/m$^3$), brine density (1,045 kg/m$^3$), $scCO_2$ viscosity (3.95 x $10^{-5}$ Pa s), and brine viscosity (2.535 x $10^{-4}$ Pa s). Fluid density and viscosity in STOMP-CO2e are computed as a function of temperature, pressure, and composition. To bypass this standard approach, an option was added to STOMP-CO2e to read in fluid density and viscosity from the input file. The option is invoked using the key words "Invariant Fluid Density and Viscosity" in the *Solution Control Card*, and then entering property values for fluid aqueous density and viscosity and $scCO2_2$ density and viscosity. The reference problem 1.1 additionally uses linear relationships for the aqueous and gas relative permeability versus saturation functions and no capillary pressure. The STOMP-CO2e simulator requires a finite capillary pressure to execute. A low entry pressure head of 0.1 m, was used to model the zero capillary pressure condition.

This problem comprises four simulations; one base case and three exercises. The base-case simulation (the analog of the Stuttgart 1.1 problem) is an isothermal simulation of the $CO_2$ injection into a deep two-dimensional saline reservoir, with a leaky well 100-m from the injection well. Fixed fluid properties are used, along with linear forms for relative permeability-saturation functions. The first exercise involves using variable fluid density and viscosity and comparing the leakage rates against the base case. The second exercise involves converting the grid spacing in the injection reservoir to be uniform and comparing the injection rates and first arrival times. The third exercise (the analog of the Stuttgart 1.2 problem) involves decreasing the injection reservoir depth and then running the simulation as a non-isothermal simulation and comparing the leakage rates against the original rates for the base-case problem. The base-case and third-exercise input files are shown below.

This problem involves two aquifers separated vertically by an impermeable aquitard with a leaky well connecting the two aquifers, as shown in Figure 1. The most efficient way to model this problem in STOMP is to treat the aquitard as being inactive, as shown in the *Inactive Nodes Card*. A vertical string of active nodes at (i = 50) was reserved for the leaky well. Two rock/soil types were defined, first the entire domain, including the inactive nodes, were specified as being type "aquifer," and then the leaky well nodes were specified as being type "leaky well." The domain depth is specified via pressures in the *Initial Conditions Card*, not by altering the dimensions of the domain. For the deeper system gas and aqueous pressures are set to yield hydrostatic conditions with a pressure of 30.86 MPa at the bottom of the domain. For the shallower system initial pressures used a pressure of 8.499 MPa at the bottom of the domain. Boundary conditions on the west and east faces were set to be in equilibrium with the initial pressure fields, allowing flow of brine and sc$CO_2$ across the boundary surface. All other boundaries are no- flow boundaries.

Injection of $CO_2$ into the system was specified using the coupled well model, which allows the user to specify both an injection rate and a maximum injection pressure. This well model will solve for the injection pressure, if the injection rate can be met without exceeding the maximum injection pressure. Otherwise the well is considered to be pressure controlled and the injection rate becomes the unknown at the maximum injection pressure. An injection rate of 0.025 kg/s was selected for this problem to mimic the reference Stuttgart problem. The maximum injection pressure of 45 MPa was sufficiently high to avoid pressure-controlled conditions in the well. Simulation time for both problems is 1,000 days.

The output of interest is the $CO_2$ leakage through the leaky well as a function of time. This is defined here as the $CO_2$ mass flow at midway between top and bottom aquifers divided by the injection rate, in percent. The flow of $CO_2$ was tracked by requesting $CO_2$ mass flux across the top surface of the node just below the midpoint in the vertical leaky well, via the *Surface Flux Card*. Plot file requests were made to enable the plotting of the plume development and temperature evolution over time.

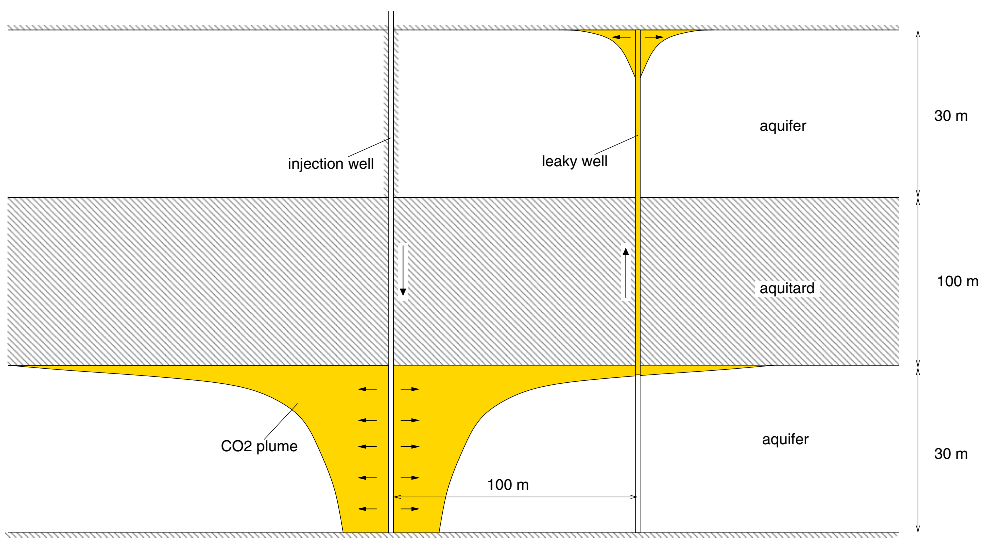


**Figure 1**. Leakage Scenario (from Class et al., 2009)

The leakage rate of $CO_2$ through the leaky well, midway through the aquitard, is shown in Figure 2. This result differs significantly from the Stuttgart 1.1 reference problem, in terms of the percent of $scCO_2$ leaking through the well, principally due to the change from a 3- to 2-dimensional geometry. In the reference problem the maximum leakage percent is 0.25%; whereas, in the 2-dimensional problem the leakage rate approaches 50% of the injection rate. A STOMP-CO2 simulation of the 3-dimensional problem yields results that are similar to those published for the reference problem. The $scCO_2$ gas saturation after 500 days is shown in Figures 3; where the vertical to horizontal scale is 5:1. After a delay of about 10 days, the flux of $scCO_2$ through the leaky well rises sharply and then reaches a plateau, once more steady flow conditions are reached. At 1,000 days $scCO_2$ is migrating across the lateral boundaries in both the lower and upper aquifers.

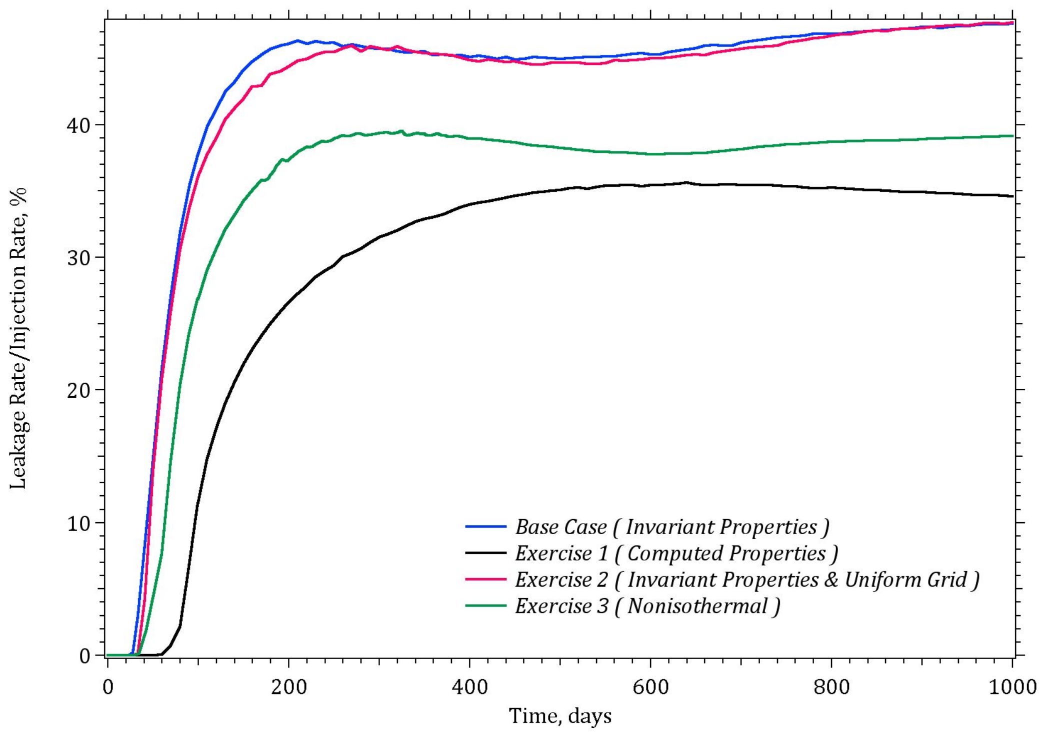


**Figure 2**. Leakage rate through the leaky-well for the Base-Case, Exercise 1, Exercise 2, and Exercise 3 simulations.

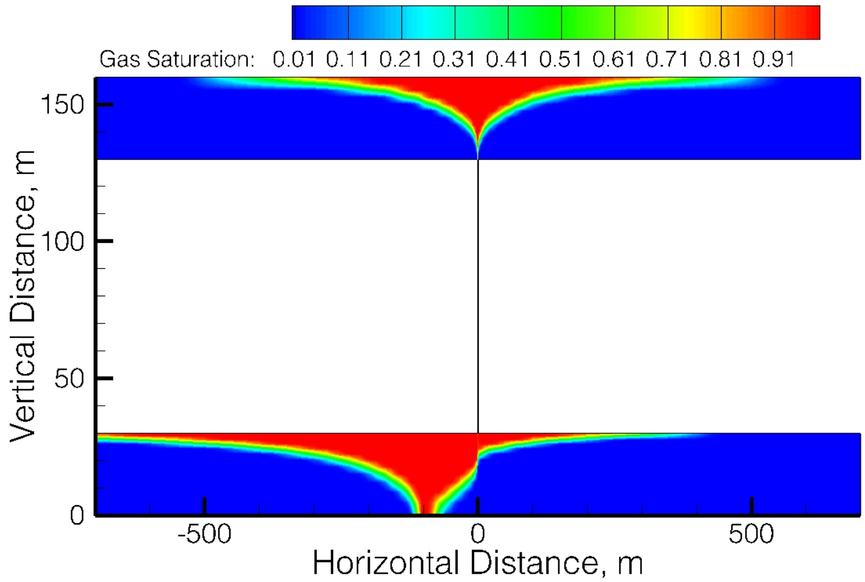


**Figure 3**. sc$CO_2$ saturation profile after 500 days for the Base Case simulation

*References*

Class, H., A. Ebigbo, R. Helmig, H. K. Dahle, J. M. Nordbotten, M. A. Celia, P. Audigane, M. Darcis, J. Ennis-King, Y. Fan, B. Flemisch, S. E. Gasda, M. Jin · S. Krug, D. Labregere, A. N. Beni, R. J. Pawar, A. Sbai, S. G. Thomas, L. Trenty, L. Wei. 2009. "A benchmark study on problems related to CO2 storage in geologic formations," *Comput. Geosci.*, 13:409-434.

Ebigbo, A., Class, H., Helmig, R. 2007. "CO2 leakage through an abandoned well: problem-oriented benchmarks," *Comput. Geosci.*, 11:103–115.

Nordbotten, J.M., Celia, M.A. 2006. "Similarity solutions for fluid injection into confined aquifers," *J. Fluid Mech.*, 561:307–327.

Nordbotten, J.M., Celia, M.A., Bachu, S. 2004. "Analytical solutions for leakage rates through abandoned wells," *Water Resour. Res.*, 40(4), W04204.

Nordbotten, J.M., Celia, M.A., Bachu, S., Dahle, H. 2005. "Semi-analytical solution for CO2 leakage through an abandoned well," *Environ. Sci. Technol.*, 39(2):602–611.

## Exercises

1. (Basic) Repeat the base-case simulation with internally computed properties for fluid density and viscosity.
2. (Moderate) Repeat the base-case problem with a uniform grid spacing of 5.0 m in the vertical direction. This exercise requires changing grid indices in several cards.

3. (Difficult) Repeat the exercise 1 problem with the bottom of the domain moved from a depth of 3,000 m to 800 m, and consider the impact of non-isothermal conditions.

# Input Files

## Base-Case Simulation Input File

```
~Simulation Title Card
1,
STOMP Example Problem CO2e-1,
Mark White,
Pacific Northwest Laboratory,
01 June 2011,
09:37 PDT,
8,
2.1 Definition of benchmark problem 1: CO2 plume evolution and
leakage through an abandoned well
2.1.1 Formulated by A. Ebigbo, J. Nordbotten and H. Class
Problem description CO2 is injected into an aquifer; spreads within the
aquifer and, upon reaching a leaky well, rises up to a shallower
aquifer. A quantification of the leakage rate which depends on the
pressure build- up in the aquifer due to injection and on the plume
evolution is the goal of the simulation.

~Solution Control Card
Normal,
STOMP-CO2e Isothermal w/ Invariant Fluid Density and Viscosity,
1,
0,day,1000,day,1,s,10,day,1.25,16,1.e-06,0.001,s,0.2,
10000,
Variable Aqueous Diffusion,
Variable Gas Diffusion,
1045,kg/m^3,2.535e-4,Pa s,479,kg/m^3,3.950e-5,Pa s,
0,

~Grid Card
Cartesian,
89,1,44,
-700.000,m,-675.000,m,-650.000,m,-625.000,m,
-600.000,m,-575.000,m,-550.000,m,-525.000,m,
-500.000,m,-475.000,m,-450.000,m,-425.000,m,-400.000,m,-375.000,m,
-350.000,m,-325.000,m,-300.000,m,-275.000,m,-255.000,m,-235.000,m,
-215.000,m,-200.000,m,-185.000,m,-170.000,m,-160.000,m,-150.000,m,
-140.000,m,-130.000,m,-122.500,m,-115.000,m,-107.500,m,-102.500,m,
-97.500,m,-92.500,m,-85.000,m,-77.500,m,-70.000,m,-60.000,m,
-50.000,m,-40.000,m,-30.000,m,-20.000,m,-12.500,m,-8.000,m,
-5.000,m,-2.800,m,-1.500,m,-0.800,m,-0.400,m,-0.133,m,
0.133,m,0.400,m,0.800,m,1.500,m,2.800,m,5.000,m,
8.000,m,12.500,m,20.000,m,30.000,m,40.000,m,50.000,m,
60.000,m,70.000,m,85.000,m,100.000,m,125.000,m,150.000,m,
175.000,m,200.000,m,225.000,m,250.000,m,275.000,m,300.000,m,
325.000,m,350.000,m,375.000,m,400.000,m,425.000,m,450.000,m,
475.000,m,500.000,m,525.000,m,550.000,m,575.000,m,600.000,m,
```

```
625.000,m,650.000,m,675.000,m,700.000,m,
0.000,m,1.000,m,
0.0,m,4.41,m,8.32,m,11.80,m,14.90,m,17.65,m,20.09,m,22.27,m,24.20,m,
25.92,m,27.44,m,28.80,m,30.0,m,20@5.000,m,12@2.500,m,

~Inactive Nodes Card
2,
1,49,1,1,13,32,
51,89,1,1,13,32,

~Rock/Soil Zonation Card
2,
aquifer,1,89,1,1,1,44,
leaky well,50,50,1,1,1,44,

~Mechanical Properties Card
aquifer,2650,kg/m^3,0.15,0.15,Compressibility,1.e-9,1/psi,,,constant,1.0,1.0,
leaky well,2650,kg/m^3,0.15,0.15,Compressibility,1.e-9,1/psi,,,constant,1.0,1.0,

~Hydraulic Properties Card
aquifer,2.e-14,m^2,2.e-14,m^2,2.e-14,m^2,
leaky well,1.e-12,m^2,1.e-12,m^2,1.e-12,m^2,


~Saturation Function Card
aquifer,Brooks and Corey,0.1,m,2.0,,,
leaky well,Brooks and Corey,0.1,m,2.0,,,

~Aqueous Relative Permeability Card
aquifer,tabular,2,
0.0,0.0,
1.0,1.0,
leaky well,tabular,2,
0.0,0.0,
1.0,1.0,

~Gas Relative Permeability Card
aquifer,tabular,2,
0.0,0.0,
1.0,1.0,
leaky well,tabular,2,
0.0,0.0,
1.0,1.0,

~Salt Transport Card
aquifer,0.0,ft,0.0,ft,
leaky well,0.0,ft,0.0,ft,

~Initial Conditions Card
Gas Pressure,Aqueous Pressure,
3,
Gas Pressure,30.81955,MPa,,,,,-0.01025,1/m,1,89,1,1,1,44,
Aqueous Pressure,30.81955,MPa,,,,,-0.01025,1/m,1,89,1,1,1,44,
Temperature,34,C,,,,,,,1,89,1,1,1,44,

~Boundary Conditions Card
2,
West,Aqu. Initial Condition,Gas Initial Condition,Aqu. Mass Frac.,
```

```
1,1,1,1,1,44,1,
0,s,,,,,,,0.0,,,,
East,Aqu. Initial Condition,Gas Initial Condition,Aqu. Mass Frac.,
89,89,1,1,1,44,1,
0,s,,,,,,,0.0,,,,

~Coupled Well Card
1,
CO2 Injection Well,Water Relative Saturation,1.0,0.5,1.0,0.383184,MMT,
1,
-100.0,m,0.5,m,30.0,m,-100.0,m,0.5,m,0.0,m,0.15,m,0.0,screened,
1,
0.0,hr,0.025,kg/s,45,MPa,0.0,
#0.0,hr,4.435,kg/s,45,MPa,0.0,

~Output Options Card
5,
32,1,1,
32,1,12,
50,1,12,
50,1,22,
50,1,33,
1,1,day,m,6,6,6,
16,
Phase Condition,,
Gas Saturation,,
Gas Relative Permeability,,
#Trapped Gas Saturation,,
Integrated CO2 Mass,kg,
Integrated CO2 Aqueous Mass,kg,
Integrated CO2 Gas Mass,kg,
Integrated CO2 Trapped-Gas Mass,kg,
Salt Aqueous Mass Fraction,,
CO2 Aqueous Mass Fraction,,
Gas Density,kg/m^3,
Aqueous Density,kg/m^3,
Gas Viscosity,Pa s,
Aqueous Viscosity,Pa s,
Gas Pressure,MPa,
Aqueous Pressure,MPa,
#Diffusive Porosity,,
Coupled-Well Press,1,MPa,
#Coupled-Well CO2 Mass Rate,1,kg/s,
#Coupled-Well CO2 Mass Integral,1,kg,
8,
0.1,day,
0.5,day,
1.0,day,
5.0,day,
10.0,day,
50.0,day,
100.0,day,
500.0,day,
13,
Rock/Soil Type,,
Gas Saturation,,
Trapped Gas Saturation,,
Salt Saturation,,
```

```
CO2 Aqueous Concentration,gm/cm^3,
Salt Aqueous Mass Fraction,,
CO2 Aqueous Mass Fraction,,
Gas Pressure,MPa,
Aqueous Pressure,MPa,
Diffusive Porosity,,
Gas Density,kg/m^3,
Aqueous Density,kg/m^3,
Phase Condition,,

~Surface Flux Card
1,
CO2 Mass Flux,kg/s,kg,top,50,50,1,1,22,22,
```

## Exercise 3 (Non-isothermal) Input File

```
~Simulation Title Card
1,
STOMP Example Problem CO2e-1: Exercise 3,
Mark White,
Pacific Northwest Laboratory,
01 June 2011,
09:37 PDT,
8,
2.1 Definition of benchmark problem 1: CO2 plume evolution and
leakage through an abandoned well
2.1.1 Formulated by A. Ebigbo, J. Nordbotten and H. Class
Problem description CO2 is injected into an aquifer; spreads within the
aquifer and, upon reaching a leaky well, rises up to a shallower
aquifer. A quantification of the leakage rate which depends on the
pressure build- up in the aquifer due to injection and on the plume
evolution is the goal of the simulation.

~Solution Control Card
Normal,
STOMP-CO2e,
1,
0,day,1000,day,1,s,10,day,1.25,16,1.e-06,0.001,s,0.2,
10000,
Variable Aqueous Diffusion,
Variable Gas Diffusion,
0,

~Grid Card
Cartesian,
89,1,44,
-700.000,m,-675.000,m,-650.000,m,-625.000,m,
-600.000,m,-575.000,m,-550.000,m,-525.000,m,
-500.000,m,-475.000,m,-450.000,m,-425.000,m,-400.000,m,-375.000,m,
-350.000,m,-325.000,m,-300.000,m,-275.000,m,-255.000,m,-235.000,m,
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-140.000,m,-130.000,m,-122.500,m,-115.000,m,-107.500,m,-102.500,m,
-97.500,m,-92.500,m,-85.000,m,-77.500,m,-70.000,m,-60.000,m,
-50.000,m,-40.000,m,-30.000,m,-20.000,m,-12.500,m,-8.000,m,
-5.000,m,-2.800,m,-1.500,m,-0.800,m,-0.400,m,-0.133,m,
0.133,m,0.400,m,0.800,m,1.500,m,2.800,m,5.000,m,
8.000,m,12.500,m,20.000,m,30.000,m,40.000,m,50.000,m,
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325.000,m,350.000,m,375.000,m,400.000,m,425.000,m,450.000,m,
475.000,m,500.000,m,525.000,m,550.000,m,575.000,m,600.000,m,
625.000,m,650.000,m,675.000,m,700.000,m,
0.000,m,1.000,m,
0.0,m,4.41,m,8.32,m,11.80,m,14.90,m,17.65,m,20.09,m,22.27,m,24.20,m,
25.92,m,27.44,m,28.80,m,30.0,m,20@5.000,m,12@2.500,m,

~Inactive Nodes Card
2,
1,49,1,1,13,32,
51,89,1,1,13,32,

~Rock/Soil Zonation Card
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aquifer,1,89,1,1,1,44,
leaky well,50,50,1,1,1,44,

~Mechanical Properties Card
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leaky well,2650,kg/m^3,0.15,0.15,Compressibility,1.e-9,1/psi,,,constant,1.0,1.0,


~Hydraulic Properties Card
aquifer,2.e-14,m^2,2.e-14,m^2,2.e-14,m^2,
leaky well,1.e-12,m^2,1.e-12,m^2,1.e-12,m^2,

~Saturation Function Card
aquifer,Brooks and Corey,0.1,m,2.0,,,
leaky well,Brooks and Corey,0.1,m,2.0,,,

~Aqueous Relative Permeability Card
aquifer,tabular,2,
0.0,0.0,
1.0,1.0,
leaky well,tabular,2,
0.0,0.0,
1.0,1.0,

~Gas Relative Permeability Card
aquifer,tabular,2,
0.0,0.0,
1.0,1.0,
leaky well,tabular,2,
0.0,0.0,
1.0,1.0,

~Thermal Properties Card
aquifer,parallel,0.582,W/m K,0.582,W/m K,0.582,W/m K,1000,J/kg K,
leaky well,parallel,0.582,W/m K,0.582,W/m K,0.582,W/m K,1000,J/kg K,

~Salt Transport Card
aquifer,0.0,ft,0.0,ft,
leaky well,0.0,ft,0.0,ft,

~Initial Conditions Card
Gas Pressure,Aqueous Pressure,
```

```
3,
Gas Pressure,8.45855,MPa,,,,,-0.01025,1/m,1,89,1,1,1,44,
Aqueous Pressure,8.45855,MPa,,,,,-0.01025,1/m,1,89,1,1,1,44,
Temperature,36.93385,C,,,,,-0.03,1/m,1,89,1,1,1,44,

~Boundary Conditions Card
4,
West,Energy Initial Condition,Aqu. Initial Condition,Gas Initial Condition,Aqu. Mass Frac.,
1,1,1,1,1,44,1,
0,s,,,,,,,,0.0,,,,
East,Energy Initial Condition,Aqu. Initial Condition,Gas Initial Condition,Aqu. Mass Frac.,
89,89,1,1,1,44,1,
0,s,,,,,,,,0.0,,,,
Bottom,Energy Dirichlet,Aqu. Zero Flux,Gas Zero Fluxn,Aqu. Mass Frac.,
1,89,1,1,1,1,1,
0,s,37.0,C,,,,,,0.0,,,,
Top,Energy Dirichlet,Aqu. Zero Flux,Gas Zero Fluxn,Aqu. Mass Frac.,
1,89,1,1,44,44,1,
0,s,32.2,C,,,,,,0.0,,,,



~Coupled Well Card
1,
CO2 Injection Well,Water Relative Saturation,1.0,0.5,1.0,0.383184,MMT,
1,
-100.0,m,0.5,m,30.0,m,-100.0,m,0.5,m,0.0,m,0.15,m,0.0,screened,
1,
0.0,hr,0.025,kg/s,45,MPa,0.0,33.6,C,

~Output Options Card
5,
32,1,1,
32,1,12,
50,1,12,
50,1,22,
50,1,33,
1,1,day,m,6,6,6,
16,
Temperature,C,
Gas Saturation,,
Gas Relative Permeability,,
#Trapped Gas Saturation,,
Integrated CO2 Mass,kg,
Integrated CO2 Aqueous Mass,kg,
Integrated CO2 Gas Mass,kg,
Integrated CO2 Trapped-Gas Mass,kg,
Salt Aqueous Mass Fraction,,
CO2 Aqueous Mass Fraction,,
Gas Density,kg/m^3,
Aqueous Density,kg/m^3,
Gas Viscosity,Pa s,
Aqueous Viscosity,Pa s,
Gas Pressure,MPa,
Aqueous Pressure,MPa,
#Diffusive Porosity,,
Coupled-Well Press,1,MPa,
#Coupled-Well CO2 Mass Rate,1,kg/s,
```

```
#Coupled-Well CO2 Mass Integral,1,kg,
8,
0.1,day,
0.5,day,
1.0,day,
5.0,day,
10.0,day,
50.0,day,
100.0,day,
500.0,day,
13,
Temperature,C,
Gas Saturation,,
Trapped Gas Saturation,,
Salt Saturation,,
CO2 Aqueous Concentration,gm/cm^3,
Salt Aqueous Mass Fraction,,
CO2 Aqueous Mass Fraction,,
Gas Pressure,MPa,
Aqueous Pressure,MPa,
Diffusive Porosity,,
Gas Density,kg/m^3,
Aqueous Density,kg/m^3,
Phase Condition,,

~Surface Flux Card
1,
CO2 Mass Flux,kg/s,kg,top,50,50,1,1,22,22,
```

## Solution to Selected Exercises

### Exercise 1

sc$CO_2$ density and viscosity computed internally were in the 950 kg/m$^3$ and 1.05x10$^{-4}$ Pa-s, ranges for the pressure and temperature conditions of the problem, which differ significantly from those used in the base-case simulation of 479 kg/m$^3$ and 3.95x10$^{-5}$ Pa-s. This results in reduced bouyancy forces, yielding lower leakage rates, as shown in the leakage rate plot (Figure 2) and the gas saturation profile at 500 days in Figure 4.

### Exercise 2

In the 3-dimensional simulation of the reference Stuttgart problem it was found that the vertical grid spacing was critical to computing the proper leakage rates. Coarse grid spacing allow the underside of the aquitard yielded delayed arrival times for $CO_2$ in the leaky well and reduced peak leakage rates. For the 2-dimensional domain the impact of the grid resolution is far less, as shown in the leakage rate plot (Figure 2) and the gas saturation profile at 500 days in Figure 5. The lack of a radial flow impact is the principal reason for the reduce impact of the grid. The 3-dimensional simulation, however, strongly demonstrates the importance of grid convergence on simulation results.

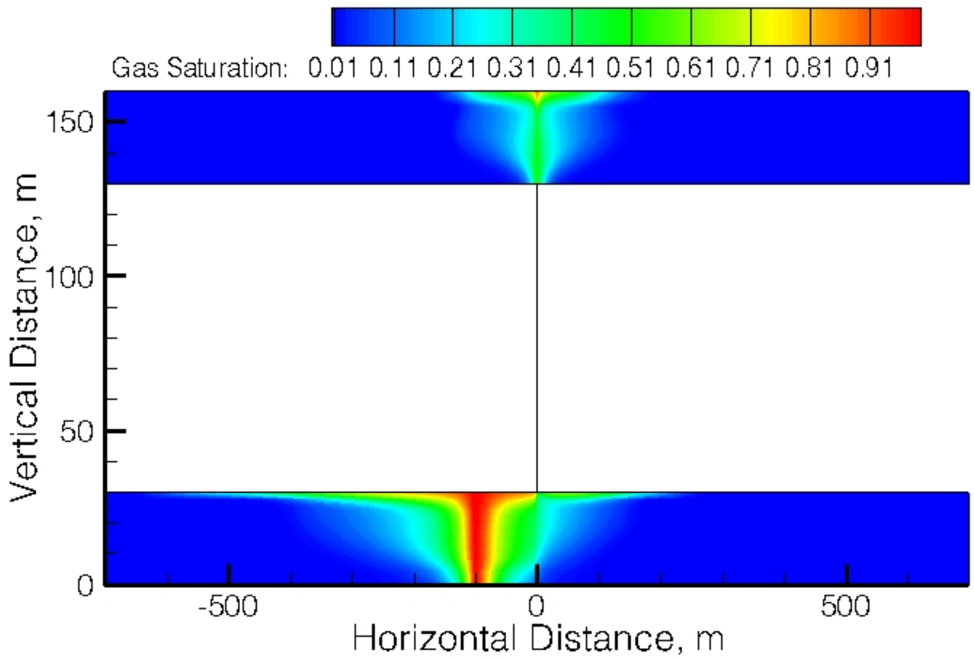


**Figure 4**. $scCO_2$ saturation profile after 500 days for the Exercise 1 simulation

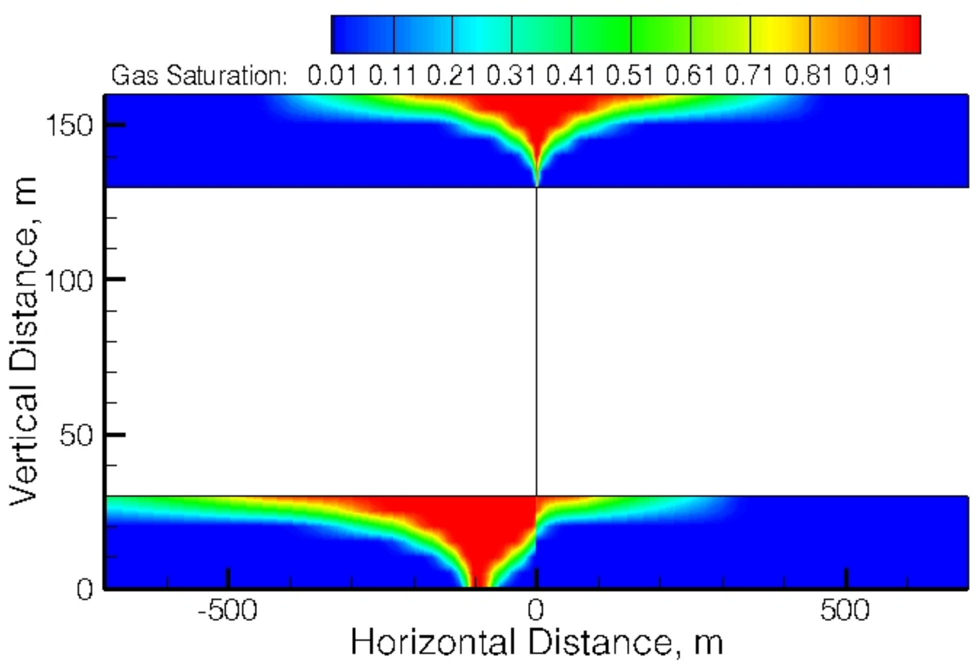


**Figure 5**. $scCO_2$ saturation profile after 500 days for the Exercise 2 simulation

**Exercise 3**

To account for heat transfer and nonisothermal effects the STOMP-CO2e simulator is used in full nonisothermal mode. By choosing to consider nonisothermal conditions, the number of equations solved at each grid cell increase. For isothermal conditions, the STOMP-CO2e simulator solves the conservation equations for water mass, $CO_2$ mass, and salt mass at each grid cell; whereas, invoking the nonisothermal mode requires STOMP-CO2e to solve an additional equation for the conservation of energy. As would be expected, this also requires additional input over the isothermal option. A *Thermal Properties Card* is required for specifying the effective thermal conductivity and the specific heat of the geologic media and an energy boundary condition specification in the *Boundary Condition Card* is required for active boundaries.

To change the system depth from the basecase (3,000 m) to the specified depth of 800 m, the gas and aqueous pressures in both the initial and boundary conditions were lowered. This produces a domain whose pressure falls below the critical pressure for $CO_2$. Therefore as $CO_2$ migrates up the leaky well it transitions from supercritical to sub-critical conditions, both in terms of pressure and temperature. $CO_2$ from the injection well enters the system between 8 and 16 MPa over the 1,000-day period, at 33.6˚C, which is sc$CO_2$. During the migration up the leaky well the $CO_2$ fluid density drops, accelerating the rising $CO_2$, as shown in Figure 2. Color scaled profiles of gas saturation and temperature are shown in Figures 6 and 7, respectively.

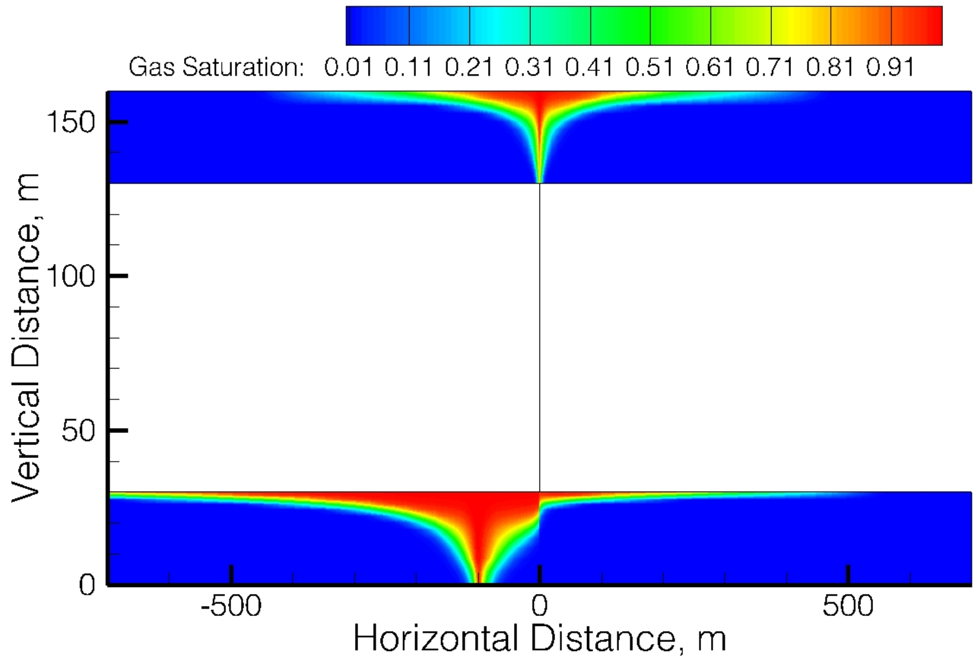


**Figure 6**. $scCO_2$ saturation profile after 500 days

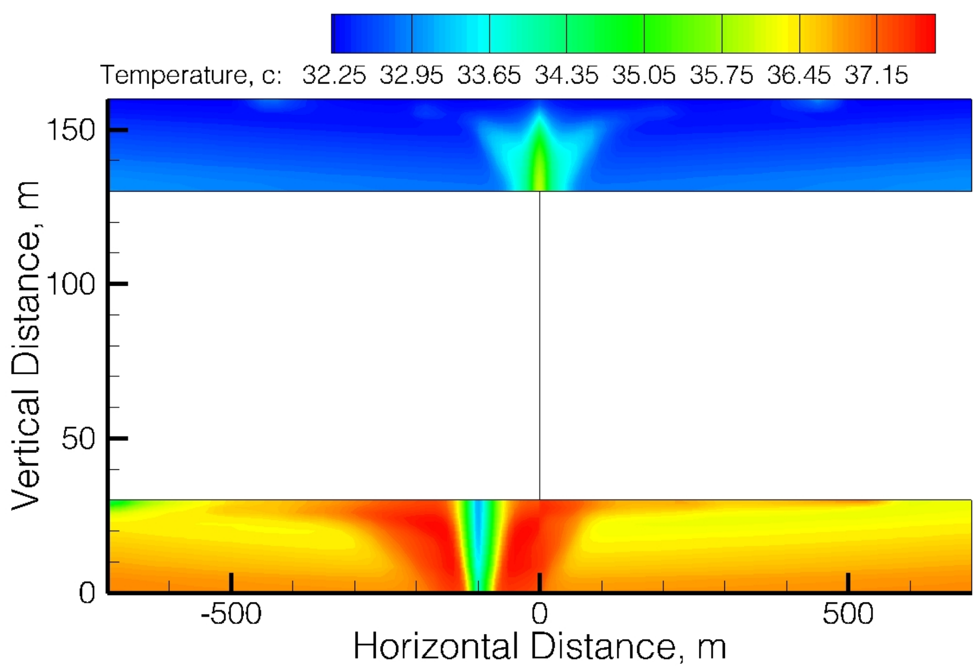


**Figure 7**. Temperature profile after 500 days