TOUGH
Training Courses

Problem ECO2N: Radial Flow from a CO2 Injection Well

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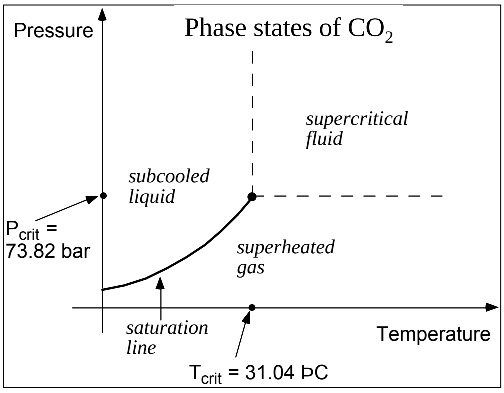
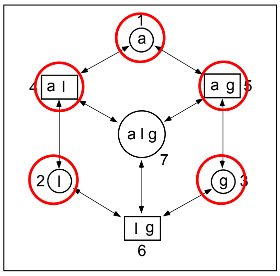
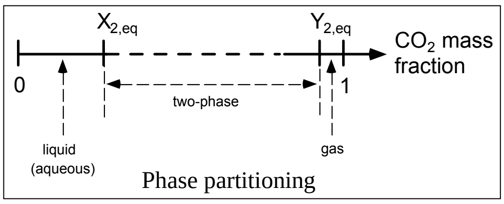
ECO2N for Water-NaCl-CO_2

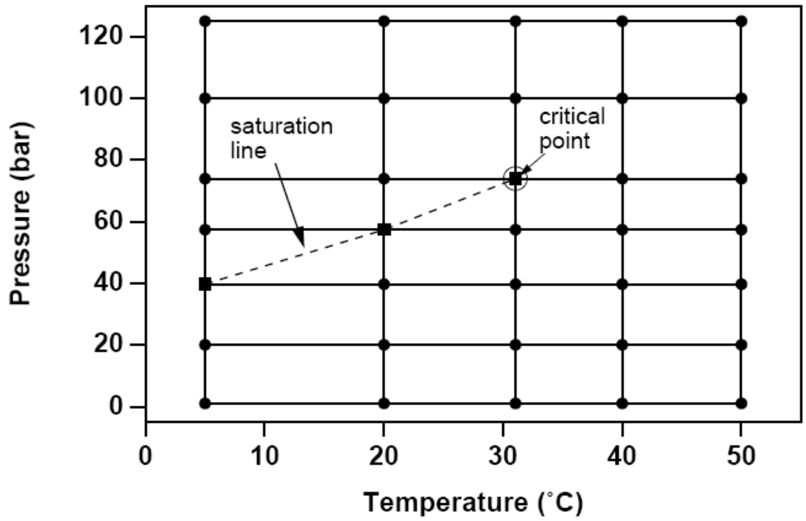






Possible phase combinations in the system water-CO_2:
a – aqueous
l - liquid CO_2
g - gaseous CO_2.
Separate liquid and gas phases exist only at subcritical conditions.

Tabulation of CO_2 Properties



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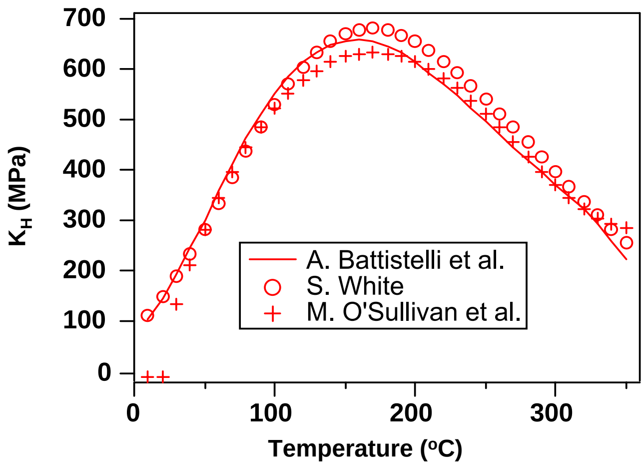
Henry's Coefficient for Dissolution of CO_2 in Liquid Water



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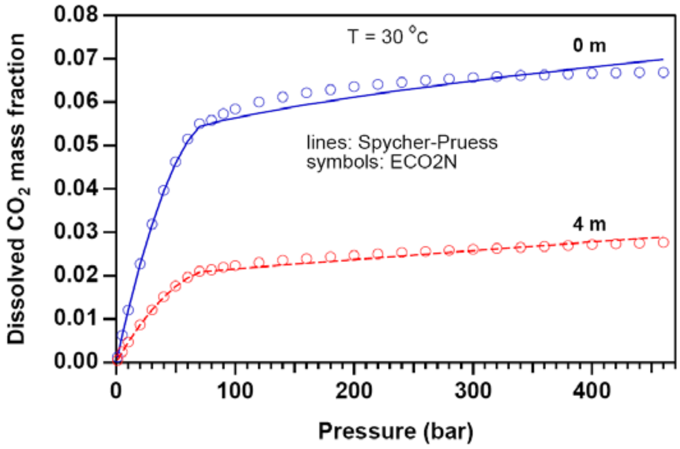
Dissolution of CO_2 in Brine



Dissolved CO_2 mass fractions in two-phase system at T = 30 °C for pure water (0 m) and 4-molal NaCl brine. Lines represent the original correlation of Spycher and Pruess (2005) that uses a Redlich-Kwong EOS for molar volume of CO_2. Symbols represent data calculated by ECO2N in which the molar volume of CO_2 is obtained from the correlations of Altunin (1975)

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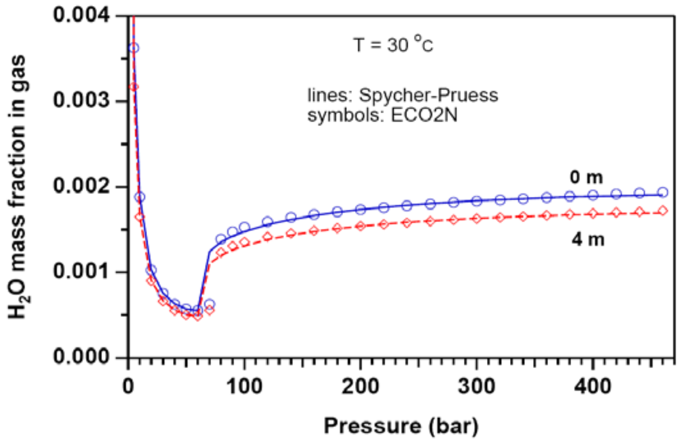
H_2O Mass Fraction in CO_2-Rich Phase



H_2O mass fractions in gas in two-phase system at T = 30 °C for pure water (0 m) and 4- molal NaCl brine. Lines represent the original correlation of Spycher and Pruess (2005) that uses a Redlich-Kwong EOS for molar volume of CO2. Symbols represent data calculated by ECO2N in which the molar volume of CO2 is obtained from the correlations of Altunin (1975).

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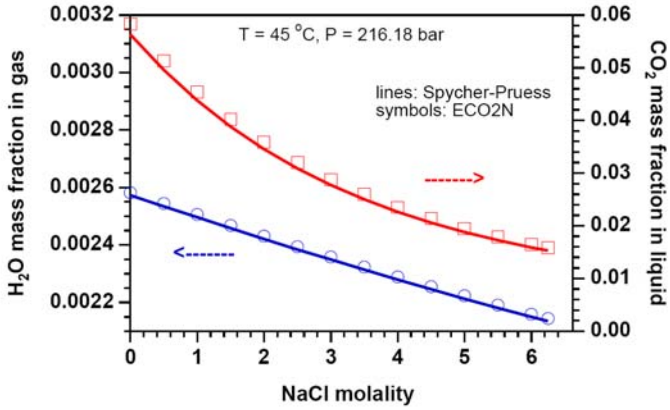
H_2O Concentration in Gas, CO_2 Concentration in Brine



Concentration of water in gas and CO_2 in the liquid (aqueous) phase at (T, P) = (45 °C, 216.18 bar), for salinities ranging from zero to fully saturated. Lines were calculated from the correlation of Spycher and Pruess (2005) that uses a Redlich-Kwong EOS for molar volume of CO_2. Symbols represent data calculated by ECO2N from a modified correlation in which the molar volume of CO_2 is obtained from the correlations of Altunin (1975).

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Summary of ECO2N

<u>Components</u> # 1: water
2: NaCl
3: CO_2

<u>Parameter choices</u>

(NK, NEQ, NPH, NB) = (3, 4, 3, 6) water, NaCl, CO_2, nonisothermal (default)

(3, 3, 3, 6) water, NaCl, CO_2, isothermal
molecular diffusion can be modeled by setting NB = 8

<u>Primary Variables</u>

single fluid phase (only aqueous, or only gas)# (P, X_{sm}, X3, T)
P - pressure
X_{sm} - salt mass fraction X_s in two-component water-salt system, or solid saturation S_s+10
X3 - CO_2 mass fraction in the aqueous phase, or in the gas phase, in the three-component system water-salt-CO_2
T - temperature

two fluid phases (aqueous and gas)# (P, X_{sm}, S_g+10, T)
P - pressure
X_s - salt mass fraction X_s in two-component water-salt system, or solid saturation S_s+10
S_g - gas phase saturation
T - temperature

in addition there may be solid salt

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SELEC Block for ECO2N (1 of 2)

- Dependence of *permeability* on the fraction $\varphi_f \; \varphi_0 = (1-S_s)$ of original pore space that remains available to fluids:
  - 0: permeability does not vary with φ_f
  - 1: $k \; k_0 = (1-S_s)\gamma$
  - 2: fractures in series
  - 3: tubes-in-series
- Model for *water solubility* in CO_2:
  - 0: after Spycher and Pruess (2005)
  - 1: evaporation model; i.e., water density in the CO_2-rich phase is calculated as density of saturated water vapor at prevailing temperature and salinity
- Dependence of *brine density* on dissolved CO_2:
  - 0: brine density varies with dissolved CO_2 concentration according to García (2001)
  - 1: brine density is independent of CO_2 concentration

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SELEC Block for ECO2N (2 of 2)

- Thermophysical properties as a function of *salinity*
  - 0: full dependence.
  - 1: no salinity dependence of thermophysical properties (except for brine enthalpy; salt solubility constraints are maintained).
- Correlation for *brine enthalpy* at saturated vapor pressure
  - 0: after Lorenz et al. (2000).
  - 1: after Michaelides (1981).
  - 2: after Miller (1978).
- PVT properties of CO_2 on file CO2TAB

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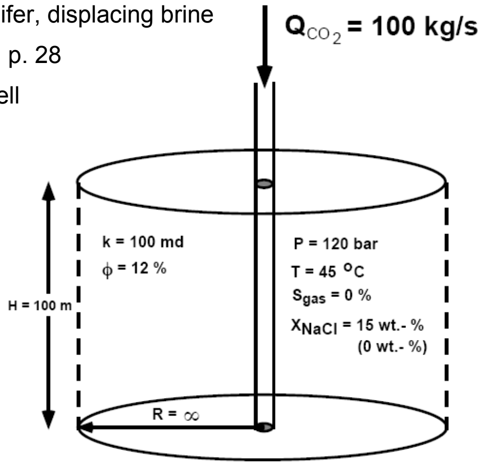
Radial Flow from a CO_2 Injection Well

- CO_2 injection into saline aquifer, displacing brine
- ECO2N manual Section 5.2, p. 28
- Sample2_CO2_Injection_Well
- Input file gcc3



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MESH Generation: Radial Flow

```
*rcc3* ... Code Intercomparison problem3: Radial flow from a CO2 Injection Well
MESHMAKER1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
RZ2D
RADII
    1
        0.
EQUID
    1             .3
LOGAR
  200           1.E3
LOGAR
  100           3.E3
LOGAR
  100           1.E4
LOGAR
   34           1.E5
LAYER----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
    1
      100.

ENDFI----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
```

```
ELEME ---   435    1    1  434    .00000100000.000
A1  1              2 .2827E+02 .5655E+00           .3000E+00          -.5000E+02
A1  2              1 .8728E+02 .1746E+01           .4532E+00          -.5000E+02
A1  3              1 .1501E+03 .3002E+01           .7630E+00          -.5000E+02
A1  4              1 .2169E+03 .4339E+01           .1079E+01          -.5000E+02
...
...

CONNE
A1  1A1  2                   1 .1500E-05 .1532E+00 .1885E+03
A1  2A1  3                   1 .1532E+00 .1565E+00 .3811E+03
A1  3A1  4                   1 .1565E+00 .1599E+00 .5778E+03
...
```

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Input File for Radial Flow Problem

```
*rcc3* ... Code Intercomparison problem3: Radial flow from a CO2 Injection Well
ROCKS----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
SAND     2  2600.e00       .12  100.e-15  100.e-15  100.e-15      2.51      920.
   4.5e-10
    7           .457       .30        1.       .05
    7           .457       .00    5.1e-5      1.e7      .999
well     2  2600.e40       .12  100.e-15  100.e-15  100.e-15      2.51      920.
   4.5e-10
    7           .457       .30        1.       .05
    7           .457       .00    5.1e-5      1.e7      .999

MULTI----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
    3    3    3    6
SELEC....2....3....4....5....6....7....8....9...10...11...12...13...14...15...16
    1                                       0    0    0    0    0    0    0    0
        .8   .8
SOLVR----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
5  Z1   O0    8.0e-1    1.0e-7
START----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
----*----1 MOP: 123456789*123456789*1234 ---*----5----*----6----*----7----*----8
PARAM----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
   1 999     9991000300000000  4    3
              8.64e8       -1.
        1.
     1.E-5     1.E00
              120.e5                 .15                 0.0                 45.
FOFT ----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
A1 49              1 .1745E+04 .2685E+03           .2570E+02          -.6500E+01
A12 2              1 .3080E+08 .4738E+07           .1080E+04          -.6500E+01

GENER----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
A1  1inj 1                         COM3       100.

INCON----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8

TIMES----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
    4
 2.592E+06  8.64E+06  8.64E+07  8.64E+08
ENDCY----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
```

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rcc3

- Generate radial mesh using MESHMAKER, RZ2D
- Edit mesh according to instructions in manual
- Look at input file rcc3 and answer the following questions prior to running the simulation:

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Questions rcc3

- Is this an isothermal or non-isothermal simulation?
  ____
- What approximate overpressure is needed for CO_2 to displace brine? ______________________
  ____
- Fully describe the initial conditions in the saline aquifer: ____________________________
  ____
  ____
  ____

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Questions rcc3

- Run rcc3; answer the following questions:
- Describe the time-stepping and convergence behavior during the first few time steps: ______________________
  ____
  ____
  ____
- Describe the system state after 100 years of CO2 injection:
  ____
  ____
  ____
  ____
  ____
  ____
  ____

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Output from Radial Flow Problem

```
 ...ITERATING...  AT [   1,  1] --- DELTEX = 0.100000E+01   MAX. RES. = 0.353732E+01  AT ELEMENT A1  1  EQUATION   3
 $$$$$$$$$$$ GAS PHASE EVOLVES AT ELEMENT *A1  1*  $$$$$    X3 = 0.267978E-01   XCO2aq = 0.262048E-01 PX = 0.136627E+08 PA
 ...ITERATING...  AT [   1,  2] --- DELTEX = 0.100000E+01   MAX. RES. = 0.246617E-01  AT ELEMENT A1  2  EQUATION   3
 $$$$$$$$ GAS PHASE DISAPPEARS AT ELEMENT *A1  1*  $$$$$    SG = -.904072E-04
 $$$$$$$$$$$ GAS PHASE EVOLVES AT ELEMENT *A1  1*  $$$$$    X3 = 0.262048E-01   XCO2aq = 0.261505E-01 PX = 0.135423E+08 PA
 ...ITERATING...  AT [   1,  3] --- DELTEX = 0.100000E+01   MAX. RES. = 0.123381E-01  AT ELEMENT A1  1  EQUATION   3
 $$$$$$$$ GAS PHASE DISAPPEARS AT ELEMENT *A1  1*  $$$$$    SG = -.100409E-03
 ...ITERATING...  AT [   1,  4] --- DELTEX = 0.100000E+01   MAX. RES. = 0.890409E-02  AT ELEMENT A1  1  EQUATION   3
 ...ITERATING...  AT [   1,  5] --- DELTEX = 0.100000E+01   MAX. RES. = 0.318444E-04  AT ELEMENT A1  1  EQUATION   3
 A1  1(   1,  6) ST = 0.100000E+01 DT = 0.100000E+01 DX1= 0.166338E+07 DX2= -.220039E-15 T =  45.000 P = 13663377. S = 0.000000E+00
 ...ITERATING...  AT [   2,  1] --- DELTEX = 0.100000E+01   MAX. RES. = 0.100000E+01  AT ELEMENT A1  1  EQUATION   3
 $$$$$$$$$$$ GAS PHASE EVOLVES AT ELEMENT *A1  1*  $$$$$    X3 = 0.515157E-01   XCO2aq = 0.264066E-01 PX = 0.141315E+08 PA
 ...ITERATING...  AT [   2,  2] --- DELTEX = 0.100000E+01   MAX. RES. = 0.986667E+00  AT ELEMENT A1  1  EQUATION   3
 ...ITERATING...  AT [   2,  3] --- DELTEX = 0.100000E+01   MAX. RES. = 0.906190E+00  AT ELEMENT A1  2  EQUATION   3
 ...ITERATING...  AT [   2,  4] --- DELTEX = 0.100000E+01   MAX. RES. = 0.171549E+00  AT ELEMENT A1  2  EQUATION   3
 ...ITERATING...  AT [   2,  5] --- DELTEX = 0.100000E+01   MAX. RES. = 0.110501E-01  AT ELEMENT A1  2  EQUATION   3
 ...ITERATING...  AT [   2,  6] --- DELTEX = 0.100000E+01   MAX. RES. = 0.115547E-03  AT ELEMENT A1  2  EQUATION   3
 A1  2(   2,  7) ST = 0.200000E+01 DT = 0.100000E+01 DX1= 0.111159E+07 DX2= 0.974701E-07 T =  45.000 P = 14270651. S = 0.000000E+00
 ...ITERATING...  AT [   3,  1] --- DELTEX = 0.100000E+01   MAX. RES. = 0.496177E+00  AT ELEMENT A1  1  EQUATION   3
 ...ITERATING...  AT [   3,  2] --- DELTEX = 0.100000E+01   MAX. RES. = 0.124120E-01  AT ELEMENT A1  1  EQUATION   3
 ...ITERATING...  AT [   3,  3] --- DELTEX = 0.100000E+01   MAX. RES. = 0.252259E-04  AT ELEMENT A1  2  EQUATION   3
 A1  1(   3,  4) ST = 0.300000E+01 DT = 0.100000E+01 DX1= 0.158370E+07 DX2= 0.972615E-05 T =  45.000 P = 17948923. S = 0.722178E-01
 ...ITERATING...  AT [   4,  1] --- DELTEX = 0.200000E+01   MAX. RES. = 0.661797E+00  AT ELEMENT A1  1  EQUATION   3
 ...ITERATING...  AT [   4,  2] --- DELTEX = 0.200000E+01   MAX. RES. = 0.745778E+00  AT ELEMENT A1  2  EQUATION   3
 ...ITERATING...  AT [   4,  3] --- DELTEX = 0.200000E+01   MAX. RES. = 0.679967E-01  AT ELEMENT A1  2  EQUATION   3
 ...ITERATING...  AT [   4,  4] --- DELTEX = 0.200000E+01   MAX. RES. = 0.594905E-03  AT ELEMENT A1  2  EQUATION   3
 A1  2(   4,  5) ST = 0.500000E+01 DT = 0.200000E+01 DX1= 0.259505E+06 DX2= -.563856E-06 T =  45.000 P = 14951272. S = 0.000000E+00
 ...ITERATING...  AT [   5,  1] --- DELTEX = 0.200000E+01   MAX. RES. = 0.523482E+00  AT ELEMENT A1  2  EQUATION   3
 ...ITERATING...  AT [   5,  2] --- DELTEX = 0.200000E+01   MAX. RES. = 0.378805E+00  AT ELEMENT A1  2  EQUATION   3
 ...ITERATING...  AT [   5,  3] --- DELTEX = 0.200000E+01   MAX. RES. = 0.890199E-02  AT ELEMENT A1  2  EQUATION   3
 A1  2(   5,  4) ST = 0.700000E+01 DT = 0.200000E+01 DX1= 0.957718E+05 DX2= -.261078E-05 T =  45.000 P = 15047044. S = 0.000000E+00
 ...ITERATING...  AT [   6,  1] --- DELTEX = 0.400000E+01   MAX. RES. = 0.132942E+01  AT ELEMENT A1  2  EQUATION   3
 $$$$$$$$$$$ GAS PHASE EVOLVES AT ELEMENT *A1  2*  $$$$$    X3 = 0.414314E-01   XCO2aq = 0.267721E-01 PX = 0.150490E+08 PA
 ...ITERATING...  AT [   6,  2] --- DELTEX = 0.400000E+01   MAX. RES. = 0.103059E+01  AT ELEMENT A1  2  EQUATION   3
 ...ITERATING...  AT [   6,  3] --- DELTEX = 0.400000E+01   MAX. RES. = 0.896260E+00  AT ELEMENT A1  3  EQUATION   3
 ...ITERATING...  AT [   6,  4] --- DELTEX = 0.400000E+01   MAX. RES. = 0.219633E+00  AT ELEMENT A1  3  EQUATION   3
 ...ITERATING...  AT [   6,  5] --- DELTEX = 0.400000E+01   MAX. RES. = 0.164693E-01  AT ELEMENT A1  3  EQUATION   3
 ...ITERATING...  AT [   6,  6] --- DELTEX = 0.400000E+01   MAX. RES. = 0.150149E-03  AT ELEMENT A1  3  EQUATION   3
 A1  3(   6,  7) ST = 0.110000E+02 DT = 0.400000E+01 DX1= 0.392177E+06 DX2= -.150040E-06 T =  45.000 P = 14761447. S = 0.000000E+00
```

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Output from Radial Flow Problem

```
*rcc3* ... Code Intercomparison problem3: Radial flow from a CO2 Injection Well

         OUTPUT DATA AFTER ( 358,  5)-2-TIME STEPS                                                  THE TIME IS 0.100000E+04 DAYS
 @@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@

  TOTAL TIME     KCYC    ITER  ITERC    KON        DX1M         DX2M         DX3M          MAX. RES.       NER    KER        DELTEX
 0.864000E+08     358       5   2476      2       0.14482E+06  0.68369E-01  0.11142E+00    0.85015E-06      59     2       0.14599E+07
 @@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@

 ELEM. INDEX    P          T        SG          SS         XNACL       YH2OG       XCO2aq       PCAP       k-red.      DG        DL
              (Pa)     (deg-C)                                                                  (Pa)                 (kg/m3)    (kg/m3)

 A1  1    1 0.22350E+08  45.00 0.93159E+00 0.68408E-01 0.00000E+00 0.00000E+00 0.15977E-01 -.94561E+07 0.10000E+01  836.33       0.00
 A1  2    2 0.22273E+08  45.00 0.95700E+00 0.42995E-01 0.00000E+00 0.00000E+00 0.15964E-01 -.94561E+07 0.10000E+01  835.64       0.00
 A1  3    3 0.22197E+08  45.00 0.95823E+00 0.41769E-01 0.00000E+00 0.00000E+00 0.15952E-01 -.94561E+07 0.10000E+01  834.95       0.00
 A1  4    4 0.22145E+08  45.00 0.95947E+00 0.40525E-01 0.00000E+00 0.00000E+00 0.15943E-01 -.94561E+07 0.10000E+01  834.49       0.00
 A1  5    5 0.22106E+08  45.00 0.96055E+00 0.39446E-01 0.00000E+00 0.00000E+00 0.15936E-01 -.94561E+07 0.10000E+01  834.14       0.00
 A1  6    6 0.22075E+08  45.00 0.96205E+00 0.37946E-01 0.00000E+00 0.00000E+00 0.15931E-01 -.94561E+07 0.10000E+01  833.86       0.00
 A1  7    7 0.22048E+08  45.00 0.96166E+00 0.38340E-01 0.00000E+00 0.00000E+00 0.15927E-01 -.94561E+07 0.10000E+01  833.62       0.00
 A1  8    8 0.22025E+08  45.00 0.96045E+00 0.39549E-01 0.00000E+00 0.00000E+00 0.15923E-01 -.94561E+07 0.10000E+01  833.41       0.00
 A1  9    9 0.22005E+08  45.00 0.96181E+00 0.38190E-01 0.00000E+00 0.00000E+00 0.15920E-01 -.94561E+07 0.10000E+01  833.23       0.00
 A1 10   10 0.21987E+08  45.00 0.96354E+00 0.36461E-01 0.00000E+00 0.00000E+00 0.15916E-01 -.94561E+07 0.10000E+01  833.06       0.00
 A1 11   11 0.21970E+08  45.00 0.96205E+00 0.37947E-01 0.00000E+00 0.00000E+00 0.15913E-01 -.94561E+07 0.10000E+01  832.91       0.00
 A1 12   12 0.21955E+08  45.00 0.96121E+00 0.38790E-01 0.00000E+00 0.00000E+00 0.15911E-01 -.94561E+07 0.10000E+01  832.77       0.00
 A1 13   13 0.21941E+08  45.00 0.96235E+00 0.37652E-01 0.00000E+00 0.00000E+00 0.15908E-01 -.94561E+07 0.10000E+01  832.64       0.00
 A1 14   14 0.21927E+08  45.00 0.96271E+00 0.37294E-01 0.00000E+00 0.00000E+00 0.15906E-01 -.94561E+07 0.10000E+01  832.52       0.00
 A1 15   15 0.21915E+08  45.00 0.96180E+00 0.38201E-01 0.00000E+00 0.00000E+00 0.15904E-01 -.94561E+07 0.10000E+01  832.40       0.00
 A1 16   16 0.21903E+08  45.00 0.96306E+00 0.36940E-01 0.00000E+00 0.00000E+00 0.15902E-01 -.94561E+07 0.10000E+01  832.30       0.00
 A1 17   17 0.21892E+08  45.00 0.96448E+00 0.35525E-01 0.00000E+00 0.00000E+00 0.15900E-01 -.94561E+07 0.10000E+01  832.19       0.00
 A1 18   18 0.21882E+08  45.00 0.96256E+00 0.37440E-01 0.00000E+00 0.00000E+00 0.15898E-01 -.94561E+07 0.10000E+01  832.10       0.00
 A1 19   19 0.21872E+08  45.00 0.96256E+00 0.37438E-01 0.00000E+00 0.00000E+00 0.15897E-01 -.94561E+07 0.10000E+01  832.01       0.00
 A1 20   20 0.21862E+08  45.00 0.96446E+00 0.35544E-01 0.00000E+00 0.00000E+00 0.15895E-01 -.94561E+07 0.10000E+01  831.92       0.00
```

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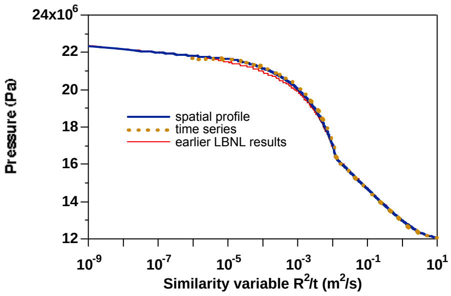
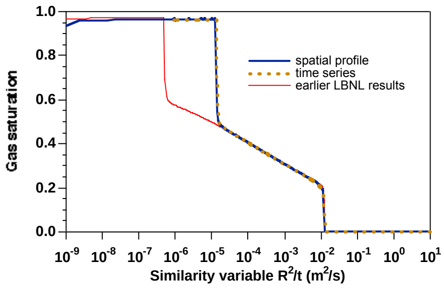
Pressure and Saturation Profiles from Radial Flow Problem





Similarity variable: R^2/t
Spatial profile at $t = 8.64 \times 10^7$ s
Time series at $R = 25.25$ m
Thin line: earlier LBNL results with "evaporation model"

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Questions rcc3

- Modify rcc3, for example:
  - Make simulation non-isothermal
  - Add permeability reduction due to salt precipitation
  - Change thermodynamic models in SELEC block
  - Refine or coarsen mesh
  - Stop CO_2 injection; observe pressure recovery and phase redistribution
  - Change capillary pressure and relative permeability functions and observe impact in residual CO_2 trapping
- For each modification, discuss effect on simulation results

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