Example Problem CO2-1

Radial Flow of Supercritical CO_2 from an Injection Well (GeoSeq # 3)

Abstract: *Radial flow of injected supercritical CO_2 into simplified fresh-water and saline aquifers is compared. This problem is identical to Problem 3 of the code intercomparison problems developed under the GeoSeq Project (Pruess et al. 2002) and addresses two-fluid flow of CO_2 and aqueous for a simplified flow geometry and aquifer properties. A constant mass injection rate of CO_2 is applied from a line source at the center of the infinite radial domain into an aquifer with homogeneous and isotropic hydrologic properties. Gravity and inertial effects are ignored by using a one-dimensional radial computational domain. The problem has a similarity solution, where dependence on the radial distance (r) and time (t), is replaced by the similarity variable ($\xi = r^2 / t$), (O'Sullivan 1981; Doughty and Pruess 1992).*

Problem Description

Geologic sequestration of anthropologic CO_2 into subsurface reservoirs, including brine aquifers, partially or fully depleted oil and gas reservoirs, and coal beds, is currently being implemented or evaluated globally. Numerical simulation has shown and will continue to be useful in determining the feasibility of sequestering CO_2 into particular reservoirs, developing injection protocols, and monitoring sequestration. The credibility of numerical simulation to accurately model the multifluid subsurface flow, transport, and reactive processes needs to be established before it will become an accepted engineering tool. The primary objective of the code intercomparison exercises of the GeoSeq Project (Pruess et al. 2002), was to evaluate the ability of numerical simulators to model critical processes associated with CO_2 sequestration in geologic reservoirs.

This problem involves the injection of supercritical CO_2 into an infinite-acting one-dimensional radial domain with an aquifer thickness of 100 m. The porous medium is assumed homogenous and isotropic and gravity effects are ignored. Injection occurs at a constant rate of 100 kg/s. The multifluid processes of interest for this problem are two-phase flow of CO_2 and brine, subject to relative permeability and capillarity effects, the effects of pressure and salinity on phase density, phase viscosity and CO_2 solubility and precipitation of salt with dry-out of the formation. Whereas, this problems contains nonlinearities in the thermodynamic and hydrologic transport properties, the problem solution for time and radial distance can be reduced through the similarity variable $\xi = r^2 / t$. This allows results to be reported using radial profiles at a fixed time or a time series at a fixed radial distance. The original GeoSeq problem requested that results be reported over the similarity variable range $10^{-8}\ m^2 / s \le \xi \le 10^{-1} m^2 / s$.

The capillary pressure-saturation relation is described using the van Genuchten formulation (van Genuchten 1980):

$$\bar{s}_l = \left[1 + \left(\beta_{gl}\ \alpha\ h_{gl} \right)^n \right]^{-m} ;\ \bar{s}_l = \frac{s_l - s_{lr}}{1 - s_{lr}} ;\ m = 1 - \frac{1}{n} \quad (1)$$

where β_{gl} is the gas-aqueous scaling factor, h_{gl} is the gas-aqueous capillary head (m), and other parameters are described in Table 1.

The aqueous relative permeability relation is described using the van Genuchten capillary pressure function with the Mualem porosity distribution function (van Genuchten 1980):

$$k_{rl} = \sqrt{\bar{s}_l} \left\{ 1 - \left(1 - \bar{s}_l^{\,(1/m)} \right)^m \right\}^2 \quad (2)$$

The gas relative permeability relation is described using the Corey formulation, which includes an irreducible gas saturation:

$$k_{rg} = \left(1-\hat{s}\right)^2 \left(1-\hat{s}^2\right); \;\; \hat{s} = \frac{s_l - s_{lr}}{1 - s_{lr} - s_{gr}} \quad (3)$$

Simulation parameters are shown in Table 1.

Table 1. Simulation Parameter Values

Parameter Description		Parameter Value
Intrinsic Permeability		10^{-13} m^2
Porosity		0.12
Pore Compressibility		4.5 x 10^{-10} Pa^{-1}
Aquifer Thickness		100 m
Saturation Function	s_{lr}	0.0
Saturation Function	n	1.84162
Saturation Function	α	0.5 m^{-1}
Aqu. Rel. Perm.	s_{lr}	0.30
Aqu. Rel. Perm.	m	0.457
Gas. Rel. Perm.	s_{gr}	0.05
Gas Rel. Perm.	s_{lr}	0.30
Initial Aquifer Pressure		120 bar
Initial Aquifer Temperature		45°C
Initial Aquifer Salinity		15 wt.% NaCl
CO_2 Injection Rate		100 kg/s

Time stepping and grid spacing were not specified as part of the original GeoSeq problem description but were instead left to the discretion of the modeler. For this problem a domain ranging from 0.3 to 100,000.0 m was specified using 100 grid cells, with the grid spacing increasing exponentially. An initial time step of 0.001 seconds was specified with an ending time of 10,000 days.

The evolution of the gas front is shown in Figure 1 for four points in time. The coarse grid spacing for the outer radial nodes tends to smear the leading edge of the front profile. Accuracy of the numerical simulation can be examined by plotting the results in terms of the similarity variable. Figure 2 shows the results for pressure as a function of the similarity variable at four different times (30, 100, 1000 and 10000 days) and one radial distance (904.76 m). The agreement of the results between the different time points and radial distance is good, verifying the similarity property of the numerical solution. Figures 3 and 4 show gas saturation and aqueous dissolved CO_2 mass fraction.

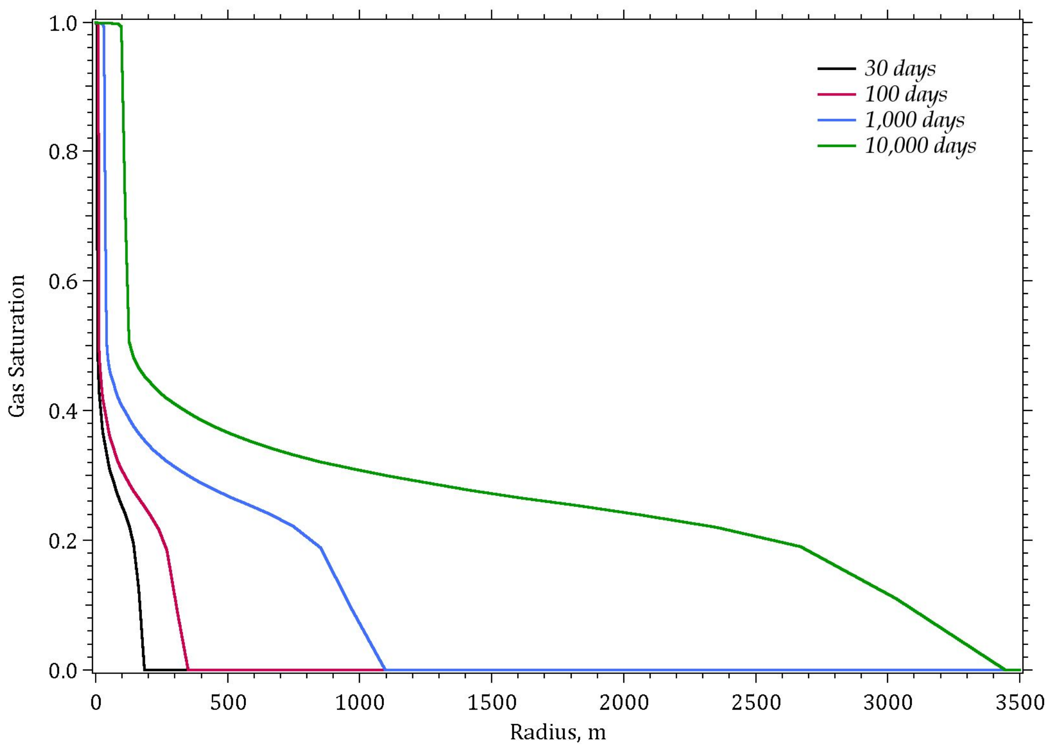

Figure 1. Gas saturation front (zero salinity)

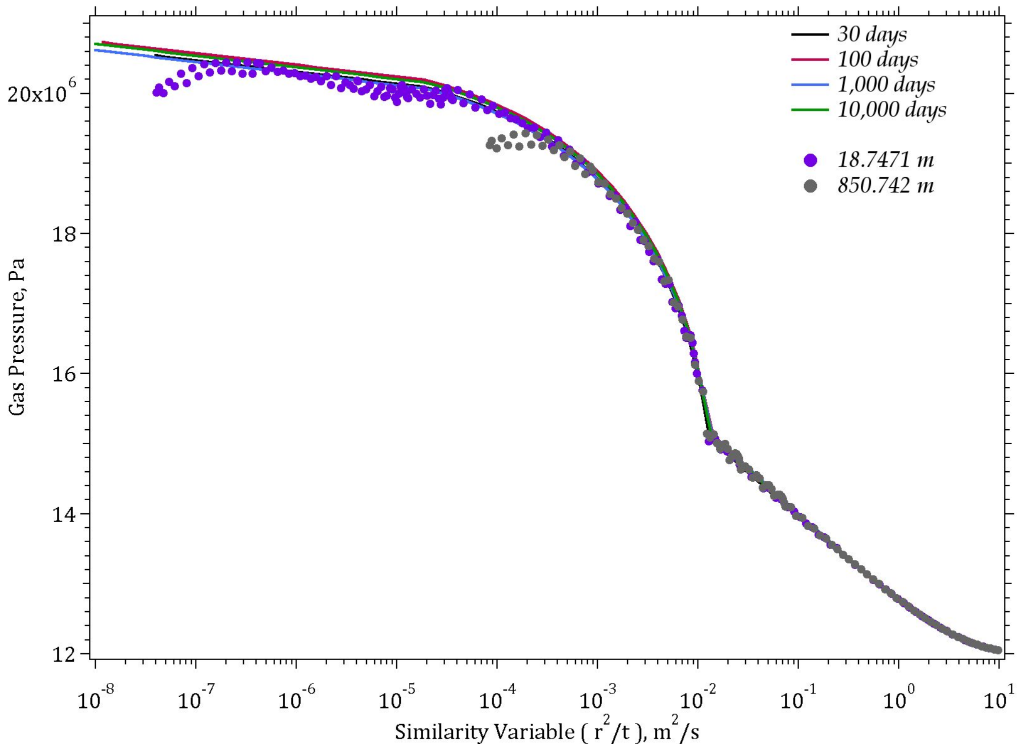

Figure 2. Pressure as a function of similarity variable

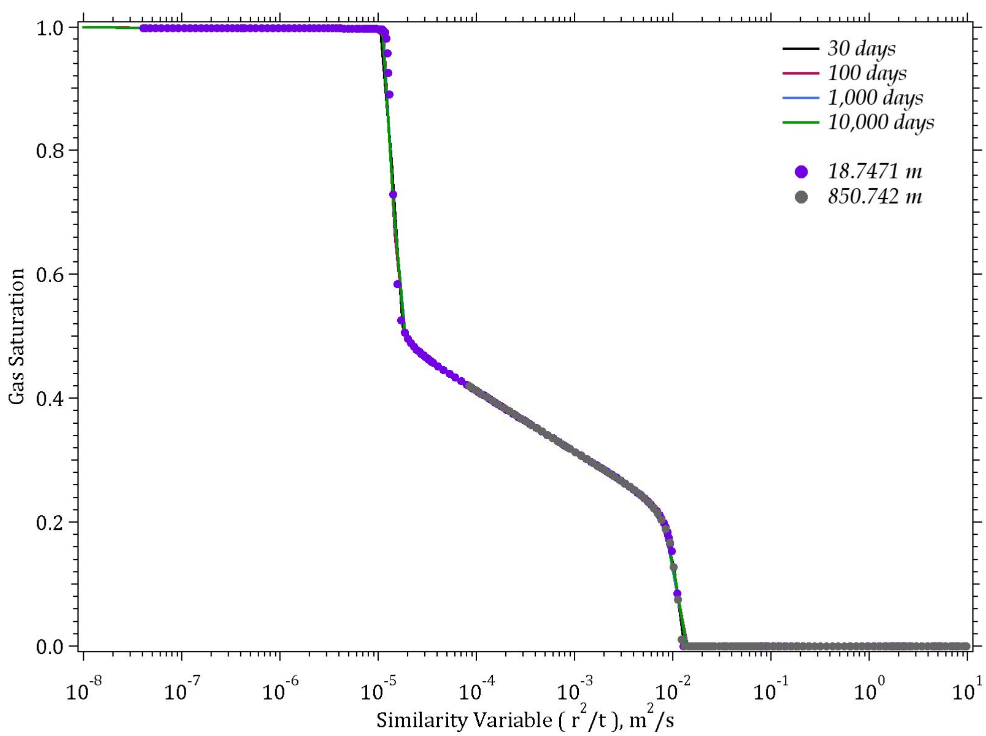

Figure 3. Gas saturation as a function of similarity variable

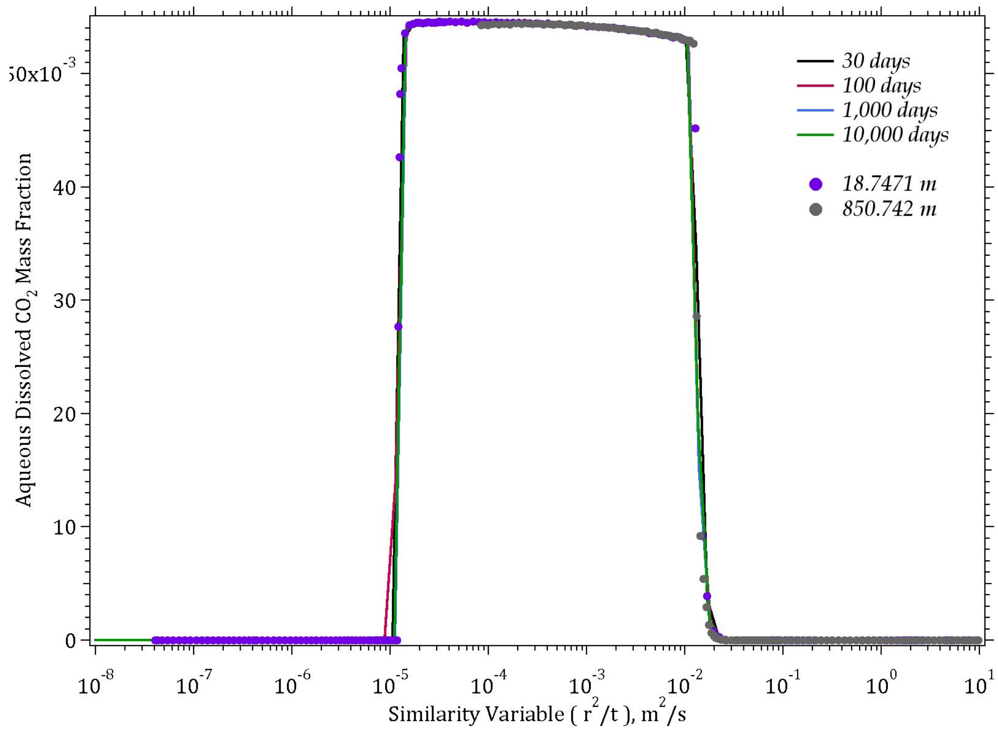

Figure 4. Aqueous dissolved mass fraction as a function of similarity variable

References

Doughty, C. a. K. P. 1992. "A similarity solution for two-phase water, air and heat flow near a linear heat source in porous medium." *Journal of Geophysical Research*. 97(B2):1821-1838.

O'Sullivan, M. J. 1981. "A similarity method for geothermal well test analysis." *Water Resources Research*. 17(2):390-398.

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. 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. (Basic) Repeat the simulation using the provided input file and generate the similarity plots shown in Figures 2 through 4. Check the results against those reported herein.
2. (Basic) Repeat the simulation using an initial 15 weight-% NaCl salinity with the input file provided under the salinity folder and generate the similarity plots shown in Figures 2 and 4. Contrast the simulation results against those reported for zero salinity.
3. (Intermediate) Create an input file to compute the density and viscosity of the aqueous and gas phase and aqueous dissolved CO_2 mass fraction at a temperature of 45 C, pressures of 120, 160, 200, and 240 bar, and aqueous NaCl salinities of 0 and 15 weight-%. (Hint: Conduct a simulation of zero time steps using a unique grid cell for each temperature, pressure, salinity combination.)

Input Files

Zero-Salinity Input File

```
~Simulation Title Card
1,
STOMP Example Problem CO2-1 Zero Salinity,
M.D. White,
Pacific Northwest Laboratory,
21 May 2002,
09:45 AM PST,
10,
Intercomparison of simulation models for CO2 disposal in
underground storage reservoirs.
Test Problem 3: Radial Flow from a CO2 Injection Well
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 x = R2/t (O'Sullivan 1981; Doughty and Pruess 1992).

~Solution Control Card
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Variable Gas Diffusion,
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~Grid Card
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2.294995583,m,2.606217409,m,2.959643684,m,3.360997708,m,3.81677891,m,
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8.185962079,m,9.296051391,m,10.55667869,m,11.98825828,m,13.61397279,m,
15.46014866,m,17.55668242,m,19.9375248,m,22.64123061,m,25.71158298,m,
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0.0,m,100.0,m,

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Quirk,

~Hydraulic Properties Card
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Aquifer,van Genuchten,0.5,1/m,1.84162,0.0,0.457,0.0,

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~Gas Relative Permeability Card
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Gas Saturation,,
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Gas Density,kg/m^3,
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Gas Relative Permeability,,
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Water Gas Mass Fraction,,
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Gas Saturation,,
Aqueous Density,kg/m^3,
Gas Density,kg/m^3,
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Gas Viscosity,Pa s,
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Gas Relative Permeability,,
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Water Gas Mass Fraction,,
X Node Centroid,m,
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15 wt.-% Salinity Input File

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~Simulation Title Card
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STOMP Example Problem CO2-1 Salinity,
M.D. White,
Pacific Northwest Laboratory,
21 May 2002,
09:45 AM PST,
10,
Intercomparison of simulation models for CO2 disposal in
underground storage reservoirs.
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variable x = R2/t (O'Sullivan 1981; Doughty and Pruess 1992).

~Solution Control Card
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STOMP-CO2,
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Variable Gas Diffusion,
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~Grid Card
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4726.16741,m,5367.077773,m,6094.901285,m,6921.424143,m,7860.030856,m,
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~Hydraulic Properties Card
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~Saturation Function Card
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~Aqueous Relative Permeability Card
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~Gas Relative Permeability Card
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~Salt Transport Card
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Aqueous Pressure,120.0,Bar,,,,,,1,100,1,1,1,1,
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Salt Saturation,,
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CO2 Aqueous Mass Fraction,,
Gas Pressure,Pa,
Diffusive Porosity,,
Similitude Variable,,
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30,day,
100,day,
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1000,day,
10000,day,
7,
Gas Saturation,,
Salt Saturation,,
Salt Aqueous Mass Fraction,,
CO2 Aqueous Mass Fraction,,
Gas Pressure,Pa,
Diffusive Porosity,,
Similitude Variable,,
```

Solutions to Selected Exercises

Exercise 2

Salt in the aqueous phase changes the aqueous-gas interfacial tension, increases the density and viscosity of the aqueous phase, and induces the processes associated with precipitation of the salt with desiccation of the pore space near the injection well. The increased viscosity of the aqueous phase with salinity results in higher pressures as shown in Figure 5. In spite of the increased pressure, viscosity and density, there is little change in the gas saturation profiles, as shown in Figure 6. The aqueous dissolved CO_2 mass fraction profile appears significantly differ near the well, as shown in Figure 7. Salt concentrations in the aqueous phase are at saturated conditions because of the desiccation by the entering dry CO_2. This results in precipitated NaCl, which modifies the media intrinsic permeability, and reduced aqueous dissolved CO_2 concentrations near the injection well.

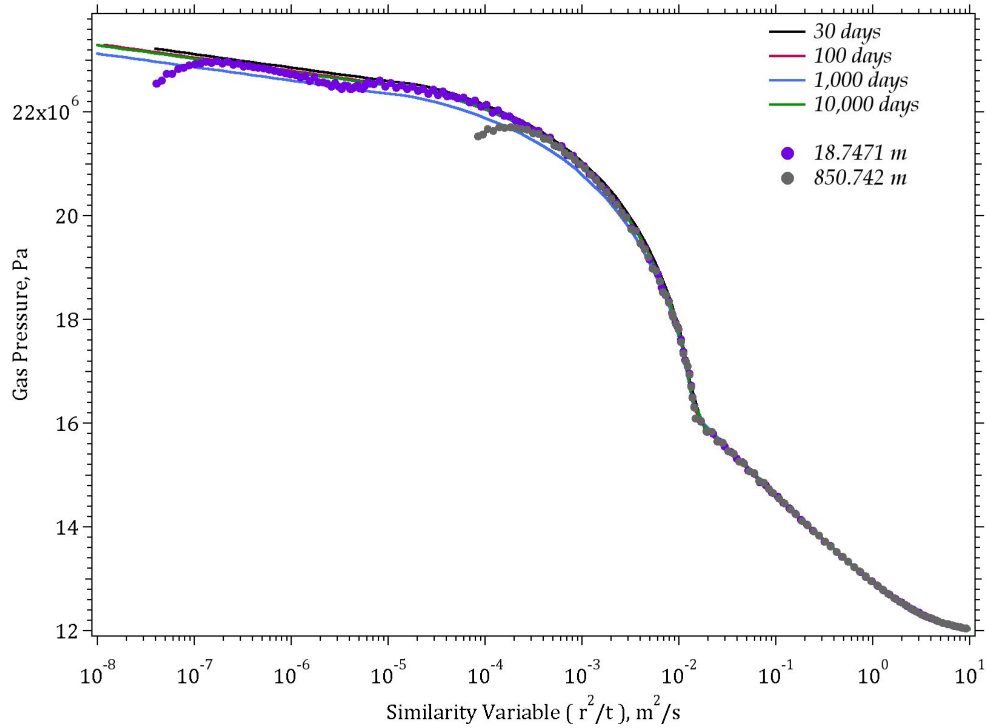

Figure 5. Gas pressure as a function of similarity for 15 wt.-% salinity

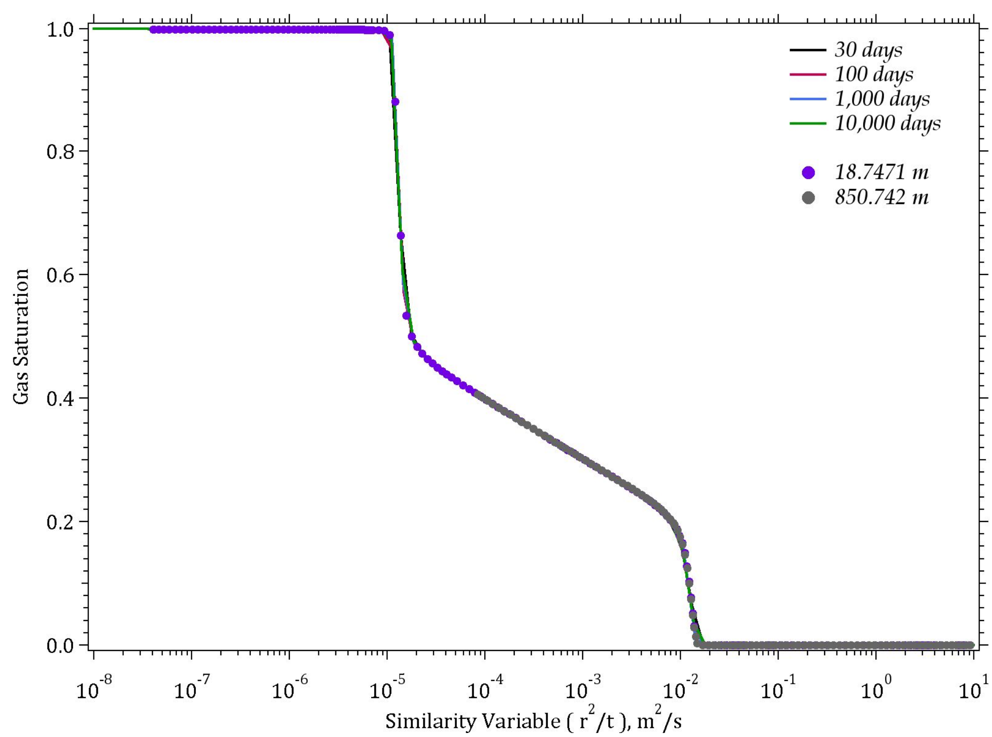

Figure 6. Gas saturation as a function of similarity for 15 wt.-% salinity

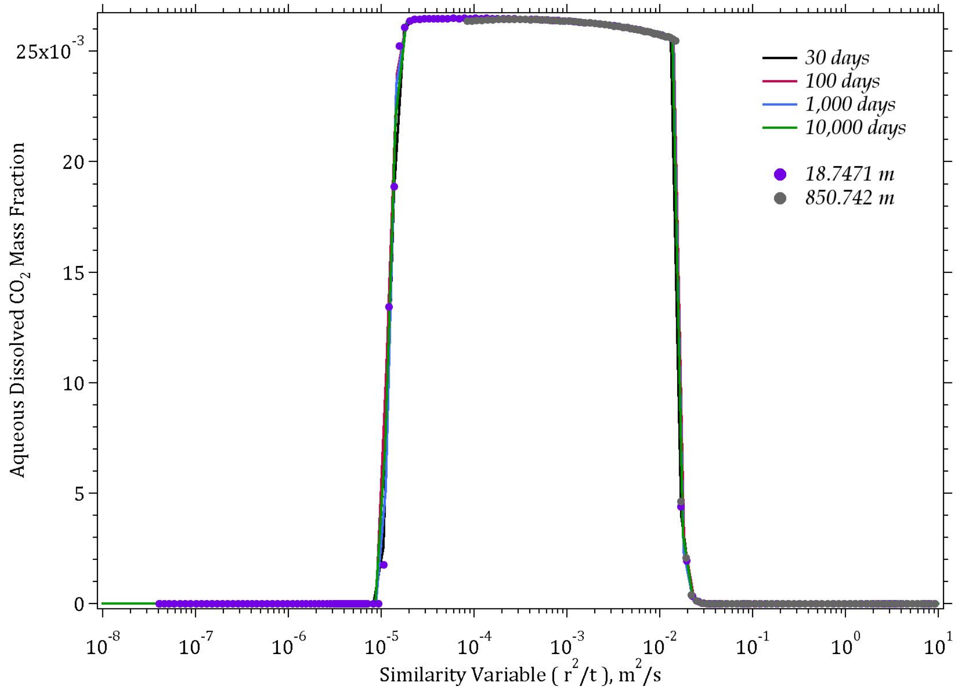

Figure 7. Aqueous dissolved mass fraction for 15 wt.-% salinity

Exercise 3

Property checks are invaluable in verifying a numerical simulator's accuracy. Property data can be generated with the STOMP simulator, by executing the simulator through the thermodynamic and transport property routines printing output and then stopping the execution. This procedure can be implemented in STOMP by requesting zero time steps on the *Solution Control Card*. To simultaneously compute properties for the range of pressures and salinities in Exercise 3, a computational domain of 8 grid cells was created, with each cell having different initial conditions for pressure and salinity. Two-phase (aqueous-gas) conditions were created by specifying a gas pressure greater than the aqueous pressure plus scaled entry pressure, as shown in the input file:

```
~Simulation Title Card
1,
STOMP Example Problem CO2-1 Exercise 3,
M.D. White,
Pacific Northwest Laboratory,
21 May 2002,
09:45 AM PST,
9,
```

Intercomparison of simulation models for CO2 disposal in underground storage reservoirs.
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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 x = R2/t (O'Sullivan 1981; Doughty and Pruess 1992).

```
~Solution Control Card
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STOMP-CO2,
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Variable Aqueous Diffusion,
Variable Gas Diffusion,
0,

~Grid Card
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1.0,m,
1.0,m,

~Rock/Soil Zonation Card
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~Mechanical Properties Card
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~Hydraulic Properties Card
Aquifer,1.e-13,m^2,,,,,0.8,0.8,

~Saturation Function Card
Aquifer,van Genuchten,0.5,1/m,1.84162,0.0,0.457,0.0,

~Aqueous Relative Permeability Card
Aquifer,Mualem Irreducible,0.457,0.30,

~Gas Relative Permeability Card
Aquifer,Corey,0.3,0.05,

~Salt Transport Card
Aquifer,0.0,m,0.0,m,

~Initial Conditions Card
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Gas Density,kg/m^3,
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#Gas Viscosity,Pa s,
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Salt Aqueous Mass Fraction,,
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#Gas Saturation,,
Gas Pressure,bar,
Aqueous Density,kg/m^3,
Gas Density,kg/m^3,
#Aqueous Viscosity,Pa s,
#Gas Viscosity,Pa s,
CO2 Aqueous Mass Fraction,,
Salt Aqueous Mass Fraction,,
```

When the simulation is executed, properties are reported to the screen and in the reference-node section of the output file:

```
---  Reference Node Output Record  ---

Reference Node(s) (  1,  1,  1:     1) (  2,  1,  1:     2) (  3,  1,  1:     3) (  4,  1,  1:     4) (  5,  1,  1:     5) (  6,  1,  1:
6) (  7,  1,  1:     7) (  8,  1,  1:     8)
  Step  Node    Time       Timestep  Itr    PG        RHOL        RHOG        XLA        XLS
              [s    ]    [s    ]        [bar    ]   [kg/m^3 ]   [kg/m^3 ]
     0     1  0.00000E+00  8.69565E-04  0  1.20000E+02  1.00692E+03  6.55187E+02  5.12950E-02  0.00000E+00
     0     2  0.00000E+00  8.69565E-04  0  1.20000E+02  1.11112E+03  6.55240E+02  2.41464E-02  1.50000E-01
     0     3  0.00000E+00  8.69565E-04  0  1.60000E+02  1.00910E+03  7.58341E+02  5.36436E-02  0.00000E+00
     0     4  0.00000E+00  8.69565E-04  0  1.60000E+02  1.11278E+03  7.58393E+02  2.52512E-02  1.50000E-01
     0     5  0.00000E+00  8.69565E-04  0  2.00000E+02  1.01117E+03  8.11211E+02  5.56128E-02  0.00000E+00
     0     6  0.00000E+00  8.69565E-04  0  2.00000E+02  1.11439E+03  8.11267E+02  2.61770E-02  1.50000E-01
     0     7  0.00000E+00  8.69565E-04  0  2.40000E+02  1.01318E+03  8.46765E+02  5.73661E-02  0.00000E+00
     0     8  0.00000E+00  8.69565E-04  0  2.40000E+02  1.11596E+03  8.46825E+02  2.70010E-02  1.50000E-01
NOTE: Simulation Stopped:
```