Example Problem CO2-2
Discharge of Sequestered CO_2 Along a Fault Zone
(GeoSeq #4)

Abstract: *Loss of CO_2 from a deep fresh-water aquifer through a leaky fault is investigated. This problem is identical to Problem 4 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 one-dimensional vertical flow geometry. The problem is designed to investigate the transport of CO_2 from the disposal aquifer to another aquifer 500 m above, through an intersecting vertical fault. The vertical fault is idealized using a one-dimensional geometry and constant pressure boundary conditions (Pruess and Garcia 2002).*

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 leakage of CO_2 from the injection aquifer to another aquifer situated 500 m above, through an idealized 25-m leaky fault as shown in Figure 1.

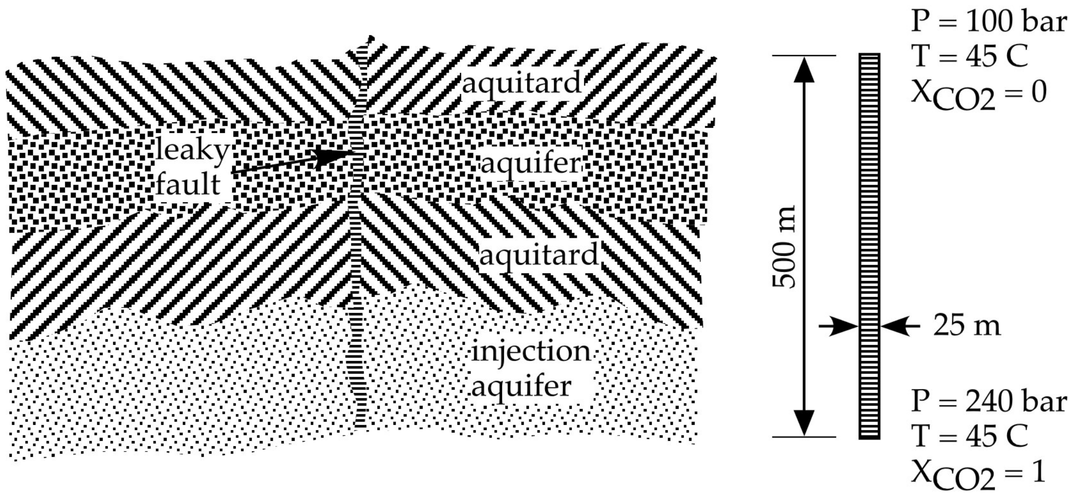

Figure 1. Schematic of fault-connected aquifers and idealized fault with boundary conditions

Initially the system is under saturated hydrostatic conditions (pure water) relative to the 100–bar pressure in the upper aquifer. Temperature is held constant throughout the simulation at 45 C. At time zero the gas pressure in the lower aquifer is increased to 240 bar causing an immiscible displacement of water by upward migrating CO_2 with concurrent dissolution of CO_2 into the aqueous phase.

Results to be calculated are CO_2 mass fluxes (kg/m^2 s) over both gas and aqueous phases at the fault inlet (bottom) and outlet (top). Aqueous phase flux (kg/m^2 s) is to be calculated at the fault outlet. Fluxes are to be reported for a range of times from 10^3 to 10^{11} seconds. Profiles of gas saturation and dissolved CO_2 mass fraction at times of 1 x 10^7 and 2 x 10^7 s are to reported, along with the CO_2 inventory in the aqueous and gas phases at those times.

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

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

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

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

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

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

Simulation parameters are shown in Table 1.

Time stepping and grid spacing were not specified as part of the original GeoSeq problem description; left to the discretion of the modeler. For this problem the 500-m fault was modeled using 100 vertical grid cells with a uniform height of 5 m. The width of the domain matched the width of the fault (25 m) and a 1-m depth was used. To achieve hydrostatic conditions an initial simulation was executed for a period of 10^{11} seconds imposing 100-bar pressure conditions at the fault top and zero flux boundary conditions at the fault bottom. The results from this initial simulation were then used as initial conditions for the transient simulation, which used an initial time step of 1 second, with a time-step acceleration factor of 1.25 for a total time of 10^{11} seconds.

Table 1. Simulation Parameter Values

Parameter Description		Parameter Value
Intrinsic Permeability		10^{-13} m^2
Porosity		0.35
Pore Compressibility		4.5 x 10^{-10} Pa^{-1}
Fault Height		500 m
Fault Width		25 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		hydrostatic w/ 100 bar at top
Initial Aquifer Temperature		45˚C
Initial Aquifer Salinity		0 wt.% NaCl
CO_2 Injection Pressure		240 bar at bottom

In response to a step change in pressure at the lower fault boundary condition CO_2 migrates up the fault, displacing the aqueous phase and concurrently dissolving into the aqueous phase. Gas saturation profiles at 1 x 10^7 and 2 x 10^7 seconds are shown in Figure 2. Aqueous dissolved CO_2 mass fraction profiles at 1 x 10^7 and 2 x 10^7 seconds are shown in Figure 3. Dissolution of CO_2 in the aqueous phase for the thermodynamic conditions of this problem is subject to strong non-idealities. The STOMP simulator contains two solubility formulations, with and without the Poynting correction factor. Without the Poynting correction factor the CO_2 solubility increases with pressure, thus, the slope in dissolved CO_2 mass fraction with depth, as shown in Figure 3. The Poynting correction factor reduces this solubility at higher pressures. The time dependence of CO_2 and water mass fluxes is shown in Figures 4 through 6. Because of the step change in boundary pressure, initially the CO_2 flux entering the fault is large, but then decreases until CO_2 breaks through the fault top, at approximately 2.75 x 10^7 seconds. As with the CO_2 flux, water flux at the fault top increases rapidly, transitions to a quasi-steady flux and then decreases rapidly after CO_2 breakthrough at the fault top. Aqueous flux then slowly declines as water evaporates into the dry CO_2 stream. Total CO_2 inventories in the aqueous and gas phases at 1 x 10^7 s are 100.5 and 397.2 tonnes, respectively; and at 2 x 10^7 s are 170.4 and 686.2 tonnes, respectively.

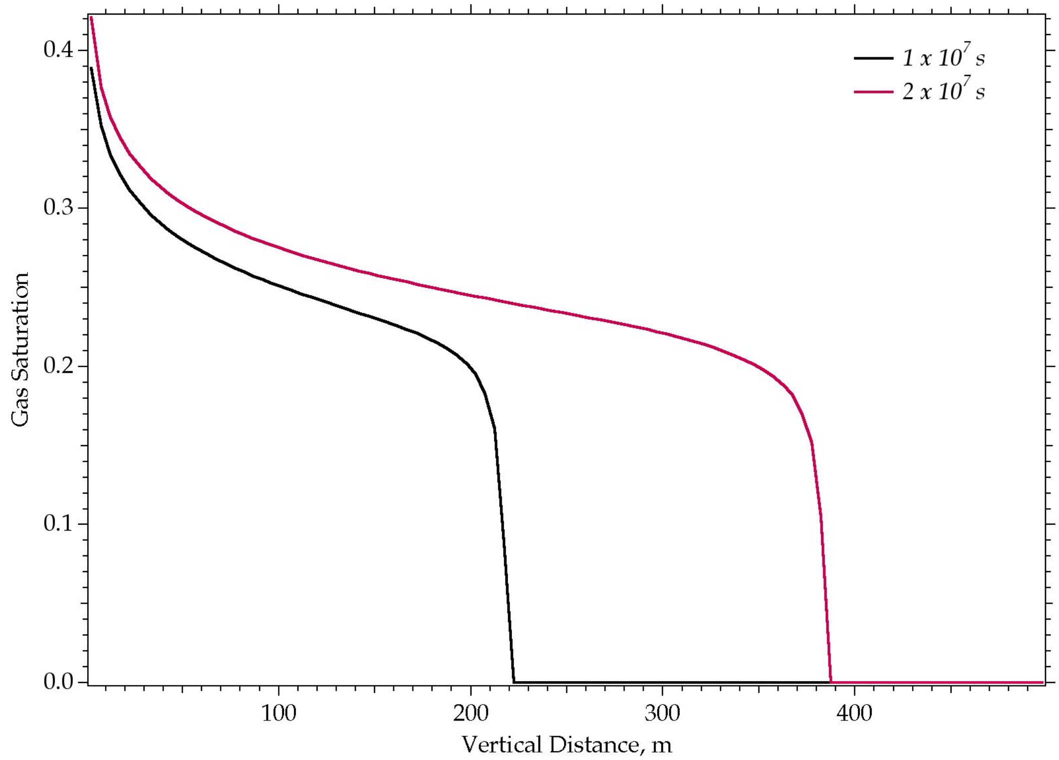

Figure 2. Gas saturation profiles at 1 x 10^7 and 2 x 10^7 s

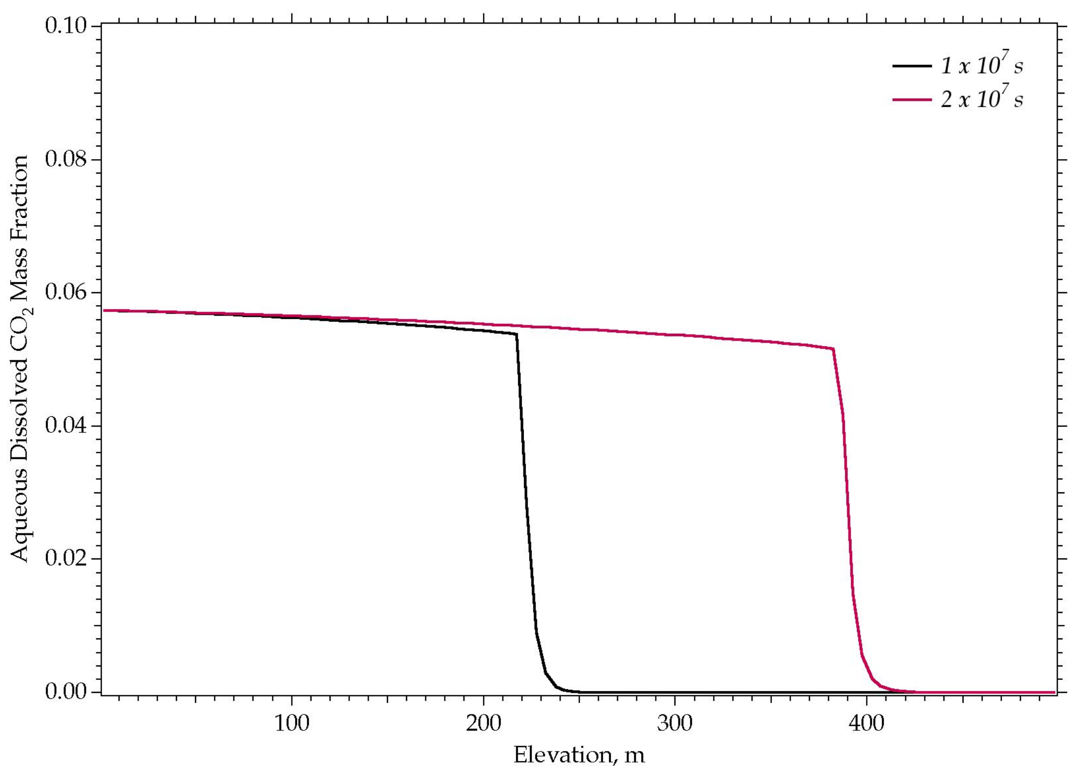

Figure 3. Dissolved CO_2 mass fraction profiles at 1 x 10^7 and 2 x 10^7 s

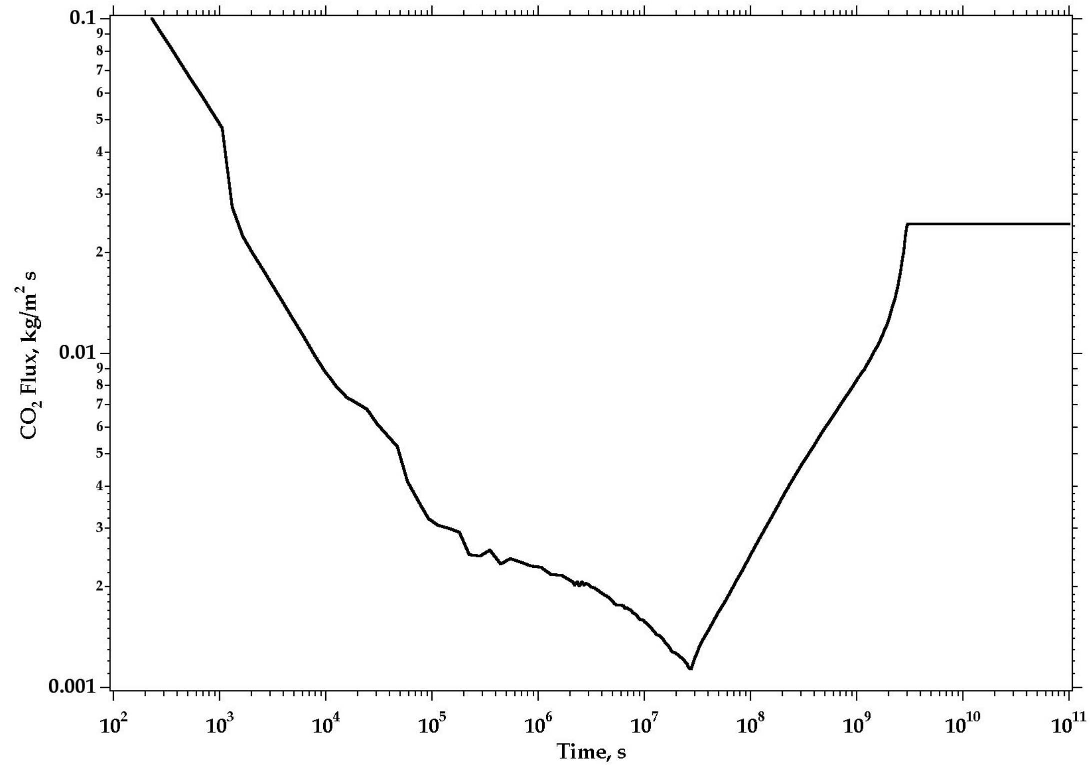

Figure 4. CO_2 flux at the fault bottom, kg/m^2 s

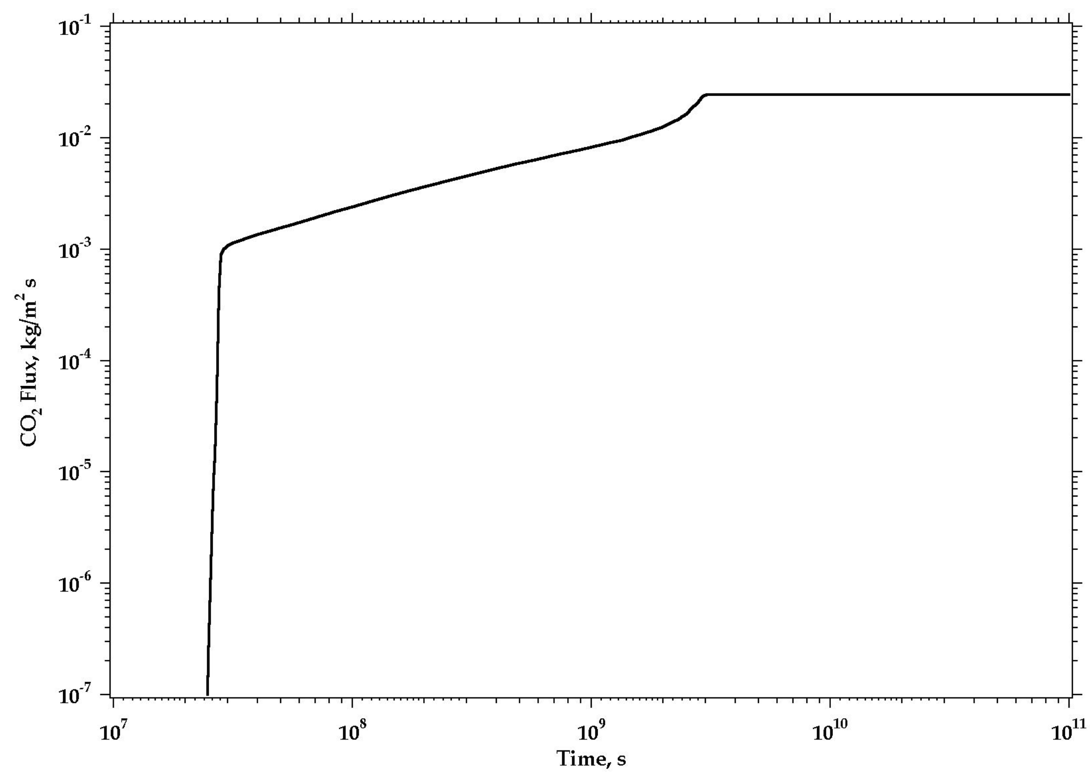

Figure 5. CO_2 flux at the fault top, kg/m^2 s

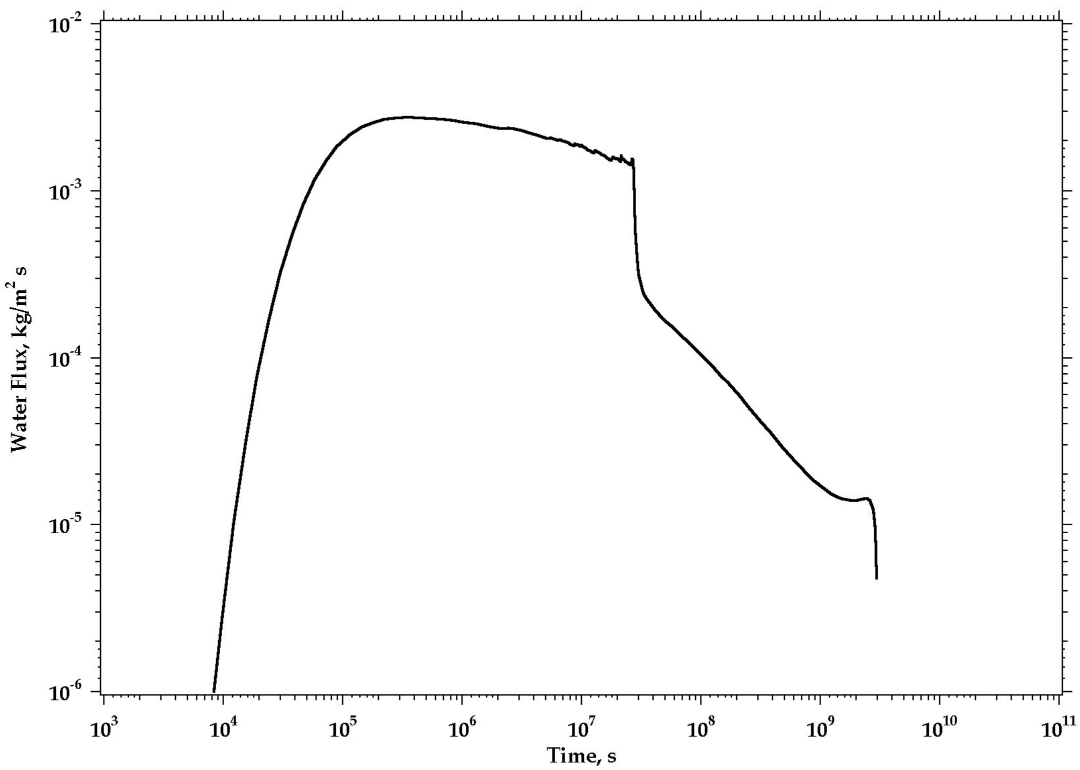

Figure 6. Water flux at the fault top, kg/m^2 s

References

Pruess, K., and J. Garcia. 2002. "Multiphase flow dynamics during CO2 injection into saline aquifers." *Environmental Geology*. 42:282-295.

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 Poynting correction. Contrast the simulation results against those reported for no Poynting correction.
2. (Basic) Repeat the simulation using 15 weight-% NaCl salinity. Contrast the simulation results against those reported for zero salinity.

Input Files

Initial Condition Input File

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M.D. White,
Pacific Northwest Laboratory,
26 August 2002,
14:45 AM PST,
10,
Intercomparison of simulation models for CO2 disposal in
underground storage reservoirs.
Test Problem 4: CO2 Discharge Along a Fault Zone
This problem explores CO2 loss from storage through a leaky fault,
using a highly simplified 1-D linear flow geometry. It is envisioned
that an aquifer into which CO2 disposal is made is intersected by a
vertical fault, which establishes a connection through an otherwise
impermeable caprock to another aquifer 500 m above the storage aquifer.
This situation is idealized by assuming 1-D flow geometry and constant
pressure boundary conditions (Pruess and Garcia, 2000).
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Transient Input File

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Pacific Northwest Laboratory,
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underground storage reservoirs.
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pressure boundary conditions (Pruess and Garcia, 2002).

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