

STOMP Short Course

June 19-20, 2003

Delft University

Problem 9: Simulation of Supercritical CO₂ into a Deep Saline Aquifer (CO₂ Sequestration)

Abstract: *One viable scenario for geologic sequestration of anthropogenic CO₂ is its injection into deep saline aquifers. To evaluate the potential for a field application of this scenario, numerical simulations of the CO₂ injection process will be necessary. In the absence of long-term field experiments, which will be cost and time prohibitive for most applications, numerical simulation is the most comprehensive means for predicting the complex behavior of multiple fluids under complex hydrogeologic conditions and evaluating the feasibility for geologic sequestration of CO₂. Numerical simulations will additionally provide critical information required to obtain regulatory permits and satisfy stakeholder concerns prior to injecting CO₂, including reservoir pressure, CO₂ migration and dissolution behavior, and the potential for leakage to the ground surface.*

To numerically simulate CO₂ sequestration in deep saline aquifers, several special features are needed in the numerical model. First, the simulator must have multifluid capabilities with algorithms for handling phase transitions (i.e., phase appearances and disappearances). Depending on the system pressure and temperature, injected CO₂ occurs as liquid, gas, or supercritical fluid. A precondition for efficient and safe storage of CO₂ is that it not transition from a liquid or supercritical fluid state into a gas state, during the sequestration process. Numerical simulators for geologic sequestration of CO₂ should, therefore, be able to predict when such phase transitions occur. Long-term sequestration of CO₂ in deep saline aquifers is envisioned to occur via CO₂ dissolution in the brine or chemical complexation with the formation. To accurately model CO₂ dissolution the numerical simulator must have capabilities for buoyancy driven flow, Rayleigh instability fingering, aqueous dissolution, molecular diffusion, hydrodynamic

dispersion, and phase transitions. The $H_2O-NaCl-CO_2$ and $H_2O-NaCl-CO_2-Energy$ operational modes of the STOMP simulator have the capabilities described above for modeling sequestration of CO_2 in deep saline aquifers.

Problem Description and Input Parameters

The CO_2 injection simulation involves a two-dimensional radial domain (36° wedge) with the injection well situated at the center of the domain. Radially the computational domain extends from the well radius of 0.25 to 3350 ft. Vertically the computational domain ranges from 6400 to 4900 ft below ground surface. The bottom nine grid rows represent the injection formation, sandstone. The overlying six grid rows constitute the immediate caprock above the injection layer. The inner-radial vertical boundary, representing the well casing is treated as a zero flux boundary and the outer-radial vertical boundary uses a unit hydraulic gradient boundary, representing hydrostatic conditions remote from the well. Upper and lower horizontal surfaces are considered zero flux boundaries. These boundary conditions allow displaced brine to only flow out the outer-radial vertical boundary. CO_2 injection is simulated by specifying a CO_2 mass injection rate for the lowest nine grid cells adjacent to the well casing, representing a screened well over the sandstone interval. An injection rate of 1 mt/yr of CO_2 was used, adjusted to 100 kt/yr (13727.5 lb-mole/d) for the 36° domain of the model. The simulation was executed for 20 years of injection followed by 20 years of post injection. Soil moisture retention was described using the Brooks and Corey formulation, as shown in Equation (9.1). Aqueous and gas relative permeability were described using a modified Corey function, as shown in Equation (9.2) and (9.3). Hydrogeologic simulation parameters are listed in Table 9-1.

$$S_l = \frac{h_{gl}}{h} \left[1 - S_m \right] + S_m = \bar{S}_l \left[1 - S_m \right] + S_m \text{ for } h_{gl} > h$$

$$S_l = 1 = \bar{S}_l \text{ for } h_{gl} \leq h$$
(9.1)

$$k_{rl} = k_{rl}^{ref} \frac{S_l \square S_{lr}}{1 \square S_{lr} \square S_{gr}} \quad (9.2)$$

$$k_{rg} = k_{rg}^{ref} \frac{S_l \square S_{lr}}{1 \square S_{lr} \square S_{gr}} \quad (9.3)$$

Table 9-1. Simulation Parameter Values

Parameter Description	Rock/Soil	Parameter Value
Porosity	Eau Claire Carbonate	0.32
	Eau Claire Shale	0.28
	Lower Eau Claire	0.064
	Upper Mt. Simon	0.065
	Middle Mt. Simon	0.093
	Lower Mt. Simon	0.044
Saturated Hydraulic Conductivity	Eau Claire Carbonate	3.0 x 10 ⁻⁷ Darcy
	Eau Claire Shale	7.0 x 10 ⁻⁹ Darcy
	Lower Eau Claire	3.0 x 10 ⁻⁶ Darcy
	Upper Mt. Simon	3.8 x 10 ⁻³ Darcy
	Middle Mt. Simon	2.1 x 10 ⁻² Darcy
	Lower Mt. Simon	7.1 x 10 ⁻³ Darcy
Brooks and Corey \square	Eau Claire Carbonate	1.404 x 10 ⁻² m
	Eau Claire Shale	2.239 x 10 ⁻² m
	Lower Eau Claire	3.14 x 10 ⁻² m
	Upper Mt. Simon	1.109 x 10 ⁻² m
	Middle Mt. Simon	2.179 x 10 ⁻² m
	Lower Mt. Simon	1.842 x 10 ⁻² m
Brooks and Corey \square	all formations	0.5
Brooks and Corey residual saturation	all formations	0.2
Aqueous Free Corey k_{rl}^{ref} Rel. Perm. Endpoint	all formations	1.0
Aqueous Free Corey \square Rel. Perm. Exponent	all formations	3.25
Aqueous Free Corey S_{lr} Residual Aqu. Saturation	all formations	0.2
Aqueous Free Corey S_{gr} Residual Gas. Saturation	all formations	0.1
Gas Free Corey k_{rg}^{ref} Rel. Perm. Endpoint	all formations	0.9

Gas Free Corey \square	all formations	2.9
Rel. Perm. Exponent		
Gas Free Corey S_{gr}	all formations	0.2
Residual Aqu. Saturation		
Gas Free Corey S_{gr}	all formations	0.1
Residual Gas. Saturation		
Salt Transport	all formations	20 ft
Longitudinal Dispersivity		
Salt Transport	all formations	5 ft
Transverse Dispersivity		

The input file for this simulation, listed in Appendix A.9, shows how to introduce a “plug” source. The *Source Card* has one source, representing the injection of CO₂ mass into the column of nine nodes adjacent to the well screen. The injection period starts at time zero and continues at a constant rate of 0.352413 kg/s for each grid cell for 20 years (i.e., 7300 days). For a source with multiple time entries, the first and last time entries represents the start and stop times, respectively. By default, the simulator matches time steps with times for execution periods, sources, boundary conditions, and plot files.

Simulation results in terms of gas-saturation contours at years 10, 20, 30, and 40 are shown in Figures 9.1 through 9.4, respectively. The injected CO₂ forms a distinct phase, which is less dense than the ambient brine, resulting in the gross migration of CO₂ phase toward the caprock. There appears to be minimal to no migration of CO₂ phase into the caprock. During the injection and post injection periods, a large portion of the CO₂ mass dissolved in the ambient brine. Depending on the temperature, pressure, and dissolved concentration, brine with dissolved CO₂ can be more or less dense than the ambient brine. CO₂ saturated dense brine overlying ambient brine, is an unstable situation that can lead to advective mixing of the aquifer brine, primarily via fingered flow. The computational domain was originally designed to avoid boundary condition affects on the migration behavior of the CO₂ phase. Clearly, from Figures 9.1 through 9.4 the outer-radial boundary is remote enough not to impact the plume formation and migration. This modeling approach, however, comes with the cost of slower execution. Ideally, the computational domain should be sized to minimize the impact on the multifluid flow processes and maximize the execution speed.

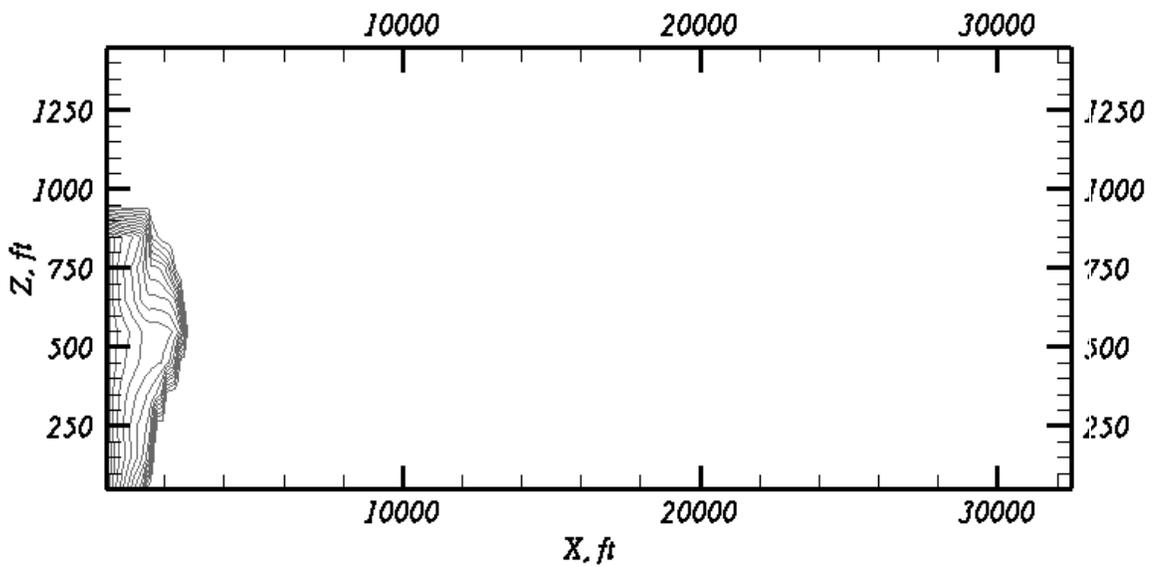


Figure 9.1. Gas Saturation Contours at 10 Years

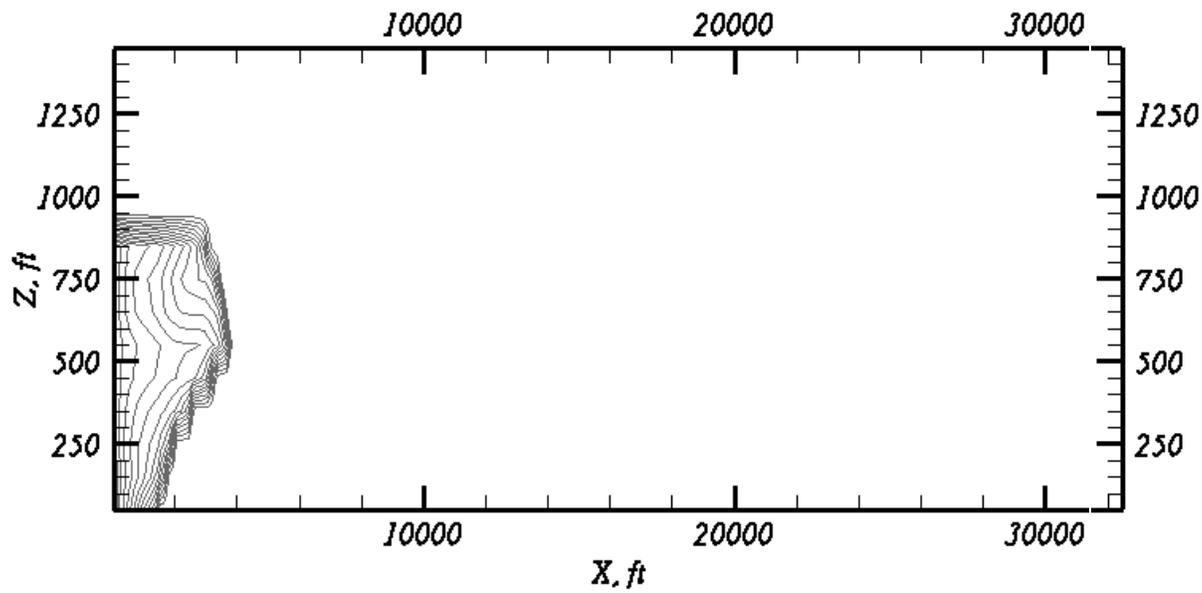


Figure 9.2. Gas Saturation Contours at 20 Years

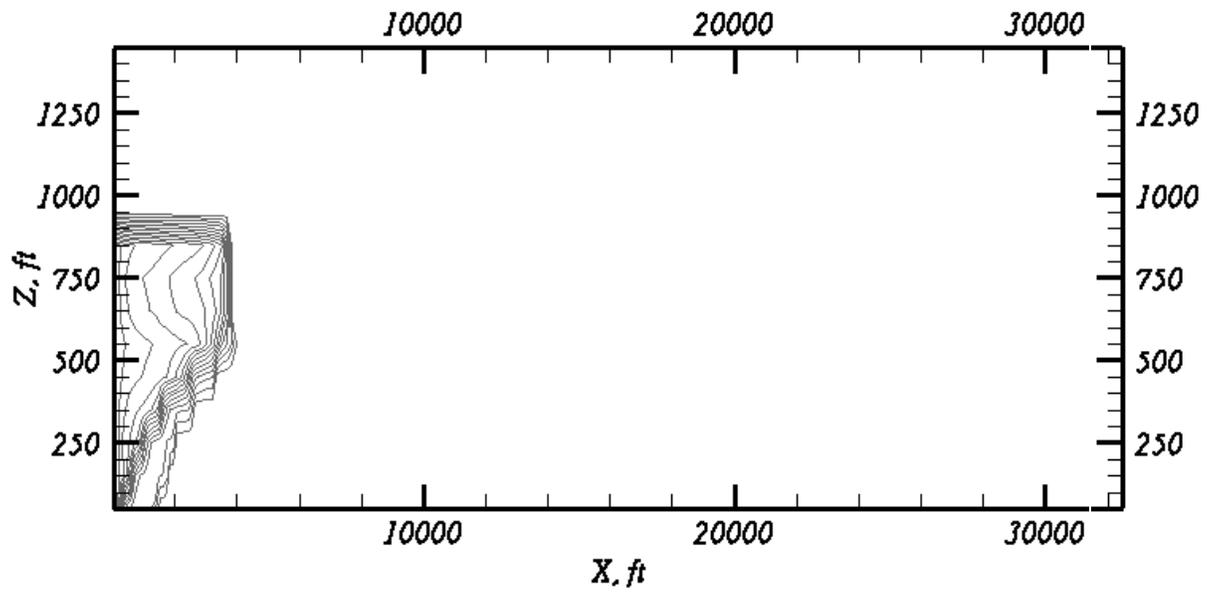


Figure 9.3. Gas Saturation Contours at 30 Years

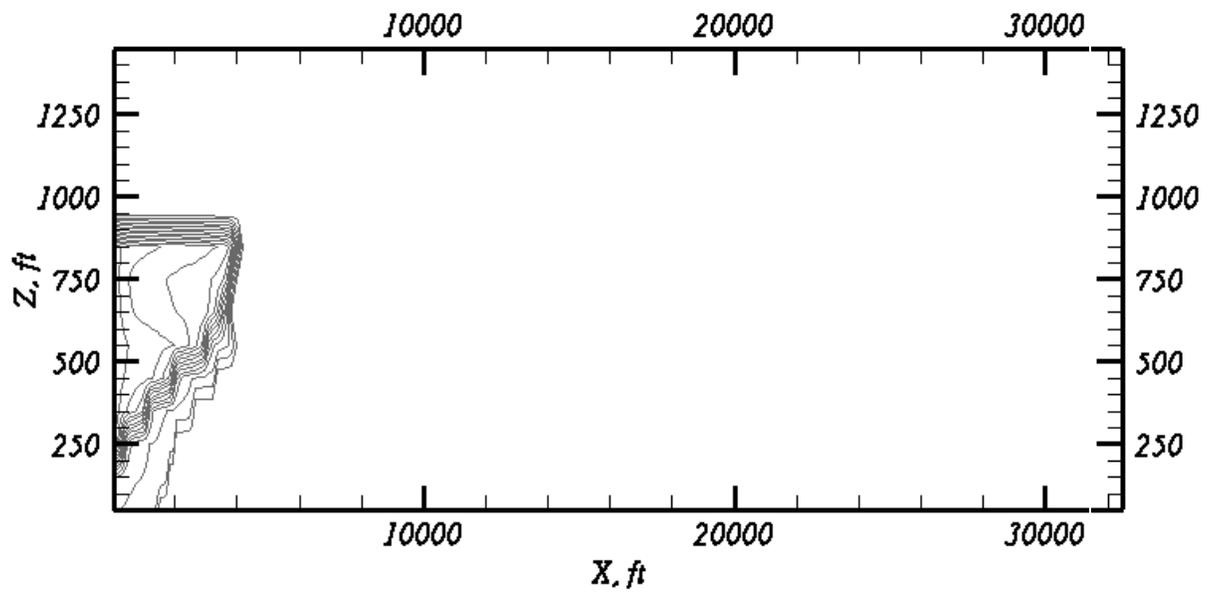


Figure 9.4. Gas Saturation Contours at 40 Years

Exercises

1. (Basic) This simulation suffers from an excessive computational domain. Repeat the two-dimensional simulation using a more efficient domain that does not impact the multifluid flow behavior.
2. (Intermediate) Use the plotting utility *plotTo.pl* or write a script to determine the fraction of CO₂ that has dissolved into the brine as a function of time.
3. (Intermediate) Use the plotting utility *plotTo.pl* or write a script to determine the maximum system pressure as a function of time.
4. (Advanced) Design and execute a simulation to determine the solubility of CO₂ as a function of NaCl concentration over the range from 0 to 100% NaCl saturated solutions at 20 C and 13.8 MPa.
5. (Advanced) Design and execute a simulation to determine the density of CO₂ saturated brine as a function of pressure from 0.1 MPa to 100 MPa, at a dissolved NaCl mass fraction of 0.178 and temperature of 20 C.

Appendix A.10

~Simulation Title Card

1,

BP_UTCOMP Comparison (Base Case),

M.D. White,

Pacific Northwest Laboratory,

30 October 2002,

04:06 PM PST,

23,

CC*****

CC

CC BRIEF DESCRIPTION OF DATA SET: UTCOMP (VERSION UTCOMP-3.5) *

CC

CC*****

CC Radial geometry *

CC Mt. Simon Sst. Run BPIN1 2D Full scale,radial model *

CC (phase 1=inactivewater,phase 2 = water/oil,phase 3=co2/gas *

CC LENGTH(FT): INJECTION FLUID: CO2 *

CC HEIGHT(FT): INJECTION RATE: cont. pre. *

CC WIDTH(FT): variable W/O REL. PERM: *

CC POROSITY: variable G/O REL. PERM: lindeburg *

CC ABS. PERM(MD): variable 3-PHASE REL. PERM: water endpt.=1.0 *

CC TEMP(F): .0 WETTIBILITY: *

CC PRESSURE(PSI): . psi/ft W/O CAP. PRESSURE: *

CC SOR: G/O CAP. PRESSURE: *

CC SWC: DISPLACEMENT TYPE: HORIZONTAL *

CC stop injection after 20 years run for 40 yrs,h2o k endpoint=1 *

CC ****NON-IDEAL MIXING, NO GRAVITY, WITH Pc, WITH X-FLOW **** *

CC FILE NAME: *

CC CREATED BY Neeraj Gupta *

CC MODIFIED BY Neeraj Gupta, *

CC*****

~Solution Control Card

Normal,

H2O-NaCl-CO2,

1,

0,day,14600,day,1,hr,40,day,1.25,16,1.e-06,
10000,
#Constant Aqueous Diffusion,0.0,ft^2/day,0.0,ft^2/day,
#Constant Aqueous Diffusion,4.0e-3,ft^2/day,4.0e-3,ft^2/day,
Variable Aqueous Diffusion,
Variable Gas Diffusion,
0,

~Grid Card

Cylindrical,
70,1,15,
0.25,ft,100,ft,29@100,ft,5@150,ft,5@200,ft,5@300,ft,
5@450,ft,5@700,ft,5@1000,ft,7@1500,ft,3@2000,ft,
0.0,deg,36.0,deg,
0.0,ft,15@100.0,ft,

~Rock/Soil Zonation Card

6,
Eau Claire Carbonate,1,70,1,1,14,15,
Eau Claire Shale,1,70,1,1,11,13,
Lower Eau Claire,1,70,1,1,10,10,
Upper Mt. Simon,1,70,1,1,7,9,
Middle Mt. Simon,1,70,1,1,4,6,
Lower Mt. Simon,1,70,1,1,1,3,

~Mechanical Properties Card

Eau Claire Carbonate,2650,kg/m^3,0.032,0.032,Compressibility,0.032e-
5,1/psi,14.7,psi,constant,1.0,1.0,
Eau Claire Shale,2650,kg/m^3,0.028,0.028,Compressibility,0.028e-
5,1/psi,14.7,psi,constant,1.0,1.0,
Lower Eau Claire,2650,kg/m^3,0.064,0.064,Compressibility,0.064e-
5,1/psi,14.7,psi,constant,1.0,1.0,
Upper Mt. Simon,2650,kg/m^3,0.065,0.065,Compressibility,0.065e-
5,1/psi,14.7,psi,constant,1.0,1.0,
Middle Mt. Simon,2650,kg/m^3,0.093,0.093,Compressibility,0.093e-
5,1/psi,14.7,psi,constant,1.0,1.0,
Lower Mt. Simon,2650,kg/m^3,0.044,0.044,Compressibility,0.044e-
5,1/psi,14.7,psi,constant,1.0,1.0,

~Hydraulic Properties Card

Eau Claire Carbonate,3.e-7,Darcy,,,3.e-7,Darcy,
Eau Claire Shale,7.e-9,Darcy,,,7.e-9,Darcy,
Lower Eau Claire,3.e-6,Darcy,,,3.e-6,Darcy,
Upper Mt. Simon,3.8e-3,Darcy,,,3.8e-3,Darcy,
Middle Mt. Simon,2.1e-2,Darcy,,,2.1e-2,Darcy,
Lower Mt. Simon,7.1e-3,Darcy,,,7.1e-3,Darcy,

~Saturation Function Card

Eau Claire Carbonate,Brooks and Corey,1.404e-2,m,0.5,0.2,
Eau Claire Shale,Brooks and Corey,2.239e-2,m,0.5,0.2,
Lower Eau Claire,Brooks and Corey,3.14e-2,m,0.5,0.2,
Upper Mt. Simon,Brooks and Corey,1.109e-2,m,0.5,0.2,
Middle Mt. Simon,Brooks and Corey,2.179e-2,m,0.5,0.2,
Lower Mt. Simon,Brooks and Corey,1.842e-2,m,0.5,0.2,

~Aqueous Relative Permeability Card

Eau Claire Carbonate,Free Corey,1.0,3.25,0.2,0.1,
Eau Claire Shale,Free Corey,1.0,3.25,0.2,0.1,
Lower Eau Claire,Free Corey,1.0,3.25,0.2,0.1,
Upper Mt. Simon,Free Corey,1.0,3.25,0.2,0.1,
Middle Mt. Simon,Free Corey,1.0,3.25,0.2,0.1,
Lower Mt. Simon,Free Corey,1.0,3.25,0.2,0.1,

~Gas Relative Permeability Card

Eau Claire Carbonate,Free Corey,0.9,2.9,0.2,0.1,
Eau Claire Shale,Free Corey,0.9,2.9,0.2,0.1,
Lower Eau Claire,Free Corey,0.9,2.9,0.2,0.1,
Upper Mt. Simon,Free Corey,0.9,2.9,0.2,0.1,
Middle Mt. Simon,Free Corey,0.9,2.9,0.2,0.1,
Lower Mt. Simon,Free Corey,0.9,2.9,0.2,0.1,

~Salt Transport Card

Eau Claire Carbonate,20.0,ft,5.0,ft,
Eau Claire Shale,20.0,ft,5.0,ft,
Lower Eau Claire,20.0,ft,5.0,ft,
Upper Mt. Simon,20.0,ft,5.0,ft,
Middle Mt. Simon,20.0,ft,5.0,ft,
Lower Mt. Simon,20.0,ft,5.0,ft,

~Initial Conditions Card

Gas Pressure,Aqueous Pressure,

4,

Gas Pressure,2857,Psi,,,,,-0.45,1/ft,1,70,1,1,1,15,

Aqueous Pressure,2857,Psi,,,,,-0.45,1/ft,1,70,1,1,1,15,

Temperature,50.0,C,,,,,,1,70,1,1,1,15,

Salt Mass Fraction,0.178,,,,,,1,70,1,1,1,15,

~Source Card

1,

Gas Mass Rate,Water-Vapor Mass Fraction,1,1,1,1,1,9,2,

0,day,,,0.352413,kg/s,0.0,

7300,day,,,0.352413,kg/s,0.0,

~Boundary Conditions Card

1,

East,Aqu. Initial Conditions,Gas Initial Conditions,Aqu. Mass Frac.,

70,70,1,1,1,15,1,

0,s,,,0.0,,,1.0,0.178,,

~Output Options Card

4,

1,1,1,

10,1,1,

20,1,1,

30,1,1,

1,1,day,ft,deg,6,6,6,

6,

Gas Saturation,,

Integrated CO2 Mass,kg,

Salt Aqueous Mass Fraction,,

CO2 Aqueous Mass Fraction,,

Gas Pressure,psi,

Diffusive Porosity,,

19,

1,day,

10,day,

30,day,

182,day,
365,day,
730,day,
1095,day,
1460,day,
1825,day,
3650,day,
5475,day,
7300,day,
7301,day,
7330,day,
7665,day,
8030,day,
8395,day,
10950,day,
12775,day,
6,
Gas Saturation,,
CO2 Aqueous Mole Fraction,,
Salt Aqueous Mass Fraction,,
CO2 Aqueous Mass Fraction,,
Gas Pressure,psi,
Diffusive Porosity,,