Sample Problems

- serve as benchmarks to document code applications, and to check on proper code installation;
- tutorial for learning the code;
- templates for developing new applications.

TOUGH2/EOS3: water, air

Components	# 1: water # 2: air
Parameter choices	
(NK, NEQ, NPH, NB) =	(2, 3, 2, 6) water and air, nonisothermal (default) (2, 2, 2, 6) water and air, isothermal molecular diffusion can be modeled by setting NB = 8
Primary Variables*	
single-phase conditions	
(P, X, T) - (pressure, air mass fraction, temperature)	
two-phase conditions	
(P_g, S_g + 10, T) - (gas phase pressure, gas saturation plus 10, temperature)	

* By setting MOP(19) = 1, initialization can be made with TOUGH-style variables (P, T, X) for single-phase, (P_g, S_g, T) for two-phase.

Input File (Sample Problem 1)

MOP(19) = 1:
(P, T, X) for single-phase,
(P_g, S_g, T) for two-phase

```
*sam1* CODE DEMONSTRATION: PHASE TRANSITIONS, COMPONENT (DIS-)APPEARANCES
ROCKS----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
TRANS          2650.       .50    1.E-14                          2.10     1000.
SHOME    2     2650.       .50    1.E-14                          2.10     1000.
                           1.8        .1
    3            .40       .10
    1           1.E5        .2        1.

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
   2   4       1100 30 000000200711
                          -1.          F   1
      1.E2      5.E3

                45.E5                  .5               250.
FOFT ----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
F   1
abc 2
F   7

GOFT ----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
F   2
f   1
SHO 9
SHO 2
F   8

RPCAP----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
    3            .30       .05
    1                       1.
TIMES----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
    1    3               2.E3
      1.E3
ELEME----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
F   1    9    1TRANS       10.
SHO 1    9    1SHOME       10.
SHO11    1    1SHOME      1.E4

CONNE----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
F   1F   2                  1        5.        5.        1.
F   3F   4                  1        5.        5.        1.
F   5F   6                  1        5.        5.        1.

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

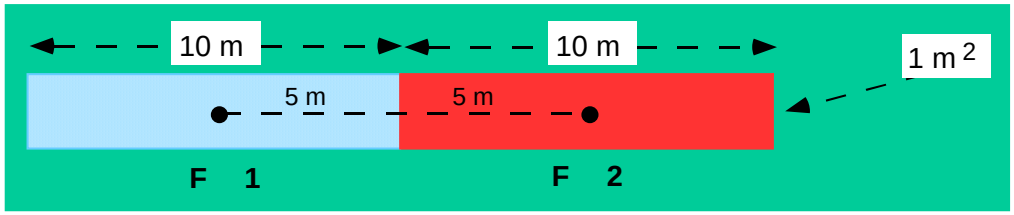
Input File (Sample Problem 1, cont'd)

MOP(19) = 1:
(P, T, X) for single-phase,
(P_g, S_g, T) for two-phase

```
INCON----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
F   1
              1.E5                 20.                  1.
F   2
              1.E6                170.                  0.
F   3
              1.E5                .001                99.5
F   4
             99.E5                .999                310.
F   5
              1.E6                100.                  0.
F   6
             10.E6                100.                  1.
F   7
              1.E5                 20.                  0.
F   8
              1.E7                300.                  0.
F   9
              1.E5                 .99                 90.
F  10
             40.E5                280.                  0.
SHO11
             50.E5                240.
SHO12
             40.E5                100.

GENER----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
f    1AIR                         AIR       5.E-3   9.882E4
F    7AIR                         AIR       5.E-3   9.882E4
F    8WEL                         MASS    -1.5E-2
F    9HOT                         HEAT       2.E6
F   10COL                         HEAT      -5.E5
SHO 1P   1                        MASS1       -1.      1.E6
SHO 2P   2                        laff         -1.
SHO 3P   3    2    1    1    4    MASS
           0.          1.E2          2.E2          4.E3
        -0.1           -0.2          -0.3          -1.1
SHO 6P   6    2    1    0    4    MASS1
           0.          1.E2          2.E2          4.E3
        -0.1           -0.2          -0.3          -1.1
         1.E6          2.E6          3.E6         1.1E7
SHO 9P   9                   1     DELV     1.E-12      1.E6
SHO10P  10                   4     WATE1
           0.          1.E2          2.E2          3.E3
         1.1            1.0           0.9           0.1
         1.E6         1.2E6         1.4E6         3.0E6
SHO11WEL00                   2     DELV     1.E-12                1.E2
SHO12WEL00                         DELV     2.E-12      1.E6      1.E2

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

```
ELEME----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
F   1    9    1TRANS       10.

CONNE----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
F   1F   2                  1        5.        5.        1.

INCON----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
F   1
                1.E5                20.                 1.
F   2
                1.E6               170.                 0.
```

$$\text{MOP(19)} = 1 \begin{cases} \text{P, T, X} & \text{single-phase} \\ \text{P}_g, \text{S}_g, \text{T} & \text{two-phase} \end{cases}$$



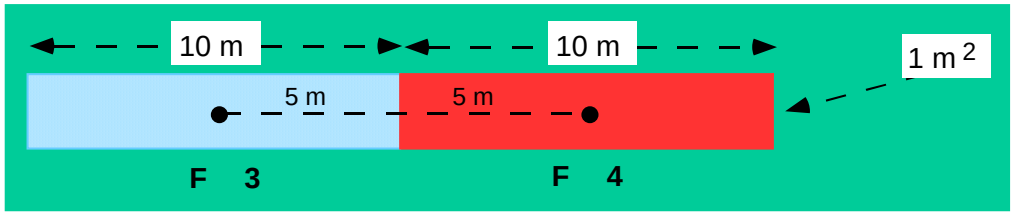
P:	1.e5	1.e6	Pa
T:	20	170	°C
X:	1 (air)	0 (water)	

"hot water being pushed into cold air"

expect: P¯ in (F 2), evolve gas (vapor) phase
P_ in (F 1), evolve aqueous phase

```
ELEME----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
F   1    9    1TRANS       10.

CONNE----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
F   3F   4                   1        5.        5.        1.

INCON----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
F   3
                1.E5                .001                99.5
F   4
               99.E5                .999                310.
```

$$\text{MOP(19)} = 1 \begin{cases} \text{P, T, X} & \text{single-phase} \\ \text{P}_g, \text{S}_g, \text{T} & \text{two-phase} \end{cases}$$



P:	1.e5	99.e5	Pa
T:	99.5	310	°C
S_g:	.001	.999	

"hot steam being pushed into colder two-phase zone"

expect: P‾ in (F 4), water evaporating; liquid phase disappearing

P_ in (F 3), incoming steam condensing; gas phase disappearing

Printed Output

```
********** VOLUME- AND MASS-BALANCES ************************************************************************************

********** [KCYC,ITER] = [    0,   0] *****                                THE TIME IS    .00000E+00 SECONDS, OR    .00000E+00 DAYS


PHASE VOLUMES IN PLACE
GAS    .49950E+02 M**3;   LIQUID   .10050E+05 M**3

MASS IN PLACE
GAS    .14263E+04 KG;     LIQUID   .89195E+07 KG;    AIR   .56359E+03 KG;    VAPOR   .86436E+03 KG;   LIQUID WATER   .89195E +07 KG

************************************************************************************************************************


...ITERATING...  AT [    1,   1] --- DELTEX =  .100000E+03   MAX. RES. =  .393471E+01  AT ELEMENT SHO 9  EQUATION   2
$$$$$$$$$$$$$ LIQUID PHASE EVOLVES AT ELEMENT *F   1*  $$$$$      PS =  .120555E+05  PSAT =  .233989E+04
$$$$$$$$$$$$$$$$ GAS PHASE EVOLVES AT ELEMENT *F   5*  $$$$$    XAIR =  .679538E -03    PX =  .240543E+07   PG =  .432994E+07
$$$$$$$$$$$$$$$$ GAS PHASE EVOLVES AT ELEMENT *F   7*  $$$$$    XAIR =  .100168E -03    PX =  .321052E+06   PG =  .625505E+06
...ITERATING...  AT [    1,   2] --- DELTEX =  .100000E+03   MAX. RES. =  .863043E+00  AT ELEMENT SHO 9  EQUATION   2
...ITERATING...  AT [    1,   3] --- DELTEX =  .100000E+03   MAX. RES. =  .803189E-02  AT ELEMENT SHO 9  EQUATION   2
F   1(    1,  4) ST =  .100000E+03 DT =  .100000E+03 DX1=  .234670E+04 DX2=  .999993E+01 T =  20.006 P =   102347. S =  .999928E+00

*sam1* CODE DEMONSTRATION: PHASE TRANSITIONS, COMPONENT (DIS-)APPEARANCES

         OUTPUT DATA AFTER (    1,   4)-2-TIME STEPS                                           THE TIME IS   .11574E -02 DAYS

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TOTAL TIME	KCYC	ITER	ITERC	KON	DX1M	DX2M	DX3M	MAX. RES.	NER	KER	DELTEX
.10000E+03	1	4	4	2	.16455E+07	.10000E+02	.14654E+02	.11503E-05	19	2	.10000E+03

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ELEM.	INDEX	P (PA)	T (DEG-C)	SG	SL	XAIRG	XAIRL	PER.MOD.	PCAP (PA)	DG (KG/M**3)	DL (KG/M**3)
F 1	1	.10235E+06	.20006E+02	.99993E+00	.715 01E-04	.98565E+00	.16076E-04	.10000E+01	.00000E+00	.12055E+01	.99832E+03
F 2	2	.84410E+06	.16999E+03	.00000E+00	.10000E+01	.00000E+00	.00000E+00	.10000E+01	.00000E+00	.00000E+00	.89734E+03
F 3	3	.10570E+06	.99591E+02	.65930E-03	.99934E+00	.84784E-01	.93960E-06	.10000E+01	.00000E+00	.64424E+00	.95842E+03
F 4	4	.98861E+07	.30990E+03	.99927E+00	.73379E-03	.32622E-02	.47952E-05	.10000E+01	.00000E+00	.54629E+02	.69093E+03
F 5	5	.26455E+07	.10005E+ 03	.37436E-03	.99963E+00	.97540E+00	.40887E-03	.10000E+01	.00000E+00	.24341E+02	.95931E+03
F 6	6	.99566E+07	.99984E+02	.10000E+01	.00000E+00	.10000E+01	.15995E -02	.10000E+01	.00000E+00	.92941E+02	.00000E+00
F 7	7	.61923E+06	.20005E+02	.13611E-03	.99986E+00	.99765E+00	.99159E-04	.10000E+01	.00000E+00	.73467E+01	.99856E+03
F 8	8	.98110E+07	.29995E+03	.00000E+00	.10000E+01	.00000E+00	.00000E+00	.10000E+01	.00000E+00	.00000E+00	.71508E+03
F 9	9	.15045E+06	.10465E+03	.99017E+00	.98254E-02	.29149E+00	.49979E-05	.10000E+01	.00000E+00	.98336E+00	.95473E+03
F 10	10	.39597E+07	.27628E+03	.10000E+01	.00000E+00	.00000E+00	.00000E+00	.10000E+01	.00000E+00	.18037E+02	.00000E+00
SHO 1	11	.44873E+07	.25017E+03	.52552E+00	.47448E+00	.14192E+00	.80067E -04	.10000E+01	-.65690E+05	.23360E+02	.79951E+03
SHO 2	12	.45000E+07	.25000E+03	.50000E+00	.50000E+00	.14823E+00	.83971E -04	.10000E+01	-.62500E+05	.23463E+02	.7997 9E+03
SHO 3	13	.43239E+07	.24902E+03	.50401E+00	.49599E+00	.12258E+00	.66147E -04	.10000E+01	-.63001E+05	.22393E+02	.80110E+03
SHO 4	14	.43239E+07	.24902E+03	.50401E+00	.49599E+00	.12258E+00	.66147E -04	.10000E+01	-.63001E+05	.22393E+02	.80110E+03
SHO 5	15	.43239E+07	.24902E+03	.50401E+00	.49599E+00	.12258E+00	.66147E -04	.10000E+01	-.63001E+05	.22393E+02	.80110E+03
SHO 6	16	.44764E+07	.24971E+03	.50405E+00	.49595E+00	.14789E+00	.83275E -04	.10000E+01	-.63006E+05	.23336E+02	.80021E+03
SHO 7	17	.44764E+07	.24971E+03	.50405E+00	.49595E+00	.14789E+00	.83275E -04	.10000E+01	-.63006E+05	.23336E+02	.80021E+03
SHO 8	18	.44764E+07	.24971E+03	.50405E+00	.49595E+00	.14789E+00	.83275E -04	.10000E+01	-.63006E+05	.23336E+02	.80021E+03
SHO 9	19	.32791E+07	.23713E+03	.55068E+00	.44932E+00	.39998E -01	.15625E-04	.10000E+01	-.68834E+05	.16588E+02	.81772E+03
SHO10	20	.45462E+07	.25026E+03	.47289E+00	.52711E+00	.15455E+00	.88636E -04	.10000E+01	-.59111E+05	.23743E+02	.79945E+03
SHO11	21	.45429E+07	.23994E+03	.00000E+00	.10000E+01	.00000E+00	.00000E+00	.10000E+01	.00000E+00	.00000E+00	.81498E+03
SHO12	22	.32957E+07	.99971E+02	.00000E+00	.10000E+01	.00000E+00	.00000E+00	.10000E+01	.00000E+00	.00000E+00	.95968E+03

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Printed Output (cont'd)

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...ITERATING...  AT [   2,  1] --- DELTEX =  .900000E+03   MAX. RES. =  .630671E+01  AT ELEMENT SHO 9  EQUATION   2
$$$$$$$$$$$$$$$$ GAS PHASE EVOLVES AT ELEMENT *F   2*  $$$$$    XAIR =  .000000E+00    PX =  .358503E+06   PG =  .791056E+06
$$$$$$$$$$$$$ GAS PHASE DISAPPEARS AT ELEMENT *F   3*  $$$$$      SG = -.234280E-02
$$$$$$$$$$ LIQUID PHASE DISAPPEARS AT ELEMENT *F   4*  $$$$$      SG =  .100161E+01
$$$$$$$$$$$$$$$$ GAS PHASE EVOLVES AT ELEMENT *F   8*  $$$$$    XAIR =  .000000E+00    PX =  .811355E+07   PG =  .853065E+07
$$$$$$$$$$$$$ LIQUID PHASE EVOLVES AT ELEMENT *F  10*  $$$$$      PS =  .359570E+07  PSAT =  .351560E+07
$$$$$$$$$$$$$$$$ GAS PHASE EVOLVES AT ELEMENT *SHO11*  $$$$$    XAIR =  .000000E+00    PX =  .292288E+07   PG =  .333073E+07
...ITERATING...  AT [   2,  2] --- DELTEX =  .900000E+03   MAX. RES. =  .117227E+01  AT ELEMENT F   9  EQUATION   1
$$$$$$$$$$$$$ GAS PHASE DISAPPEARS AT ELEMENT *F   5*  $$$$$      SG = -.155779E-02
$$$$$$$$$$ LIQUID PHASE DISAPPEARS AT ELEMENT *F   9*  $$$$$      SG =  .100503E+01
...ITERATING...  AT [   2,  3] --- DELTEX =  .900000E+03   MAX. RES. =  .208643E+01  AT ELEMENT F   6  EQUATION   1
...ITERATING...  AT [   2,  4] --- DELTEX =  .900000E+03   MAX. RES. =  .127394E+01  AT ELEMENT F   5  EQUATION   2
$$$$$$$$$$$$$$$$ GAS PHASE EVOLVES AT ELEMENT *F   5*  $$$$$    XAIR =  .274953E-02    PX =  .676786E+07   PG =  .172244E+08
...ITERATING...  AT [   2,  5] --- DELTEX =  .900000E+03   MAX. RES. =  .637298E+00  AT ELEMENT F   5  EQUATION   2
...ITERATING...  AT [   2,  6] --- DELTEX =  .900000E+03   MAX. RES. =  .819031E-01  AT ELEMENT F   5  EQUATION   2
...ITERATING...  AT [   2,  7] --- DELTEX =  .900000E+03   MAX. RES. =  .743440E-03  AT ELEMENT F   5  EQUATION   2
F   1(   2,  8) ST =  .100000E+04 DT =  .900000E+03 DX1=  .160677E+03 DX2= -.742620E-03 T =  20.186 P =   102507. S =  .999186E+00

*sam1* CODE DEMONSTRATION: PHASE TRANSITIONS, COMPONENT (DIS-)APPEARANCES

         OUTPUT DATA AFTER (   2,  8)-2-TIME STEPS                                                  THE TIME IS   .11574E-01 DAYS

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 TOTAL TIME      KCYC    ITER   ITERC    KON         DX1M          DX2M          DX3M          MAX. RES.      NER     KER        DELTEX
  .10000E+04       2       8     12       2        .57413E+07   .11000E+02    .12802E+03     .61975E-07       5      2        .90000E+03

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ELEM.  INDEX      P            T           SG           SL        XAIRG        XAIRL        PER.MOD.     PCAP         DG           DL
                 (PA)       (DEG-C)                                                                    (PA)      (KG/M**3)    (KG/M**3)

F   1      1  .10251E+06  .20186E+02  .99919E+00  .81412E-03  .98551E+00  .16098E-04  .10000E+01  .00000E+00  .12066E+01  .99829E+03
F   2      2  .79168E+06  .16998E+03  .79890E-03  .99920E+00  .15543E-14  .13099E-18  .10000E+01  .00000E+00  .41211E+01  .89732E+03
F   3      3  .48905E+07  .10056E+03  .00000E+00  .10000E+01  .00000E+00  .84691E-05  .10000E+01  .00000E+00  .00000E+00  .96001E+03
F   4      4  .96833E+07  .30936E+03  .10000E+01  .00000E+00  .32322E-02  .45940E-05  .10000E+01  .00000E+00  .52870E+02  .00000E+00
```

Version Control

```
*****************************************************************************************************************************
*                                                                                                                           *
*                                          SUMMARY OF PROGRAM UNITS USED                                                    *
*                                                                                                                           *
*****************************************************************************************************************************

     UNIT    VERSION     DATE                COMMENTS
_____________________________________________  ___________________________________________________________________________

     IO       1.0      15 APRIL     1991      OPEN FILES *VERS*, *MESH*, *INCON*, *GENER*, *SAVE*, *LINEQ*, AND *TABLE*
     SECOND   1.0       6 September 1994      CPU timing function for IBM RS/6000

     TOUGH2   2.00     20 February  20  05       MAIN PROGRAM
                                                SPECIAL VERSION FOR CONJUGATE GRADIENT PACKAGE T2CG2
                                                INCLUDES DEFINITION OF COORDINATE ARRAYS AND RADIATIVE HEAT TRANSFER CAPABILITY
                                                HAS ADDITIONAL COMMON BLOCKS FOR TMVOC

     INPUT    2.0       2 APRIL     2002      READ ALL DATA PROVIDED THROUGH FILE *INPUT*
     FLOP     1.0      11 APRIL     1991      CALCULATE NUMBER OF SIGNIFICANT DIGITS FOR FLOATING POINT ARITHMETIC

     RFILE     1.5       2 APRIL     2002      INITIALIZE DATA FROM FILES *MESH* OR *MINC*, *GENER*, AND *INCON*
                                                ALSO INITIALIZES PERMEABILITY MODIFIERS AND COORDINATE ARRAYS
                                                AND OPTIONALLY READS TABLES WITH FLOWING WELLBORE PRESSURES
     PMIN     1.0      26 September 1997      initialize block    -by-block permeability modifiers
     SINSUB   1.00      1 October   1999      initialize parameters for the solver package, and generate informative printout

     CYCIT    1.01     20 SEPTEMBER 2001      EXECUTIVE ROUTINE FOR MARCHING IN TIME

     EOS      1.01     11 January   1999      *EOS3* ... THERMOPHYSICAL PROPERTIES MODULE FOR WATER/AIR
     SAT      1.0 S    17 SEPTEMBER 1990      STEAM TABLE EQUATION: SATURATION PRESSURE AS FUNCTION OF TEMPERATURE (M. OS.)
     PCAP     1.0       9 November  1999      CAPILLARY PRESSURE AS FUNCTION OF SATURATION
     PP       1.0       1 FEBRUARY  1990      CALCULATE VAPOR PRESSURE, DENSITY, INT. ENERGY AS F(P,T,X)
     VISCO    1.0       1 FEBRUARY  1990      CALCULATE VISCOSITY OF VAPOR    -AIR MIXTURES
     COVIS    1.0       1 FEBRUARY  1990      COEFFICIENT FOR GAS PHASE VISCOSITY CALCULATION
     VISS     1.0      22 JANUARY   1990      VISCOSITY OF VAPOR AS FUNCTION OF TEMPERATURE AND PRESSURE
     VISW     1.0      22 JANUARY   1990      VISCOSITY OF LIQUID WATER AS FUNCTION OF TEMPERATUR      E AND PRESSURE
     COWAT    1.0 S    17 SEPTEMBER 1990      LIQUID WATER DENSITY AND INT. ENERGY VERSUS TEMPERATURE AND PRESSURE (M. OS.)
     SUPST    1.0 S     1 February  1991      VAPOR DENSITY AND INTERNAL ENERGY AS FUNCTION OF TEMPERATURE AND PRESSURE (M. OS.)
     RELP     1.0      26 July      1995      LIQUID AND GAS PHASE RELATIVE PERMEABILITIES AS FUNCTIONS OF SATURATION
                                                for IRP=7, use Corey    -krg when RP(4).ne. 0, with Sgr = RP(4)

     BALLA    1.0       5 MARCH     1991      PERFORM SUMMARY BALANCES FOR VOLUME, MASS, AND ENERGY
     TSTEP    1.0       4 MARCH     1991      ADJUST TIME STEPS TO COINCIDE WITH USER     -DEFINED TARGET TIMES

     MULTI    2.0       3 January   2006      ASSEMBLE ALL ACCUMULATION AND FLOW TERMS
                                                INCLUDES CAPABILITIES FOR RADIATIVE HEAT TRANSFER AND DIFFUSION IN ALL PHASES
                                                   WITH LOCAL EQUILIBRIUM PHASE PARTITIONING BETWEEN GAS AND LIQUID
                                                ALLOWS BLOCK    -BY-BLOCK PERMEABILITY MODIFICATION
                                                PERMEABILITY CHANGES FROM PRECIP. (EWASG) THROUGH PAR(NLOC2S+3)
                                                TMVOC   -COMPATIBLE VERSION; 3Jan06: no dynamic D=0 switching


     QU       2.0       2 APRIL     2002      ASSEMBLE ALL SOURCE AND SINK TERMS
                                                "RIGOROUS" STEP RATE CAPABILITY FOR MOP(12) = 2,
                                                AND CAPABILITY FOR FLOWING WELLBORE PRESSURE CORRECTIONS
     PHAS     1.0      25 OCTOBER   2  002      CALCULATE COMPOSITION AND ENTHALPY OF SOURCE FLUID
     TTAB     1.0       5 November  1997      Interpolate sink/source rates and enthalpies from tables.
     FINDL    1.0      22 JANUARY   1990      INTERPOLATE FROM A TABLE OF TIME     -DEPENDENT DATA
     QINTER   1.0      22 JANUARY   1990      PERFORM LINEAR INTERPOLATION
     HINTER   1.0      22   JANUARY   1990      PERFORM LINEAR INTERPOLATION
     PHASD    1.0      14 NOVEMBER  2001      CALCULATE COMPOSITION, RATE AND ENTHALPY FOR WELLS ON DELIVERABILITY
     GCOR     1.0      14 NOVEMBER  2001      PERFORM SIMPLE GRAVITY CORRECTION FOR FLOWING BOTTOMHOLE PRESSURE
     LINEQ    2.00      2 May       2006      Interface for linear equation solvers T2CG2
                                                 Can call a direct solver or a package of conjugate gradient solvers
     MTRXIN   1.1      10 September 2000      Routine for Z    -preprocessing of the Jacobian

     CONVER   1.0       2 May       2002      UPDATE PRIMARY VARIABLES AFTER CONVERGENCE IS ACHIEVED
     FGTAB    1.00     28 May       1998      Tabulate element, connection, and generation data vs. time for plotting

     OUT      1.1      11 January   1999      PRINT RESULTS FOR ELEMENTS, CONNECTIONS, AND SINKS/SOURCES
     WRIFI    1.0       2 May       2002      AT THE COMPLETION OF A TOUGH2 RUN, WRITE PRIMARY VARIABLES ON FILE *SAVE*

*****************************************************************************************************************************
```

Version Control

```
      SAVE ICALL
      DATA ICALL/0/
      ICALL=ICALL+1
      IF(ICALL.EQ.1) WRITE(11,899)
C 899 FORMAT(6X,'QU       1.0      22 JANUARY   1990',6X,
C 899 FORMAT(6X,'QU       1.02     18 FEBRUARY  1993',6X,
C 899 FORMAT(6X,'QU       1.1       5 NOVEMBER  1997',6X,
C 899 FORMAT(/6X,'QU       1.1      23 JANUARY   1998',6X,
C 899 FORMAT(/6X,'QU       1.1      26 OCTOBER   2000',6X,
C 899 FORMAT(/6X,'QU       1.1      10 NOVEMBER  2000',6X,
C 899 FORMAT(/6X,'QU       1.1      23 NOVEMBER  2000',6X,
C 899 FORMAT(/6X,'QU       1.1      21 DECEMBER  2000',6X,
C 899 FORMAT(/6X,'QU       1.1      12 APRIL     2001',6X,
C 899 FORMAT(/6X,'QU       2.0      23 AUGUST    2001',6X,
C 899 FORMAT(/6X,'QU       2.0      30 AUGUST    2001',6X,
  899 FORMAT(/6X,'QU       2.0       2 APRIL     2002',6X,
     X'ASSEMBLE ALL SOURCE AND SINK TERMS'/
     X47X,'"RIGOROUS" STEP RATE CAPABILITY FOR MOP(12) = 2,'/
     X47X,'AND CAPABILITY FOR FLOWING WELLBORE PRESSURE CORRECTIONS')
```

MESH

```
ELEME
F   1              1 .1000E+02 .0000E+00 .0000E+00 .0000E+00 .0000E+00 .0000E+00
F   2              1 .1000E+02 .0000E+00 .0000E+00 .0000E+00 .0000E+00 .0000E+00
F   3              1 .1000E+02 .0000E+00 .0000E+00 .0000E+00 .0000E+00 .0000E+00
F   4              1 .1000E+02 .0000E+00 .0000E+00 .0000E+00 .0000E+00 .0000E+00
F   5              1 .1000E+02 .0000E+00 .0000E+00 .0000E+00 .0000E+00 .0000E+00
F   6              1 .1000E+02 .0000E+00 .0000E+00 .0000E+00 .0000E+00 .0000E+00
F   7              1 .1000E+02 .0000E+00 .0000E+00 .0000E+00 .0000E+00 .0000E+00
F   8              1 .1000E+02 .0000E+00 .0000E+00 .0000E+00 .0000E+00 .0000E+00
F   9              1 .1000E+02 .0000E+00 .0000E+00 .0000E+00 .0000E+00 .0000E+00
F  10              1 .1000E+02 .0000E+00 .0000E+00 .0000E+00 .0000E+00 .0000E+00
SHO 1              2 .1000E+02 .0000E+00 .0000E+00 .0000E+00 .0000E+00 .0000E+00
SHO 2              2 .1000E+02 .0000E+00 .0000E+00 .0000E+00 .0000E+00 .0000E+00
SHO 3              2 .1000E+02 .0000E+00 .0000E+00 .0000E+00 .0000E+00 .0000E+00
SHO 4              2 .1000E+02 .0000E+00 .0000E+00 .0000E+00 .0000E+00 .0000E+00
SHO 5              2 .1000E+02 .0000E+00 .0000E+00 .0000E+00 .0000E+00 .0000E+00
SHO 6              2 .1000E+02 .0000E+00 .0000E+00 .0000E+00 .0000E+00 .0000E+00
SHO 7              2 .1000E+02 .0000E+00 .0000E+00 .0000E+00 .0000E+00 .0000E+00
SHO 8              2 .1000E+02 .0000E+00 .0000E+00 .0000E+00 .0000E+00 .0000E+00
SHO 9              2 .1000E+02 .0000E+00 .0000E+00 .0000E+00 .0000E+00 .0000E+00
SHO10              2 .1000E+02 .0000E+00 .0000E+00 .0000E+00 .0000E+00 .0000E+00
SHO11              2 .1000E+05 .0000E+00 .0000E+00 .0000E+00 .0000E+00 .0000E+00
SHO12              2 .1000E+05 .0000E+00 .0000E+00 .0000E+00 .0000E+00 .0000E+00

CONNE
F   1F   2                   1 .5000E+01 .5000E+01 .1000E+01 .0000E+00 .0000E+00
F   3F   4                   1 .5000E+01 .5000E+01 .1000E+01 .0000E+00 .0000E+00
F   5F   6                   1 .5000E+01 .5000E+01 .1000E+01 .0000E+00 .0000E+00
+++
    1    2    3    4    5    6
```

INCON

```
INCON
F   1            .00000000E+00
  .1000000000000E+06  .2000000000000E+02  .1000000000000E+01
F   2            .00000000E+00
  .1000000000000E+07  .1700000000000E+03  .0000000000000E+00
F   3            .00000000E+00
  .1000000000000E+06  .1000000000000E-02  .9950000000000E+02
F   4            .00000000E+00
  .9900000000000E+07  .9990000000000E+00  .3100000000000E+03
F   5            .00000000E+00
  .1000000000000E+07  .1000000000000E+03  .0000000000000E+00
F   6            .00000000E+00
  .1000000000000E+08  .1000000000000E+03  .1000000000000E+01
F   7            .00000000E+00
  .1000000000000E+06  .2000000000000E+02  .0000000000000E+00
F   8            .00000000E+00
  .1000000000000E+08  .3000000000000E+03  .0000000000000E+00
F   9            .00000000E+00
  .1000000000000E+06  .9900000000000E+00  .9000000000000E+02
F  10            .00000000E+00
  .4000000000000E+07  .2800000000000E+03  .0000000000000E+00
SHO11            .00000000E+00
  .5000000000000E+07  .2400000000000E+03  .0000000000000E+00
SHO12            .00000000E+00
  .4000000000000E+07  .1000000000000E+03  .0000000000000E+00
```

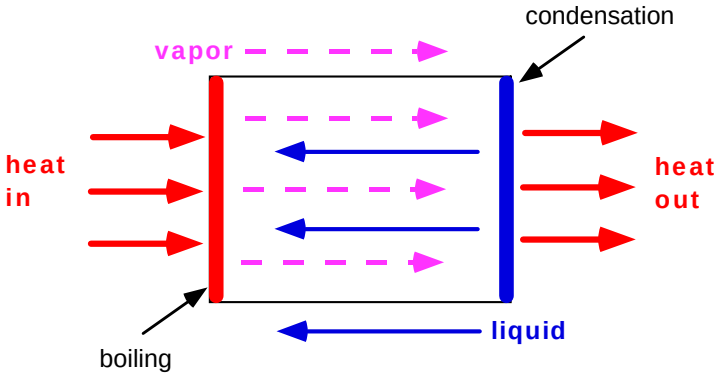
GENER

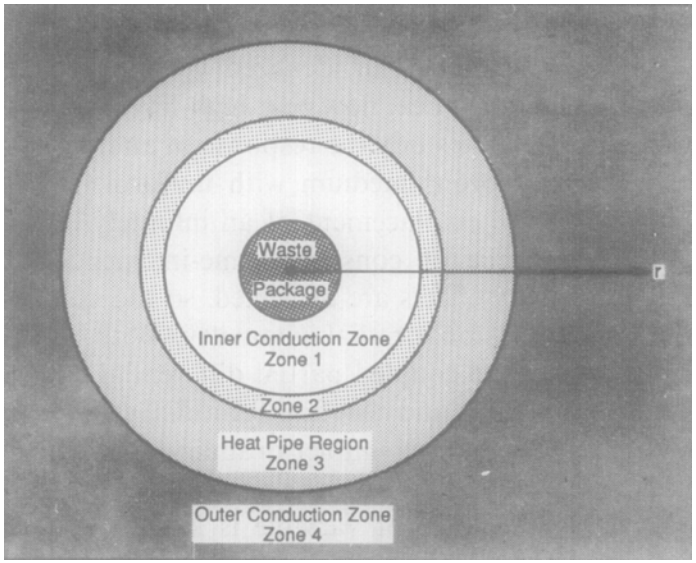
```
GENER
f   1AIR 0                   1     AIR   .5000E-02 .9882E+05 .0000E+00
F   7AIR 0                   1     AIR   .5000E-02 .9882E+05 .0000E+00
F   8WEL 0                   1     MASS -.1500E-01 .0000E+00 .0000E+00
F   9HOT 0                   1     HEAT  .2000E+07 .0000E+00 .0000E+00
F  10COL 0                   1     HEAT -.5000E+06 .0000E+00 .0000E+00
SHO 1P   1                   1     MASS1-1.000     .1000E+07 .0000E+00
SHO 2P   2                   1     laff -1.000     .0000E+00 .0000E+00
SHO 3P   3                   4     MASS  .0000E+00 .0000E+00 .0000E+00
  .0000000E+00  .1000000E+03  .2000000E+03  .4000000E+04
 -.1000000E+00 -.2000000E+00 -.3000000E+00 -.1100000E+01
SHO 4P   4                   4     MASS  .0000E+00 .0000E+00 .0000E+00
  .0000000E+00  .1000000E+03  .2000000E+03  .4000000E+04
 -.1000000E+00 -.2000000E+00 -.3000000E+00 -.1100000E+01
SHO 5P   5                   4     MASS  .0000E+00 .0000E+00 .0000E+00
  .0000000E+00  .1000000E+03  .2000000E+03  .4000000E+04
 -.1000000E+00 -.2000000E+00 -.3000000E+00 -.1100000E+01
SHO 6P   6                   4     MASS1 .0000E+00 .0000E+00 .0000E+00
  .0000000E+00  .1000000E+03  .2000000E+03  .4000000E+04
 -.1000000E+00 -.2000000E+00 -.3000000E+00 -.1100000E+01
  .1000000E+07  .2000000E+07  .3000000E+07  .1100000E+08
SHO 7P   6                   4     MASS1 .0000E+00 .0000E+00 .0000E+00
  .0000000E+00  .1000000E+03  .2000000E+03  .4000000E+04
 -.1000000E+00 -.2000000E+00 -.3000000E+00 -.1100000E+01
  .1000000E+07  .2000000E+07  .3000000E+07  .1100000E+08
SHO 8P   6                   4     MASS1 .0000E+00 .0000E+00 .0000E+00
  .0000000E+00  .1000000E+03  .2000000E+03  .4000000E+04
 -.1000000E+00 -.2000000E+00 -.3000000E+00 -.1100000E+01
  .1000000E+07  .2000000E+07  .3000000E+07  .1100000E+08
SHO 9P   9                   1     DELV  .1000E-11 .1000E+07 .0000E+00
SHO10P  10                   4     WATE1 .0000E+00 .0000E+00 .0000E+00
  .0000000E+00  .1000000E+03  .2000000E+03  .3000000E+04
  .1100000E+01  .1000000E+01  .9000000E+00  .1000000E+00
  .1000000E+07  .1200000E+07  .1400000E+07  .3000000E+07
SHO11WEL 0                   2     DELV  .1000E-11 .0000E+00 100.0
SHO12WEL 0                   1     DELV  .2000E-11 .1000E+07 100.0
+++
    0    7    8    9   10   11   13   14   15   16   17   18   19   20   21   22
```

SAVE

```
INCON -- INITIAL CONDITIONS FOR   22 ELEMENTS AT TIME   .195625E+04
F   1            .50000000E+00
  .1026783190016E+06  .1099839703607E+02  .2037588882447E+02
F   2            .50000000E+00
  .7916370186497E+06  .1000168301021E+02  .1699798522950E+03
F   3            .50000000E+00
  .7677482016712E+07  .1179335517890E-04  .1010226763824E+03
F   4            .50000000E+00
  .9572079406600E+07  .3232199089739E-02  .3091964900221E+03
F   5            .50000000E+00
  .9576155357447E+07  .1000248809440E+02  .1003047579095E+03
F   6            .50000000E+00
  .9818168919018E+07  .1000000000000E+01  .9993376313984E+02
F   7            .50000000E+00
  .1006737364472E+08  .1000283923305E+02  .2009607456794E+02
F   8            .50000000E+00
  .8537862272979E+07  .1000545748692E+02  .2995458360463E+03
F   9            .50000000E+00
  .2933407407340E+07  .2741571459748E-01  .3760295466211E+03
F  10            .50000000E+00
  .1983600803901E+07  .1099039634618E+02  .2119589075438E+03
SHO 1            .50000000E+00
  .4108087712286E+07  .8698644192479E-01  .2567204300811E+03
SHO 2            .50000000E+00
  .4500000000000E+07  .1050000000000E+02  .2500000000000E+03
SHO 3            .50000000E+00
  .8870946584688E+06  .1073526767326E+02  .1747302885933E+03
SHO 4            .50000000E+00
  .8870946584688E+06  .1073526767326E+02  .1747302885933E+03
SHO 5            .50000000E+00
  .8870946584688E+06  .1073526767326E+02  .1747302885933E+03
SHO 6            .50000000E+00
  .2858980450767E+06  .1075533722368E+02  .8069444982431E+02
SHO 7            .50000000E+00
  .2858980450767E+06  .1075533722368E+02  .8069444982431E+02
SHO 8            .50000000E+00
  .2858980450767E+06  .1075533722368E+02  .8069444982431E+02
SHO 9            .50000000E+00
  .1312984124846E+07  .1069178440957E+02  .1920452237581E+03
SHO10            .50000000E+00
  .9045343262748E+07  .1009545497753E+02  .2812831401394E+03
SHO11            .50000000E+00
  .3333056727132E+07  .1000370143276E+02  .2397486286092E+03
SHO12            .50000000E+00
  .1139849845083E+07  .0000000000000E+00  .9988050365503E+02
+++
    4   25    2  .00000000E+00  .19562500E+04
```

Heat Pipe in Radial Geometry





- partially-saturated medium (water-air)
- liquid water vaporizes near the heat source
- the vapor is driven away by pressure gradients
- vapor condenses in cooler regions
- capillary pressure gradients draw liquid back towards the heat source
- get counterflow: vapor flows away from the heat source, liquid flows towards it

Input File for Heat Pipe Problem (EOS3)

```
*rhp* 1-D RADIAL HEAT PIPE
MESHMAKER1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
RZ2D
RADII
    1
        0.
EQUID
    1              .3
LOGAR
   99           1.E2
LOGAR
   20           1.E4
EQUID
    1            0.0
LAYER----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
    1
       4.5

ROCKS----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
POMED    1     2550.       .10   20.E-15   20.E-15   20.E-15       2.0     800.0
                                  .25

MULTI----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
    2    3    2    6
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
   2 250     250000030000000002 47 1 1                   1.80
          3.15576E8       -1.
      1.E3      9.E3      9.E4      4.E5
     1.E-5     1.E00                                  1.E-7
               1.E5                0.20                 18.
diffusivity data are input as follows:
first row water, second row air; first column gas, second column aqueous
DIFFU----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
   2.13e-5     0.e-8
   2.13e-5     0.e-8
RPCAP----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
    7        0.45000    9.6E-4        1.
    7        0.45000    1.0E-3   8.0E-05      5.E8        1.
TIMES----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
    3
 3.15576E7  1.2559E8 3.15576E8
INCON----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8

GENER----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
A1  1HTR 1                         HEAT       3.E3

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

Output for Heat Pipe Problem (EOS3)

```
A1  1(   1,  2) ST = 0.100000E+04 DT = 0.100000E+04 DX1= 0.145252E+02 DX2= -.151938E-03 T =  19.065 P =   100015. S = 0.199848E+00
A1  1(   2,  3) ST = 0.100000E+05 DT = 0.900000E+04 DX1= 0.759481E+01 DX2= -.129059E-02 T =  27.246 P =   100022. S = 0.198557E+00
A1  1(   3,  4) ST = 0.100000E+06 DT = 0.900000E+05 DX1= 0.981167E+01 DX2= -.352306E-02 T =  63.142 P =   100032. S = 0.195034E+00
A1  1(   4,  7) ST = 0.500000E+06 DT = 0.400000E+06 DX1= 0.455945E+04 DX2= 0.117966E+00 T = 100.883 P =   104591. S = 0.313001E+00
A1  1(   5,  6) ST = 0.900000E+06 DT = 0.400000E+06 DX1= 0.130333E+05 DX2= 0.228700E+00 T = 104.232 P =   117625. S = 0.541701E+00
A1  1(   6,  5) ST = 0.130000E+07 DT = 0.400000E+06 DX1= 0.612673E+04 DX2= 0.670831E-01 T = 105.698 P =   123751. S = 0.608784E+00
A1  1(   7,  4) ST = 0.170000E+07 DT = 0.400000E+06 DX1= 0.427338E+04 DX2= 0.345307E-01 T = 106.686 P =   128025. S = 0.643315E+00
A1  1(   8,  7) ST = 0.250000E+07 DT = 0.800000E+06 DX1= 0.613735E+04 DX2= 0.510356E-01 T = 108.058 P =   134162. S = 0.694350E+00
A1  1(   9,  5) ST = 0.330000E+07 DT = 0.800000E+06 DX1= 0.505059E+04 DX2= 0.720326E-01 T = 109.148 P =   139213. S = 0.766383E+00
A1  1(  10,  5) ST = 0.410000E+07 DT = 0.800000E+06 DX1= 0.335887E+04 DX2= 0.523525E-01 T = 109.855 P =   142572. S = 0.818735E+00
A1  2(  11,  4) ST = 0.490000E+07 DT = 0.800000E+06 DX1= 0.297196E+04 DX2= 0.479447E-01 T = 103.471 P =   114544. S = 0.498481E+00
A1  1(  12,  7) ST = 0.650000E+07 DT = 0.160000E+07 DX1= 0.424798E+04 DX2= 0.511855E-01 T = 111.268 P =   149479. S = 0.906494E+00
A1  1(  13,  6) ST = 0.810000E+07 DT = 0.160000E+07 DX1= 0.359356E+04 DX2= 0.430199E-01 T = 111.982 P =   153072. S = 0.949514E+00
A1  1(  14,  6) ST = 0.970000E+07 DT = 0.160000E+07 DX1= 0.262995E+04 DX2= 0.232522E-01 T = 112.496 P =   155702. S = 0.972766E+00
A1  1(  15,  6) ST = 0.113000E+08 DT = 0.160000E+07 DX1= 0.216556E+04 DX2= 0.120374E-01 T = 112.913 P =   157868. S = 0.984804E+00
A1  1(  16,  8) ST = 0.129000E+08 DT = 0.160000E+07 DX1= 0.222624E+04 DX2= 0.809200E-02 T = 113.338 P =   160094. S = 0.992896E+00
A1  1(  17,  8) ST = 0.145000E+08 DT = 0.160000E+07 DX1= 0.181362E+04 DX2= 0.378796E-02 T = 113.680 P =   161908. S = 0.996684E+00
$$$$$$$$$$$$$ GAS PHASE DISAPPEARS AT ELEMENT *A1  1*  $$$$$      SG = -.821520E+00
$$$$$$$$$$$$$$$$ GAS PHASE EVOLVES AT ELEMENT *A1  1*  $$$$$    XAIR = 0.000000E+00    PX = -.377453E+05   PG = 0.170292E+06
+++++++++ REDUCE TIME STEP AT (  18,  9) +++++++++++++++   NEW DELT = 0.400000E+06
A1  1(  18,  5) ST = 0.149000E+08 DT = 0.400000E+06 DX1= 0.420592E+03 DX2= 0.539979E-03 T = 113.759 P =   162328. S = 0.997224E+00
A1  1(  19,  5) ST = 0.153000E+08 DT = 0.400000E+06 DX1= 0.398804E+03 DX2= 0.413402E-03 T = 113.834 P =   162727. S = 0.997637E+00
A1  1(  20,  5) ST = 0.157000E+08 DT = 0.400000E+06 DX1= 0.382195E+03 DX2= 0.318097E-03 T = 113.905 P =   163109. S = 0.997955E+00
A1  1(  21,  5) ST = 0.161000E+08 DT = 0.400000E+06 DX1= 0.367970E+03 DX2= 0.244910E-03 T = 113.974 P =   163477. S = 0.998200E+00
A1  1(  22,  5) ST = 0.165000E+08 DT = 0.400000E+06 DX1= 0.355310E+03 DX2= 0.188344E-03 T = 114.040 P =   163833. S = 0.998388E+00
A1  1(  23,  5) ST = 0.169000E+08 DT = 0.400000E+06 DX1= 0.343837E+03 DX2= 0.144592E-03 T = 114.104 P =   164177. S = 0.998533E+00
A1  1(  24,  5) ST = 0.173000E+08 DT = 0.400000E+06 DX1= 0.333323E+03 DX2= 0.110799E-03 T = 114.166 P =   164510. S = 0.998644E+00
A1  1(  25,  5) ST = 0.177000E+08 DT = 0.400000E+06 DX1= 0.323613E+03 DX2= 0.847531E-04 T = 114.226 P =   164833. S = 0.998728E+00
A1  1(  26,  5) ST = 0.181000E+08 DT = 0.400000E+06 DX1= 0.314604E+03 DX2= 0.647274E-04 T = 114.284 P =   165148. S = 0.998793E+00
$$$$$$$$$$ LIQUID PHASE DISAPPEARS AT ELEMENT *A1  1*  $$$$$      SG = 0.105073E+01
A1  1(  27,  5) ST = 0.185000E+08 DT = 0.400000E+06 DX1= -.629120E+03 DX2= -.109988E+02 T = 116.179 P =   164519. S = 0.100000E+01
A1  1(  28,  4) ST = 0.189000E+08 DT = 0.400000E+06 DX1= -.289016E+04 DX2= 0.000000E+00 T = 122.498 P =   161629. S = 0.100000E+01
A1  5(  29,  5) ST = 0.197000E+08 DT = 0.800000E+06 DX1= 0.370136E+03 DX2= 0.960351E-02 T =  99.745 P =   100412. S = 0.188098E+00
A1  1(  30,  5) ST = 0.205000E+08 DT = 0.800000E+06 DX1= -.773602E+04 DX2= -.450431E-17 T = 151.545 P =   146384. S = 0.100000E+01
A1  1(  31,  5) ST = 0.213000E+08 DT = 0.800000E+06 DX1= -.434906E+04 DX2= -.200931E-20 T = 158.807 P =   142035. S = 0.100000E+01
A1  1(  32,  5) ST = 0.221000E+08 DT = 0.800000E+06 DX1= -.124814E+04 DX2= 0.948520E-19 T = 161.649 P =   140787. S = 0.100000E+01
A1  1(  33,  5) ST = 0.229000E+08 DT = 0.800000E+06 DX1= 0.177759E+02 DX2= -.772333E-19 T = 162.649 P =   140805. S = 0.100000E+01
A1  2(  34,  5) ST = 0.237000E+08 DT = 0.800000E+06 DX1= 0.589749E+03 DX2= 0.661802E-02 T = 109.546 P =   141094. S = 0.974051E+00
A1  2(  35,  5) ST = 0.245000E+08 DT = 0.800000E+06 DX1= 0.536789E+03 DX2= 0.523145E-02 T = 109.659 P =   141631. S = 0.979283E+00
A1  2(  36,  5) ST = 0.253000E+08 DT = 0.800000E+06 DX1= 0.502914E+03 DX2= 0.416700E-02 T = 109.764 P =   142134. S = 0.983450E+00
A1  2(  37,  5) ST = 0.261000E+08 DT = 0.800000E+06 DX1= 0.477808E+03 DX2= 0.332475E-02 T = 109.864 P =   142612. S = 0.986774E+00
A1  2(  38,  5) ST = 0.269000E+08 DT = 0.800000E+06 DX1= 0.457283E+03 DX2= 0.264764E-02 T = 109.959 P =   143069. S = 0.989422E+00
A1  2(  39,  5) ST = 0.277000E+08 DT = 0.800000E+06 DX1= 0.439585E+03 DX2= 0.210083E-02 T = 110.050 P =   143509. S = 0.991523E+00
A1  2(  40,  5) ST = 0.285000E+08 DT = 0.800000E+06 DX1= 0.424200E+03 DX2= 0.166067E-02 T = 110.138 P =   143933. S = 0.993184E+00
A1  6(  41,  5) ST = 0.293000E+08 DT = 0.800000E+06 DX1= 0.388974E+03 DX2= 0.964454E-02 T =  99.751 P =   100434. S = 0.185657E+00
A1  2(  42,  5) ST = 0.301000E+08 DT = 0.800000E+06 DX1= 0.507631E+03 DX2= 0.126025E-02 T = 110.344 P =   144932. S = 0.995912E+00
A1  2(  43,  5) ST = 0.309000E+08 DT = 0.800000E+06 DX1= 0.453495E+03 DX2= 0.944158E-03 T = 110.438 P =   145385. S = 0.996856E+00
A1  2(  44,  5) ST = 0.315576E+08 DT = 0.657600E+06 DX1= 0.348608E+03 DX2= 0.571726E-03 T = 110.509 P =   145734. S = 0.997428E+00
```

Output for Heat Pipe Problem (EOS3)

rhp 1-D RADIAL HEAT PIPE

OUTPUT DATA AFTER (44, 5)-2-TIME STEPS   THE TIME IS 0.36525E+03 DAYS

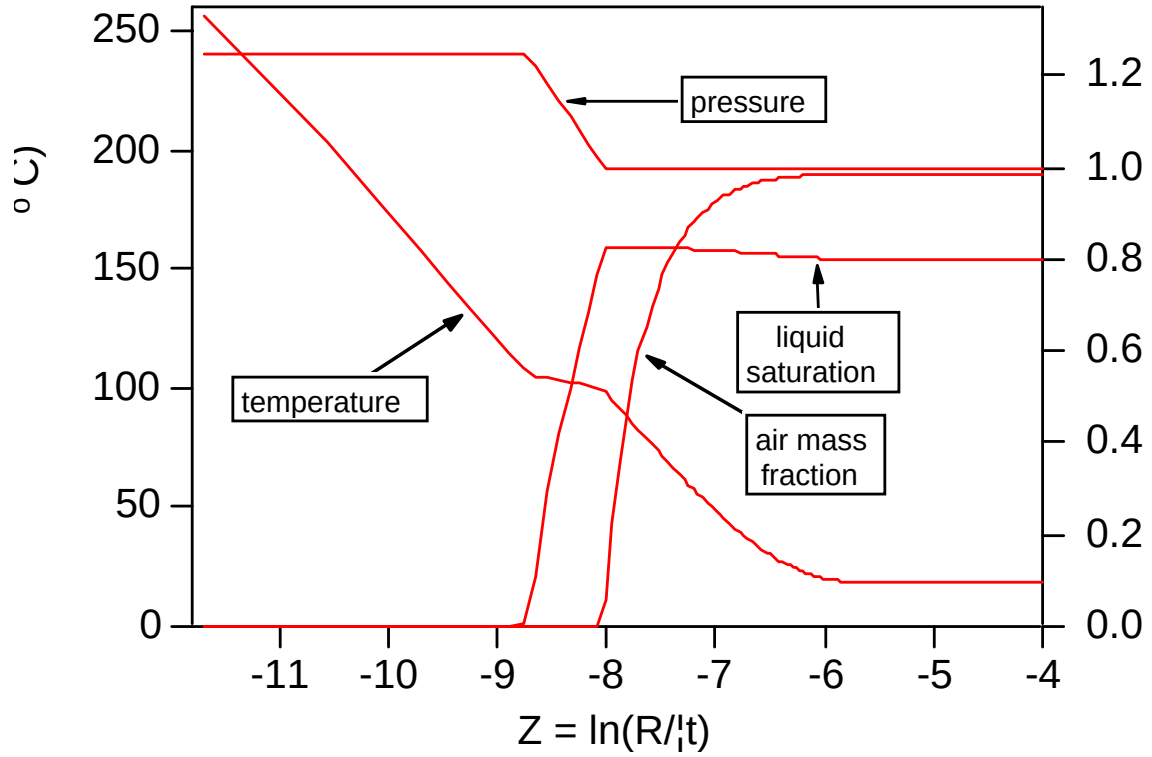
@@@

TOTAL TIME	KCYC	ITER	ITERC	KON	DX1M	DX2M	DX3M	MAX. RES.	NER	KER	DELTEX
0.31558E+08	44	5	236	2	0.42630E+03	0.11943E-01	0.58034E+00	0.10776E-06	2	1	0.65760E+06

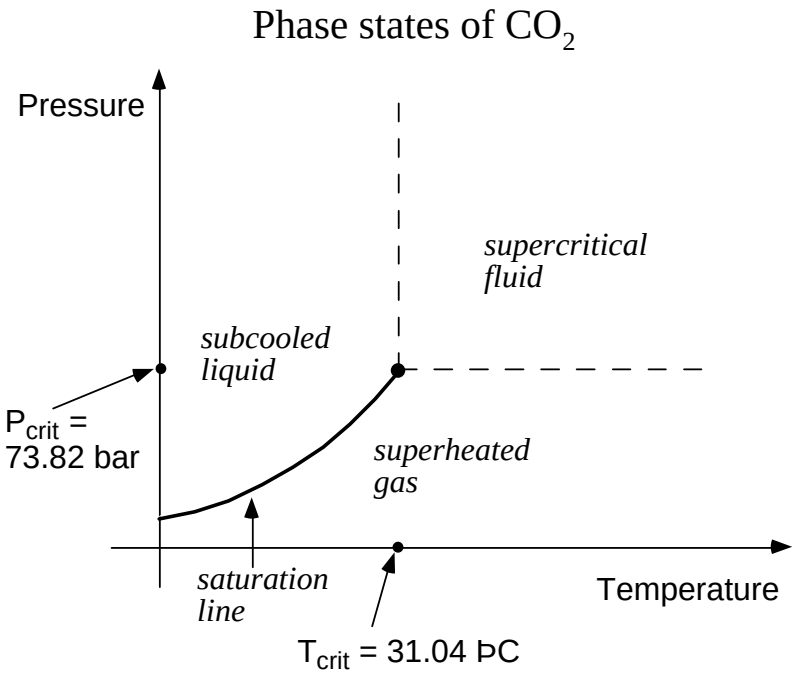
@@@

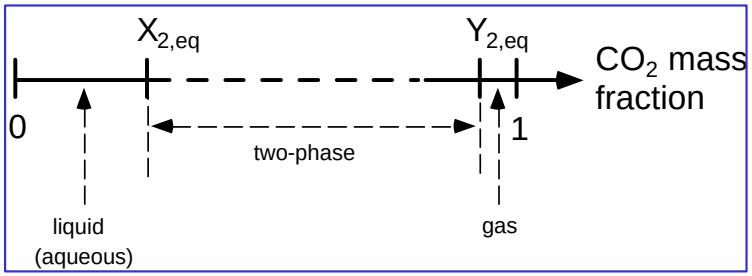
ELEM.	INDEX	P (PA)	T (DEG-C)	SG	SL	XAIRG	XAIRL	PER.MOD.	PCAP (PA)	DG (KG/M**3)	DL (KG/M**3)
A1 1	1	0.14573E+06	0.16412E+03	0.10000E+01	0.00000E+00	0.00000E+00	0.00000E+00	0.10000E+01	-.50000E+09	0.72998E+00	0.00000E+00
A1 2	2	0.14573E+06	0.11051E+03	0.99743E+00	0.25724E-02	0.00000E+00	0.00000E+00	0.10000E+01	-.33327E+08	0.83980E+00	0.95030E+03
A1 3	3	0.13007E+06	0.10715E+03	0.86852E+00	0.13148E+00	0.00000E+00	0.00000E+00	0.10000E+01	-.14955E+06	0.75504E+00	0.95285E+03
A1 4	4	0.11877E+06	0.10451E+03	0.61567E+00	0.38433E+00	0.00000E+00	0.00000E+00	0.10000E+01	-.37591E+05	0.69349E+00	0.95482E+03
A1 5	5	0.10974E+06	0.10225E+03	0.41885E+00	0.58115E+00	0.26342E-10	0.29392E-15	0.10000E+01	-.19979E+05	0.64404E+00	0.95649E+03
A1 6	6	0.10204E+06	0.10020E+03	0.22936E+00	0.77064E+00	0.26455E-05	0.27427E-10	0.10000E+01	-.10944E+05	0.60170E+00	0.95798E+03
A1 7	7	0.10004E+06	0.92930E+02	0.17304E+00	0.82696E+00	0.30601E+00	0.34979E-05	0.10000E+01	-.87795E+04	0.67657E+00	0.96312E+03
A1 8	8	0.10004E+06	0.84925E+02	0.17425E+00	0.82575E+00	0.53920E+00	0.68171E-05	0.10000E+01	-.88254E+04	0.76506E+00	0.96850E+03
A1 9	9	0.10004E+06	0.77951E+02	0.17544E+00	0.82456E+00	0.67380E+00	0.90788E-05	0.10000E+01	-.88701E+04	0.83155E+00	0.97294E+03
A1 10	10	0.10004E+06	0.71794E+02	0.17660E+00	0.82340E+00	0.75884E+00	0.10671E-04	0.10000E+01	-.89141E+04	0.88332E+00	0.97665E+03
A1 11	11	0.10004E+06	0.66307E+02	0.17775E+00	0.82225E+00	0.81587E+00	0.11820E-04	0.10000E+01	-.89575E+04	0.92479E+00	0.97978E+03
A1 12	12	0.10004E+06	0.61385E+02	0.17889E+00	0.82111E+00	0.85579E+00	0.12668E-04	0.10000E+01	-.90003E+04	0.95881E+00	0.98245E+03
A1 13	13	0.10004E+06	0.56941E+02	0.18001E+00	0.81999E+00	0.88468E+00	0.13306E-04	0.10000E+01	-.90428E+04	0.98731E+00	0.98474E+03
A1 14	14	0.10004E+06	0.52916E+02	0.18112E+00	0.81888E+00	0.90610E+00	0.13793E-04	0.10000E+01	-.90849E+04	0.10116E+01	0.98671E+03
A1 15	15	0.10004E+06	0.49260E+02	0.18223E+00	0.81777E+00	0.92233E+00	0.14170E-04	0.10000E+01	-.91266E+04	0.10325E+01	0.98840E+03
A1 16	16	0.10004E+06	0.45937E+02	0.18332E+00	0.81668E+00	0.93482E+00	0.14465E-04	0.10000E+01	-.91679E+04	0.10508E+01	0.98987E+03
A1 17	17	0.10004E+06	0.42911E+02	0.18440E+00	0.81560E+00	0.94458E+00	0.14699E-04	0.10000E+01	-.92088E+04	0.10668E+01	0.99114E+03
A1 18	18	0.10004E+06	0.40155E+02	0.18547E+00	0.81453E+00	0.95230E+00	0.14886E-04	0.10000E+01	-.92493E+04	0.10811E+01	0.99223E+03
A1 19	19	0.10004E+06	0.37648E+02	0.18652E+00	0.81348E+00	0.95848E+00	0.15036E-04	0.10000E+01	-.92894E+04	0.10937E+01	0.99318E+03
A1 20	20	0.10004E+06	0.35369E+02	0.18756E+00	0.81244E+00	0.96346E+00	0.15159E-04	0.10000E+01	-.93288E+04	0.11050E+01	0.99399E+03
A1 21	21	0.10004E+06	0.33300E+02	0.18858E+00	0.81142E+00	0.96751E+00	0.15259E-04	0.10000E+01	-.93677E+04	0.11151E+01	0.99470E+03
A1 22	22	0.10004E+06	0.31427E+02	0.18958E+00	0.81042E+00	0.97083E+00	0.15341E-04	0.10000E+01	-.94057E+04	0.11242E+01	0.99531E+03
A1 23	23	0.10004E+06	0.29736E+02	0.19056E+00	0.80944E+00	0.97356E+00	0.15409E-04	0.10000E+01	-.94427E+04	0.11323E+01	0.99583E+03
A1 24	24	0.10004E+06	0.28213E+02	0.19150E+00	0.80850E+00	0.97583E+00	0.15466E-04	0.10000E+01	-.94785E+04	0.11396E+01	0.99628E+03
A1 25	25	0.10004E+06	0.26846E+02	0.19240E+00	0.80760E+00	0.97771E+00	0.15513E-04	0.10000E+01	-.95129E+04	0.11460E+01	0.99667E+03
A1 26	26	0.10004E+06	0.25625E+02	0.19326E+00	0.80674E+00	0.97928E+00	0.15552E-04	0.10000E+01	-.95456E+04	0.11518E+01	0.99700E+03
A1 27	27	0.10004E+06	0.24539E+02	0.19407E+00	0.80593E+00	0.98060E+00	0.15586E-04	0.10000E+01	-.95765E+04	0.11569E+01	0.99728E+03
A1 28	28	0.10004E+06	0.23576E+02	0.19483E+00	0.80517E+00	0.98170E+00	0.15613E-04	0.10000E+01	-.96054E+04	0.11614E+01	0.99752E+03
A1 29	29	0.10004E+06	0.22728E+02	0.19553E+00	0.80447E+00	0.98262E+00	0.15637E-04	0.10000E+01	-.96321E+04	0.11654E+01	0.99772E+03
A1 30	30	0.10004E+06	0.21984E+02	0.19617E+00	0.80383E+00	0.98340E+00	0.15656E-04	0.10000E+01	-.96565E+04	0.11688E+01	0.99789E+03
A1 31	31	0.10004E+06	0.21336E+02	0.19674E+00	0.80326E+00	0.98405E+00	0.15673E-04	0.10000E+01	-.96786E+04	0.11719E+01	0.99804E+03
A1 32	32	0.10004E+06	0.20774E+02	0.19726E+00	0.80274E+00	0.98460E+00	0.15686E-04	0.10000E+01	-.96984E+04	0.11745E+01	0.99816E+03
A1 33	33	0.10004E+06	0.20291E+02	0.19772E+00	0.80228E+00	0.98505E+00	0.15698E-04	0.10000E+01	-.97158E+04	0.11767E+01	0.99826E+03

Output for Heat Pipe Problem after t = 10 Years (EOS4)



ECO2N for Water-NaCl-CO_2





Phase partitioning

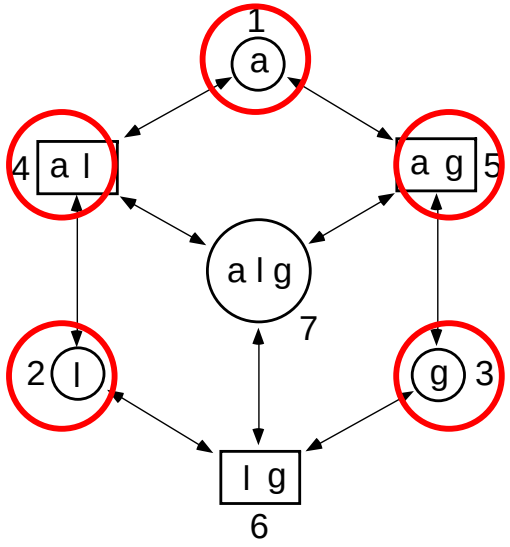


Figure 1. Possible phase combinations in the system water-CO_2. The phase designations are a - aqueous, l - liquid CO_2, g - gaseous CO_2. Separate liquid and gas phases exist only at subcritical conditions.

Summary of ECO2N

Components # 1: water
2: NaCl
3: CO_2

Parameter choices

(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

Primary Variables

single fluid phase (only aqueous, or only gas)# (P, X_{sm}, X3, T)

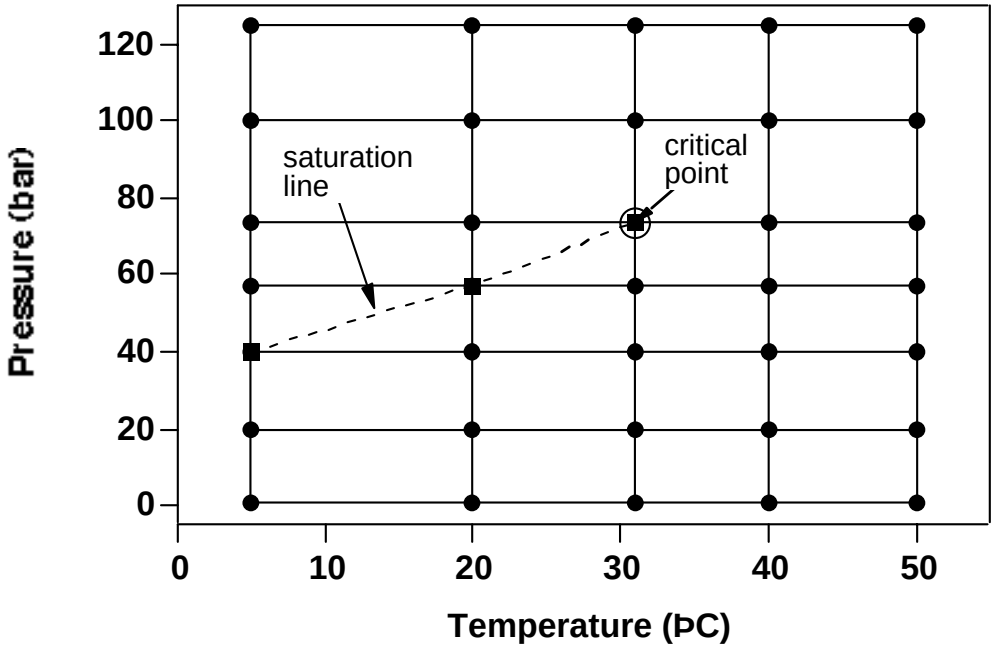
- P - pressure
- X_{sm} - salt mass fraction X_s in two-component water-salt system, or solid saturation S_s+10
- X3 - CO_2 mass fraction in the aqueous phase, or in the gas phase, in the three-component system water-salt-CO_2
- T - temperature

two fluid phases (aqueous and gas)# (P, X_{sm}, S_g+10, T)

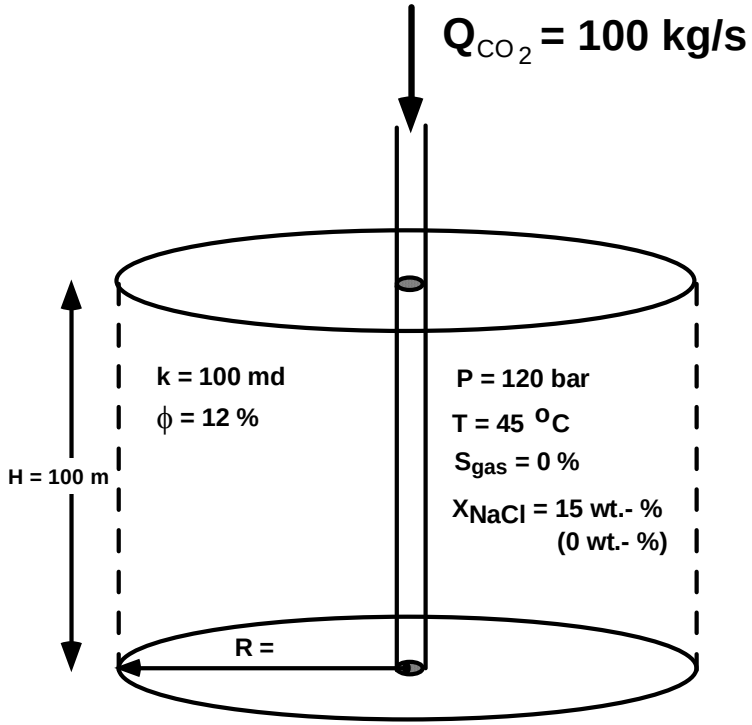
- P - pressure
- X_{sm} - salt mass fraction X_s in two-component water-salt system, or solid saturation S_s+10
- S_g - gas phase saturation
- T - temperature

in addition we may have solid salt

Tabulation of CO_2 Properties



Radial Flow from a CO_2 Injection Well



MESH Generation for Radial Flow Problem

```
*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
...
```

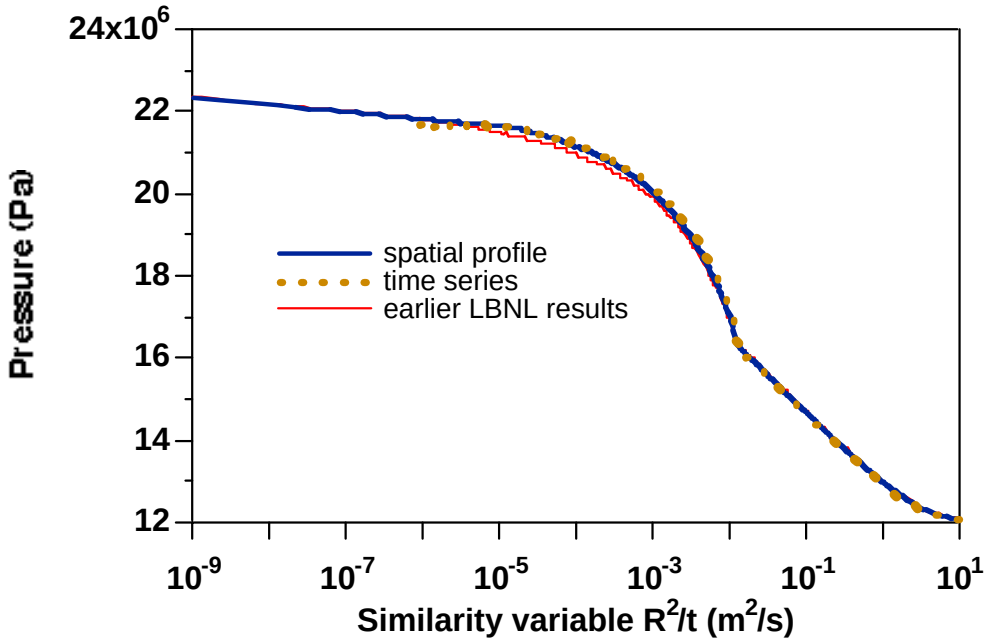
Input File for Radial Flow Problem

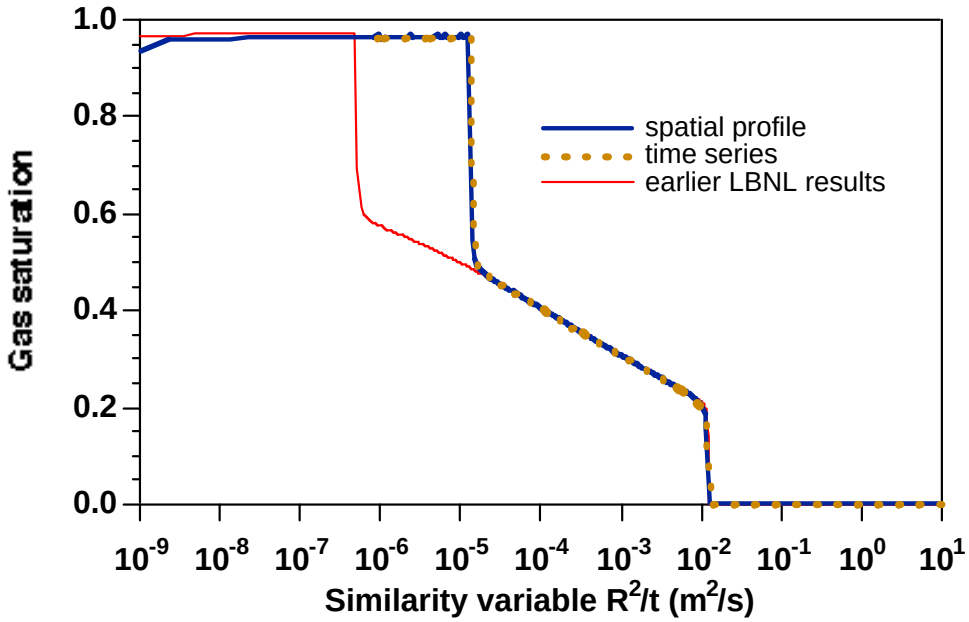
```
*rcc3* ... Code Intercomparison problem3: Radial flow from a CO2 Injection Well
ROCKS----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
SAND     2  2600.e00       .12  100.e-15  100.e-15  100.e-15      2.51      920.
   4.5e-10
    7           .457       .30        1.   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

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
```

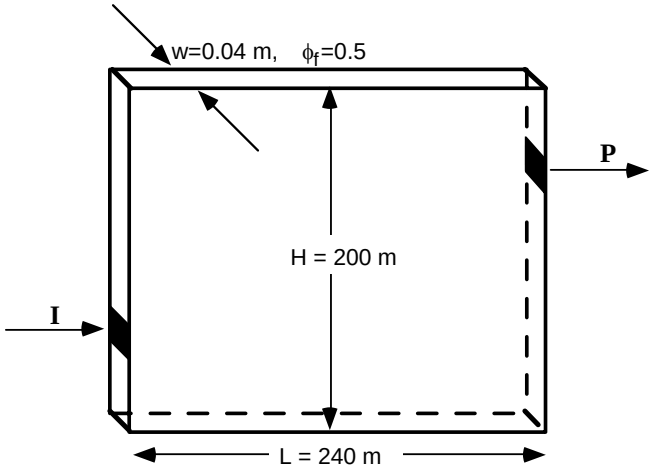
Results from Radial Flow Problem





Spatial profile at t = 8.64×10^7 s
Time series at R = 25.25 m
Thin line: earlier LBNL results with “evaporation model”

Heat Sweep in a Vertical Fracture (EOS1)



Summary of EOS1

Components	# 1: water # 2: "water 2" (optional)
Parameter choices	
(NK, NEQ, NPH, NB) =	(1, 2, 2, 6) one water component, nonisothermal (default) (1, 1, 2, 6) only liquid, or only vapor; isothermal (2, 3, 2, 6) two-waters, nonisothermal*
molecular diffusion can be modeled by setting NK = 2, NB = 8	
Primary Variables	
single-phase conditions	
(P, T, [X]) - (pressure, temperature, [mass fraction of water 2]†)	
two-phase conditions	
(P_g, S_g, [X]) - (gas phase pressure, gas saturation, [mass fraction of water 2]†)	

* two waters cannot be run in isothermal mode, because in this case temperature is not the last primary variable

† optional, for NK = 2 only

```
*rvf* - vertical fracture problem for EOS1
ROCKS----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
FRACT          2650.       .50  200.E-12  200.E-12  200.E-12      0.00     1000.
CONBD          2650.       .00    0.E-12    0.E-12    0.E-12       2.1     1000.

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  40      99100000000000001
         1.57788E8       -1.          A1312           9.81
     1.E2      9.E2      9.E3      9.E4      9.E5      2.E6      5.E6
    1.E-5
            100.E5               300.
SOLVR----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
5  Z1   O0    8.0e-1    1.0e-7
GENER----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
A18 1INJ 1                        COM1         4.     4.2E5
A1312PRO 1                        DELV     4.E-12    9.65E6

FOFT ----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
A1312

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

MULTI
    1    1    2    6
ENDCY----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
con00          CONBD
MESHMAKER1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
XYZ
      90.
NX      12       20.
NY      10       20.
NZ       1       .04


ENDFI----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
MULTI----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
    2    3    2    6
A18 1INJ 1                        COM2         4.     4.2E5
```

3 Run Segments

(1) MESH generation, followed by “hand-editing.”

(2) Obtain gravity equilibrium.

(3) Perform injection-production simulation.

MESH Pattern

```
*****************************************************************************************************
*                     CARTESIAN MESH WITH NX*NY*NZ =   12 *  10 *   1  GRID BLOCKS
*****************************************************************************************************
*
*                     THE MESH WILL BE PRINTED AS SLICES FOR K = 1 TO K = NZ =   1
*
*                     IN EACH MESH SLICE, ROWS WILL GO FROM  J = 1 TO J = NY =  10
*
*                     IN EACH ROW, COLUMNS WILL GO FROM      I = 1 TO I = NX =  12
*
*****************************************************************************************************

SLICE WITH K =   1

  COLUMN I =  1     2     3     4     5     6     7     8     9    10    11    12    13    14    15    16    17
ROWS
 J =    1   A11 1 A11 2 A11 3 A11 4 A11 5 A11 6 A11 7 A11 8 A11 9 A1110 A1111 A1112
 J =    2   A12 1 A12 2 A12 3 A12 4 A12 5 A12 6 A12 7 A12 8 A12 9 A1210 A1211 A1212
 J =    3   A13 1 A13 2 A13 3 A13 4 A13 5 A13 6 A13 7 A13 8 A13 9 A1310 A1311 A1312
 J =    4   A14 1 A14 2 A14 3 A14 4 A14 5 A14 6 A14 7 A14 8 A14 9 A1410 A1411 A1412
 J =    5   A15 1 A15 2 A15 3 A15 4 A15 5 A15 6 A15 7 A15 8 A15 9 A1510 A1511 A1512
 J =    6   A16 1 A16 2 A16 3 A16 4 A16 5 A16 6 A16 7 A16 8 A16 9 A1610 A1611 A1612
 J =    7   A17 1 A17 2 A17 3 A17 4 A17 5 A17 6 A17 7 A17 8 A17 9 A1710 A1711 A1712
 J =    8   A18 1 A18 2 A18 3 A18 4 A18 5 A18 6 A18 7 A18 8 A18 9 A1810 A1811 A1812
 J =    9   A19 1 A19 2 A19 3 A19 4 A19 5 A19 6 A19 7 A19 8 A19 9 A1910 A1911 A1912
 J =   10   A1A 1 A1A 2 A1A 3 A1A 4 A1A 5 A1A 6 A1A 7 A1A 8 A1A 9 A1A10 A1A11 A1A12

*****************************************************************************************************

MESH GENERATION COMPLETE --- EXIT FROM MODULE *MESHMAKER*
```

Semi-analytical Heat Exchange

(Vinsome and Westerveld, 1980)

- Each boundary grid block is connected to a semi-infinite conductive half-space.
- Temperature profile is assumed as a low-order polynomial with an exponential tail.

$$T(x,t) - T_i = \left(T_f - T_i + px + qx^2\right)\exp(-x/d)$$

- Penetration depth d for heat conduction is $d = \sqrt{\Theta t}/2$
- Coefficients p and q are determined during the flow simulation from two constraints, (1) energy conservation for the reservoir/caprock system, (2) diffusion equation for heat conduction must be satisfied at caprock boundary.

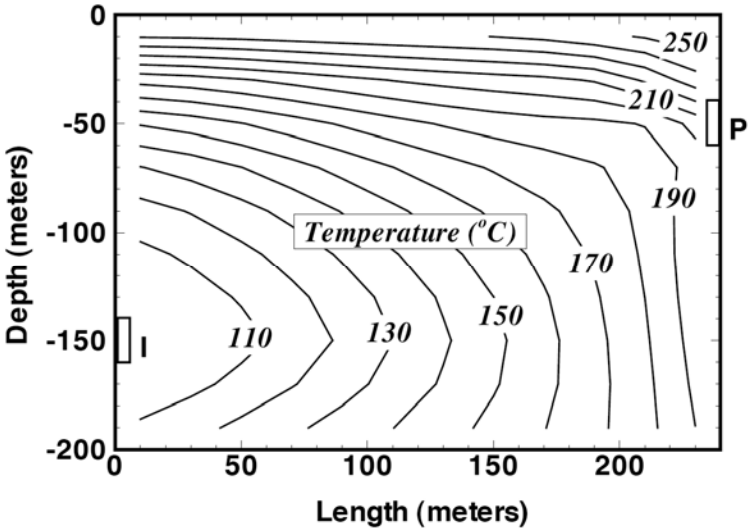
Simulation Results for Fracture Problem

```
================================================================================================================================
PERFORM SEMI-ANALYTICAL HEAT EXCHANGE CALCULATION
     THERMAL PARAMETERS ARE:
     TEMPERATURE =  0.30000E+03   HEAT CONDUCTIVITY =  0.21000E+01   DENSITY =  0.26500E+04   SPECIFIC HEAT =  0.10000E+04
     DIFFUSIVITY =  0.79245E-06
================================================================================================================================


...ITERATING...  AT [   1,  1] --- DELTEX = 0.100000E+03   MAX. RES. = 0.698170E-01  AT ELEMENT A18 1  EQUATION   1
...ITERATING...  AT [   1,  2] --- DELTEX = 0.100000E+03   MAX. RES. = 0.980877E-03  AT ELEMENT A18 1  EQUATION   2
A1312(   1,  3) ST = 0.100000E+03 DT = 0.100000E+03 DX1= 0.514076E+05 DX2= 0.105693E-01 T = 300.011 P =  9702648. S = 0.000000E+00
...ITERATING...  AT [   2,  1] --- DELTEX = 0.900000E+03   MAX. RES. = 0.141105E+00  AT ELEMENT A18 1  EQUATION   2
...ITERATING...  AT [   2,  2] --- DELTEX = 0.900000E+03   MAX. RES. = 0.196414E-01  AT ELEMENT A18 1  EQUATION   1
...ITERATING...  AT [   2,  3] --- DELTEX = 0.900000E+03   MAX. RES. = 0.526790E-04  AT ELEMENT A18 1  EQUATION   1
A1312(   2,  4) ST = 0.100000E+04 DT = 0.900000E+03 DX1= 0.523779E+05 DX2= 0.265024E-02 T = 300.013 P =  9755026. S = 0.000000E+00
...ITERATING...  AT [   3,  1] --- DELTEX = 0.900000E+04   MAX. RES. = 0.150119E+01  AT ELEMENT A18 1  EQUATION   2
...ITERATING...  AT [   3,  2] --- DELTEX = 0.900000E+04   MAX. RES. = 0.497225E+00  AT ELEMENT A18 1  EQUATION   1
...ITERATING...  AT [   3,  3] --- DELTEX = 0.900000E+04   MAX. RES. = 0.192776E-02  AT ELEMENT A19 1  EQUATION   1
...ITERATING...  AT [   3,  4] --- DELTEX = 0.900000E+04   MAX. RES. = 0.128494E-04  AT ELEMENT A18 1  EQUATION   1
A1312(   3,  5) ST = 0.100000E+05 DT = 0.900000E+04 DX1= 0.147957E+05 DX2= -.104035E-01 T = 300.003 P =  9769821. S = 0.000000E+00
...ITERATING...  AT [   4,  1] --- DELTEX = 0.900000E+05   MAX. RES. = 0.123039E+02  AT ELEMENT A18 1  EQUATION   2
...ITERATING...  AT [   4,  2] --- DELTEX = 0.900000E+05   MAX. RES. = 0.588510E+01  AT ELEMENT A18 1  EQUATION   1
...ITERATING...  AT [   4,  3] --- DELTEX = 0.900000E+05   MAX. RES. = 0.344128E-01  AT ELEMENT A19 1  EQUATION   1
...ITERATING...  AT [   4,  4] --- DELTEX = 0.900000E+05   MAX. RES. = 0.423972E-03  AT ELEMENT A1A 2  EQUATION   1
A1312(   4,  5) ST = 0.100000E+06 DT = 0.900000E+05 DX1= 0.447701E+04 DX2= -.143131E-01 T = 299.989 P =  9774298. S = 0.000000E+00
...ITERATING...  AT [   5,  1] --- DELTEX = 0.900000E+06   MAX. RES. = 0.698636E+02  AT ELEMENT A18 1  EQUATION   2
...ITERATING...  AT [   5,  2] --- DELTEX = 0.900000E+06   MAX. RES. = 0.369906E+02  AT ELEMENT A1A 3  EQUATION   1
...ITERATING...  AT [   5,  3] --- DELTEX = 0.900000E+06   MAX. RES. = 0.149552E+01  AT ELEMENT A18 3  EQUATION   2
...ITERATING...  AT [   5,  4] --- DELTEX = 0.900000E+06   MAX. RES. = 0.367687E-01  AT ELEMENT A1A 3  EQUATION   1
...ITERATING...  AT [   5,  5] --- DELTEX = 0.900000E+06   MAX. RES. = 0.161956E-03  AT ELEMENT A1A 3  EQUATION   1
A1312(   5,  6) ST = 0.100000E+07 DT = 0.900000E+06 DX1= 0.151037E+04 DX2= -.245659E+00 T = 299.743 P =  9775809. S = 0.000000E+00
...
...
```

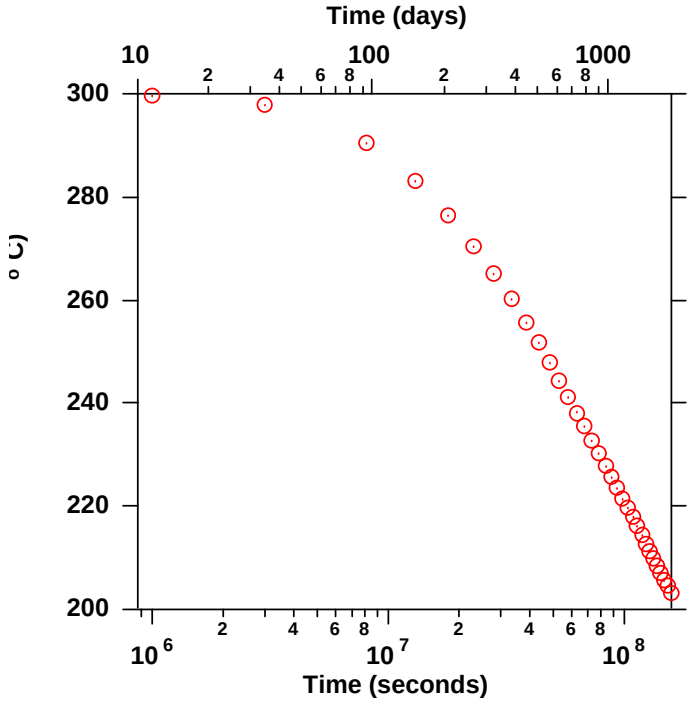
Simulation Results for Fracture Problem

```
...
...
 ...ITERATING...  AT [  37,  1] --- DELTEX = 0.478800E+07   MAX. RES. = 0.101777E+01  AT ELEMENT A12 1  EQUATION   2
 ...ITERATING...  AT [  37,  2] --- DELTEX = 0.478800E+07   MAX. RES. = 0.814304E-01  AT ELEMENT A1112  EQUATION   1
 ...ITERATING...  AT [  37,  3] --- DELTEX = 0.478800E+07   MAX. RES. = 0.137360E-03  AT ELEMENT A1312  EQUATION   1
 A1312(  37,  4) ST = 0.157788E+09 DT = 0.478800E+07 DX1= 0.662944E+03 DX2= -.117867E+01 T = 203.245 P =  9804004. S = 0.000000E+00

 *rvf* - vertical fracture problem for EOS1

          OUTPUT DATA AFTER (  37,  4)-2-TIME STEPS                                                          THE TIME IS  0.18262E+04 DAYS

 @@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@

   TOTAL TIME    KCYC    ITER  ITERC    KON    DX1M          DX2M          DX3M                      RERM         NER     KER    DELTEX
  0.15779E+09     37      4    159      2 0.226297E+04 0.189794E+01 0.000000E+00              0.616901E-07   112     1 0.478800E+07

 @@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@

 ELEM.  INDEX     P           T           SG          SW          X1          X2        PCAP                      DG          DW
               (PA)       (DEG-C)                                                        (PA)                   (KG/M**3)   (KG/M**3)

 A11 1     1 0.95547E+07 0.23076E+03 0.00000E+00 0.10000E+01 0.10000E+01 0.00000E+00 0.00000E+00             0.14192E+02 0.83273E+03
 A12 1     2 0.97248E+07 0.18326E+03 0.00000E+00 0.10000E+01 0.10000E+01 0.00000E+00 0.00000E+00             0.55399E+01 0.88931E+03
 A13 1     3 0.99054E+07 0.15080E+03 0.00000E+00 0.10000E+01 0.10000E+01 0.00000E+00 0.00000E+00             0.26002E+01 0.92145E+03
 A14 1     4 0.10094E+08 0.12962E+03 0.00000E+00 0.10000E+01 0.10000E+01 0.00000E+00 0.00000E+00             0.14807E+01 0.94005E+03
 A15 1     5 0.10289E+08 0.11607E+03 0.00000E+00 0.10000E+01 0.10000E+01 0.00000E+00 0.00000E+00             0.99691E+00 0.95103E+03
 A16 1     6 0.10493E+08 0.10749E+03 0.00000E+00 0.10000E+01 0.10000E+01 0.00000E+00 0.00000E+00             0.76327E+00 0.95763E+03
 A17 1     7 0.10708E+08 0.10223E+03 0.00000E+00 0.10000E+01 0.10000E+01 0.00000E+00 0.00000E+00             0.64360E+00 0.96157E+03
 A18 1     8 0.10948E+08 0.99278E+02 0.00000E+00 0.10000E+01 0.10000E+01 0.00000E+00 0.00000E+00             0.58345E+00 0.96378E+03
 A19 1     9 0.11096E+08 0.10288E+03 0.00000E+00 0.10000E+01 0.10000E+01 0.00000E+00 0.00000E+00             0.65745E+00 0.96128E+03
 A1A 1    10 0.11269E+08 0.11178E+03 0.00000E+00 0.10000E+01 0.10000E+01 0.00000E+00 0.00000E+00             0.87383E+00 0.95479E+03
 A11 2    11 0.95537E+07 0.23141E+03 0.00000E+00 0.10000E+01 0.10000E+01 0.00000E+00 0.00000E+00             0.14361E+02 0.83186E+03
 A12 2    12 0.97235E+07 0.18550E+03 0.00000E+00 0.10000E+01 0.10000E+01 0.00000E+00 0.00000E+00             0.58134E+01 0.88693E+03
 A13 2    13 0.99034E+07 0.15447E+03 0.00000E+00 0.10000E+01 0.10000E+01 0.00000E+00 0.00000E+00             0.28490E+01 0.91806E+03
 A14 2    14 0.10090E+08 0.13402E+03 0.00000E+00 0.10000E+01 0.10000E+01 0.00000E+00 0.00000E+00             0.16733E+01 0.93635E+03
...
...
```

Simulation Results for Fracture Problem



Temperature distribution in fracture plane after 5 years. Injection and production regions are marked I and P, respectively.



Produced fluid temperature versus time.

Five-Spot Geothermal Production/Injection Problem (EOS1)

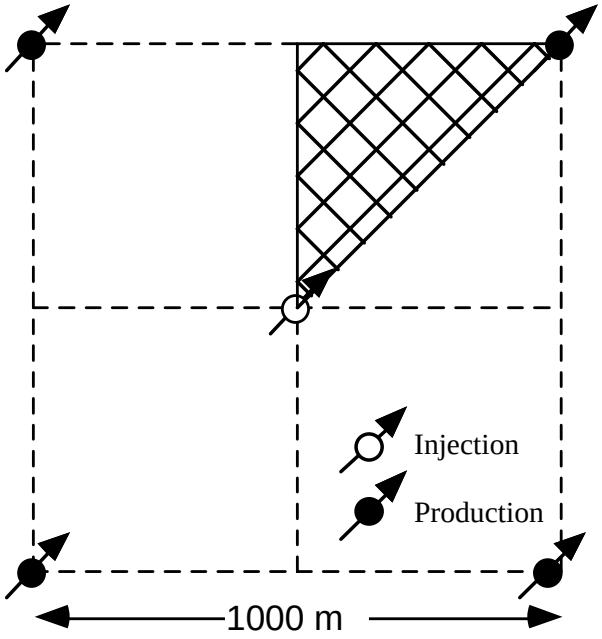


Table 14.1. Parameters for five-spot problem

Formation	
Rock grain density	2650 kg/m^3
Specific heat	1000 J/kgÞC
Heat conductivity	2.1 W/mÞC
Permeable volume fraction	2%
Porosity in permeable domain	50%
Impermeable blocks: cubes with side length	50m, 250 m
Permeability	6.0x10^{-15} m^2
Thickness	305 m
Relative permeability: Corey curves	
irreducible liquid saturation	0.30
irreducible gas saturation	0.05
Initial Conditions	
Temperature	300 ÞC
Liquid saturation	0.99
Pressure	85.93 bar
Production/Injection	
Pattern area	1 km^2
Distance between producers and injectors	707.1 m
Production rate*	30 kg/s
Injection rate*	30 kg/s
Injection enthalpy	500 kJ/kg

* Full well basis

Input File for Five-Spot Problem (EOS1)

Summary of EOS1

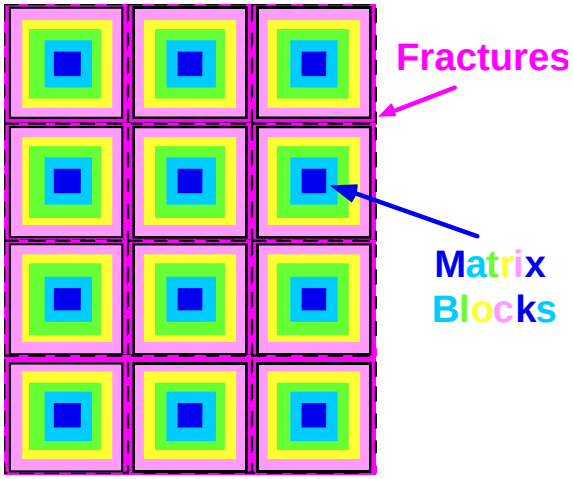
Components	# 1: water
	# 2: "water 2" (optional)
Parameter choices	
(NK, NEQ, NPH, NB) =	(1, 2, 2, 6) one water component, nonisothermal (default)
	(1, 1, 2, 6) only liquid, or only vapor; isothermal
	(2, 3, 2, 6) two-waters, nonisothermal*
molecular diffusion can be modeled by setting NK = 2, NB = 8	
Primary Variables	
single-phase conditions	
(P, T, [X]) - (pressure, temperature, [mass fraction of water 2]†)	
two-phase conditions	
(P_g, S_g, [X]) - (gas phase pressure, gas saturation, [mass fraction of water 2]†)	

* two waters cannot be run in isothermal mode, because in this case temperature is not the last primary variable

† optional, for NK = 2 only

```
*rfp* - 36 BLOCKS PARALLEL FIVE-SPOT GRID (CF. SPE-18426)
ROCKS----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
POMED          2650.       .01    6.E-15    6.E-15    6.E-15       2.1     1000.
FRACT          2650.       .50    6.E-15    6.E-15    6.E-15       2.1     1000.
MATRX          2650.    1.E-10    0.E-15    0.E-15    0.E-15       2.1     1000.

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  99      9900000000000000 4 0
         1.151852E9       -1. 3.15576E7 KA 1
      1.E5
     1.E-5                                                1.E-8
               300.                0.01                 5.E5
RPCAP----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
    3     .30       .05
    1              1.
TIMES----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
    2    2
 1.57788E8 7.88940E8
GENER----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
 AA 1INJ 1                        MASS       3.75     5.0E5
 KA 1PRO 1                        MASS      -3.75

ELEME----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
 AA 1          POMED0.1906E+060.1250E+04          0.        0.        0.1525E+03
 BA 1          POMED0.7625E+060.5000E+04          0.7071E+020.        0.1525E+03
 CA 1          POMED0.7625E+060.5000E+04          0.1414E+030.        0.1525E+03
 DA 1          POMED0.7625E+060.5000E+04          0.2121E+030.        0.1525E+03
 EA 1          POMED0.7625E+060.5000E+04          0.2828E+030.        0.1525E+03
 FA 1          POMED0.7625E+060.5000E+04          0.3536E+030.        0.1525E+03
 GA 1          POMED0.7625E+060.5000E+04          0.4243E+030.        0.1525E+03
 HA 1          POMED0.7625E+060.5000E+04          0.4950E+030.        0.1525E+03
 IA 1          POMED0.7625E+060.5000E+04          0.5657E+030.        0.1525E+03
 JA 1          POMED0.7625E+060.5000E+04          0.6364E+030.        0.1525E+03
 KA 1          POMED0.1906E+060.1250E+04          0.7071E+030.        0.1525E+03
 BB 1          POMED0.7625E+060.5000E+04          0.7071E+020.7071E+020.1525E+03
 CB 1          POMED0.1525E+070.1000E+05          0.1414E+030.7071E+020.1525E+03
...
 GE 1          POMED0.7625E+060.5000E+04          0.4243E+030.2828E+030.1525E+03
 FF 1          POMED0.3812E+060.2500E+04          0.3536E+030.3536E+030.1525E+03
HTX00          POMED        0.

CONNE----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
 AA 1 BA 1                   10.3536E+020.3536E+020.1078E+05
 BA 1 CA 1                   10.3536E+020.3536E+020.1078E+05
 BA 1 BB 1                   20.3536E+020.3536E+020.2157E+05
 CA 1 DA 1                   10.3536E+020.3536E+020.1078E+05
...
 FE 1 GE 1                   10.3536E+020.3536E+020.2157E+05
 FE 1 FF 1                   20.3536E+020.3536E+020.2157E+05

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

MESHMAKER1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
MINC
PART THRED     DFLT
  5  4OUT        50.
       .02       .08       .20       .35

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

MINC Preprocessing for Five-Spot Problem



MINC sub-gridding

```
*****************************************************************************************************
*                  MESHMAKER - MINC: GENERATE MULTIPLE INTERACTING CONTINUA MESH FOR FRACTURED MEDIUM
*****************************************************************************************************

FILE *MINC* EXISTS --- OPEN AS AN OLD FILE

CHOICE OF MATRIX-MATRIX FLOW HANDLING: "DFLT "

                     THE OPTIONS ARE: "     " (DEFAULT), NO GLOBAL MATRIX-MATRIX FLOW; GLOBAL FLOW ONLY THROUGH F
                                      "MMVER", GLOBAL MATRIX-MATRIX FLOW IN VERTICAL DIRECTION ONLY
                                      "MMALL", GLOBAL MATRIX-MATRIX FLOW IN ALL DIRECTIONS


=================== GEOMETRY DATA, NORMALIZED TO A DOMAIN OF UNIT VOLUME ========================

 CONTINUUM     IDENTIFIER       VOLUME      NODAL DISTANCE      INTERFACE AREA    INTERFACE DISTANCE
                                                                                    FROM FRACTURES

 1-FRACTURES      * *          .20000E-01      .00000E+00
                                                                .11760E+00         .00000E+00
 2-MATRIX         *2*          .80000E-01      .34984E+00
                                                                .11111E+00         .69967E+00
 3-MATRIX         *3*          .20000E+00      .97637E+00
                                                                .93970E-01         .26524E+01
 4-MATRIX         *4*          .35000E+00      .23051E+01
                                                                .59197E-01         .72627E+01
 5-MATRIX         *5*          .35000E+00      .35475E+01

=====================================================================================================

READ PRIMARY MESH FROM FILE *MESH*
           THE PRIMARY MESH HAS   37 ELEMENTS (   36 ACTIVE) AND   55 CONNECTIONS (INTERFACES) BETWEEN THEM

WRITE SECONDARY MESH ON FILE *MINC*
         THE SECONDARY MESH HAS  181 ELEMENTS (  180 ACTIVE) AND  199 CONNECTIONS (INTERFACES) BETWEEN THEM

*****************************************************************************************************

MESH GENERATION COMPLETE --- EXIT FROM MODULE *MESHMAKER*
```

Selected Output for Five-Spot Problem

```
 KA 1(   1,  6) ST = 0.100000E+06 DT = 0.100000E+06 DX1= -.187193E+06 DX2= 0.199814E+00 T = 298.440 P =  8405499. S = 0.209814E+00
 KA 1(   2,  5) ST = 0.200000E+06 DT = 0.100000E+06 DX1= -.299737E+06 DX2= 0.772235E-01 T = 295.886 P =  8105763. S = 0.287037E+00
 KA 1(   3,  5) ST = 0.300000E+06 DT = 0.100000E+06 DX1= -.330969E+06 DX2= 0.266975E-01 T = 292.981 P =  7774793. S = 0.313735E+00
 KA 1(   4,  4) ST = 0.400000E+06 DT = 0.100000E+06 DX1= -.338081E+06 DX2= 0.171490E-01 T = 289.914 P =  7436712. S = 0.330884E+00
 KA 1(   5,  4) ST = 0.600000E+06 DT = 0.200000E+06 DX1= -.749332E+06 DX2= 0.325956E-01 T = 282.716 P =  6687380. S = 0.363479E+00
 KA 1(   6,  6) ST = 0.100000E+07 DT = 0.400000E+06 DX1= -.972591E+06 DX2= 0.260141E-01 T = 272.391 P =  5714789. S = 0.389494E+00
 KA 1(   7,  4) ST = 0.140000E+07 DT = 0.400000E+06 DX1= -.187123E+06 DX2= -.145613E-01 T = 270.253 P =  5527666. S = 0.374932E+00
 KA 1(   8,  4) ST = 0.220000E+07 DT = 0.800000E+06 DX1= 0.151570E+06 DX2= -.262760E-01 T = 271.989 P =  5679236. S = 0.348656E+00
 KA 1(   9,  4) ST = 0.380000E+07 DT = 0.160000E+07 DX1= 0.103832E+06 DX2= -.138883E-01 T = 273.158 P =  5783068. S = 0.334768E+00
 KA 1(  10,  4) ST = 0.700000E+07 DT = 0.320000E+07 DX1= -.384188E+05 DX2= -.573952E-02 T = 272.728 P =  5744649. S = 0.329028E+00
 KA 1(  11,  5) ST = 0.134000E+08 DT = 0.640000E+07 DX1= -.265089E+05 DX2= -.714484E-02 T = 272.429 P =  5718140. S = 0.321884E+00
 KA 1(  12,  4) ST = 0.198000E+08 DT = 0.640000E+07 DX1= 0.268056E+06 DX2= -.181049E-01 T = 275.399 P =  5986196. S = 0.303779E+00
 KA 1(  13,  5) ST = 0.326000E+08 DT = 0.128000E+08 DX1= -.452421E+03 DX2= -.184674E-02 T = 275.394 P =  5985744. S = 0.301932E+00
 KA 1(  14,  4) ST = 0.454000E+08 DT = 0.128000E+08 DX1= -.720842E+05 DX2= 0.817172E-03 T = 274.606 P =  5913660. S = 0.302749E+00
 KA 1(  15,  4) ST = 0.710000E+08 DT = 0.256000E+08 DX1= -.277187E+06 DX2= 0.741455E-02 T = 271.503 P =  5636472. S = 0.310164E+00
 KA 1(  16,  8) ST = 0.102558E+09 DT = 0.315576E+08 DX1= -.567330E+05 DX2= -.246617E-02 T = 270.854 P =  5579740. S = 0.307697E+00
 KA 1(  17,  5) ST = 0.134115E+09 DT = 0.315576E+08 DX1= -.586688E+05 DX2= -.702594E-03 T = 270.177 P =  5521071. S = 0.306995E+00
 KA 1(  18,  5) ST = 0.157788E+09 DT = 0.236728E+08 DX1= -.659228E+05 DX2= 0.861114E-03 T = 269.410 P =  5455148. S = 0.307856E+00

*rfp* - 36 BLOCKS PARALLEL FIVE-SPOT GRID (CF. SPE-18426)

         OUTPUT DATA AFTER (  18,  5)-2-TIME STEPS                                                    THE TIME IS  0.18262E+04 DAYS

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  TOTAL TIME    KCYC   ITER  ITERC    KON    DX1M          DX2M          DX3M                          RERM         NER     KER    DELTEX
 0.15779E+09     18      5     86      2 0.637088E+06 0.299967E+03 0.000000E+00              0.496278E-08    51      2 0.236728E+08

@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@

ELEM.  INDEX      P           T           SG          SW          X1          X2         PCAP                      DG          DW
                 (PA)      (DEG-C)                                                       (PA)                   (KG/M**3)   (KG/M**3)

 AA 1     1 0.10328E+08 0.13023E+03 0.00000E+00 0.10000E+01 0.10000E+01 0.00000E+00 0.00000E+00             0.15064E+01 0.93966E+03
2AA 1     2 0.28326E+06 0.13159E+03 0.24435E+00 0.75565E+00 0.10000E+01 0.00000E+00 0.00000E+00             0.15648E+01 0.93320E+03
3AA 1     3 0.33065E+06 0.13689E+03 0.24068E+00 0.75932E+00 0.10000E+01 0.00000E+00 0.00000E+00             0.18092E+01 0.92862E+03
4AA 1     4 0.48442E+06 0.15066E+03 0.23053E+00 0.76947E+00 0.10000E+01 0.00000E+00 0.00000E+00             0.25906E+01 0.91616E+03
5AA 1     5 0.89267E+06 0.17501E+03 0.21023E+00 0.78977E+00 0.10000E+01 0.00000E+00 0.00000E+00             0.46191E+01 0.89215E+03
 BA 1     6 0.93995E+07 0.18697E+03 0.00000E+00 0.10000E+01 0.10000E+01 0.00000E+00 0.00000E+00             0.59990E+01 0.88513E+03
2BA 1     7 0.12159E+07 0.18856E+03 0.19746E+00 0.80254E+00 0.10000E+01 0.00000E+00 0.00000E+00             0.62051E+01 0.87764E+03
3BA 1     8 0.13842E+07 0.19451E+03 0.19147E+00 0.80853E+00 0.10000E+01 0.00000E+00 0.00000E+00             0.70289E+01 0.87097E+03
4BA 1     9 0.18559E+07 0.20863E+03 0.17620E+00 0.82380E+00 0.10000E+01 0.00000E+00 0.00000E+00             0.93389E+01 0.85447E+03
5BA 1    10 0.27881E+07 0.22981E+03 0.14996E+00 0.85004E+00 0.10000E+01 0.00000E+00 0.00000E+00             0.13948E+02 0.82757E+03
 CA 1    11 0.91035E+07 0.25422E+03 0.00000E+00 0.10000E+01 0.10000E+01 0.00000E+00 0.00000E+00             0.21500E+02 0.79864E+03
2CA 1    12 0.43340E+07 0.25513E+03 0.11161E+00 0.88839E+00 0.10000E+01 0.00000E+00 0.00000E+00             0.21837E+02 0.79146E+03
3CA 1    13 0.45774E+07 0.25845E+03 0.10584E+00 0.89416E+00 0.10000E+01 0.00000E+00 0.00000E+00             0.23116E+02 0.78634E+03
4CA 1    14 0.51584E+07 0.26587E+03 0.92199E-01 0.90780E+00 0.10000E+01 0.00000E+00 0.00000E+00             0.26214E+02 0.77455E+03
5CA 1    15 0.60265E+07 0.27584E+03 0.71923E-01 0.92808E+00 0.10000E+01 0.00000E+00 0.00000E+00             0.30976E+02 0.75784E+03
 DA 1    16 0.89587E+07 0.28748E+03 0.00000E+00 0.10000E+01 0.10000E+01 0.00000E+00 0.00000E+00             0.37564E+02 0.74015E+03
```
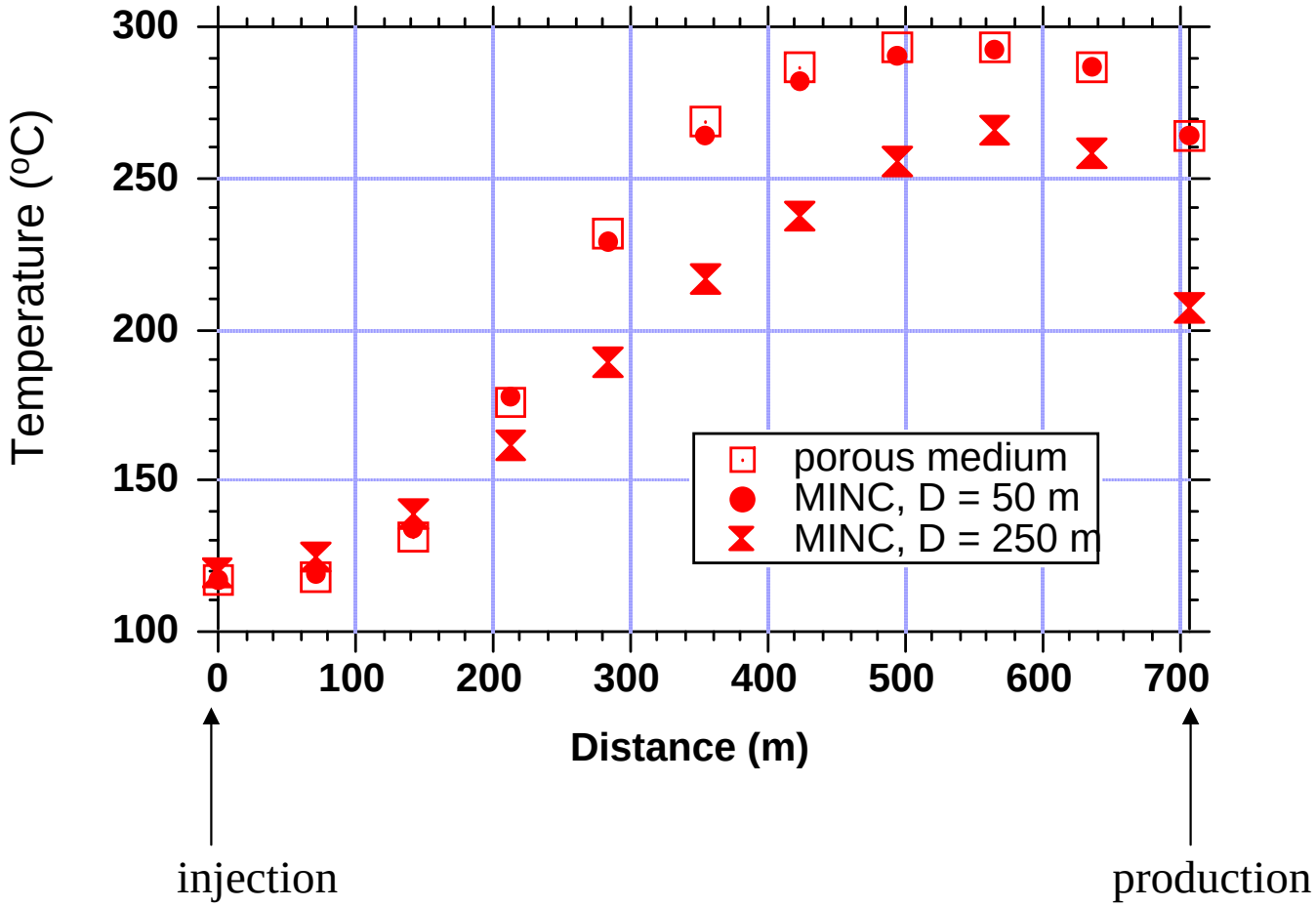

Temperature Profiles for Five-Spot after 36.5 yrs along a Line from Injection to Production Well



EOS9

Components	# 1: water
Parameter choices (NK, NEQ, NPH, NB) =	(1, 1, 1, 6) water, isothermal (default; no other choices available)
Primary Variables *† saturated conditions (P_{liq}) - (water pressure: P_{liq} P_{gas}) unsaturated conditions (S_{liq}) - (water saturation: $0 < S_{liq} < 1$)	

* The first primary variable may be initialized as X1 < 0, in which case it will be taken to denote capillary pressure, and will be converted internally to S_{liq} in the initialization phase.

† Reference gas phase pressure, flow system temperature, and (optionally) thermophysical parameters of water density, viscosity, and compressibility may be specified through a fictitious ROCKS domain `'REFCO'`.

reos9a Input File

```
*reos9a* ... input file for demonstrating EOS9 capabilities
&&&&&&&&&&&&&&&&&&&&&&&&&&&&&&&&&&&&&&&&&&&&&&&&&&&&&&&&&&&&&&&&&&&&&&&&&&&&
     Permeability modifiers (multipliers) will be applied when a domain
     'SEED' is present. A detailed description is provided in the output file.
&&&&&&&&&&&&&&&&&&&&&&&&&&&&&&&&&&&&&&&&&&&&&&&&&&&&&&&&&&&&&&&&&&&&&&&&&&&&
**************************************************************************
     Water properties at reference pressure and temperature conditions
     will be used. Default reference conditions are P = 1.013e5 Pa,
     T = 15.0 deg-C. These defaults can be overwritten by specifying
     appropriate data in a fictitious domain 'REFCO', as follows:

      reference pressure:     DROK of REFCO   ] defaults will be used
      reference temperature:  POR of REFCO    ] if left blank
      liquid density:         PER(1) of REFCO     ) if any of the PER(i) are
      liquid viscocity:       PER(2) of REFCO     ) zero or blank, values for
      liquid compressibility: PER(3) of REFCO     ) reference (P,T) will be used

     An option for initializing with gravity-capillary equilibrium is
     available. To use it, assign

      reference elevation of water table: CWET of REFCO; for CWET = 0 no
         special assignment will be made.

     This option requires that z-coordinates (elevations) are specified in
     the ELEME-data. (Note that internal MESH generation will do this
     automatically.) By convention, z-axis is considered to point upward.

     A further option is available, as follows. By specifying SPHT to a non-
     zero number, unsaturated zone saturation can be assigned to irreducible
     values for grid blocks for which Pcap is so strong that otherwise Sl
     would be below irreducible. The irreducible saturation will be taken
     to be RP(int(SPHT)); e.g., for IRP = 7, specify SPHT = 2. to use this
     feature.
**************************************************************************
```

reos9a Input File (cont'd)

```
MESHMAKER1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
XYZ
        0.
NX       1        1.
NY       1        1.
NZ      10       10.


ROCKS----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
SAND     2  2600.e00       .35    1.e-13   1.0e-13    1.e-13      2.51      920.

    7           .457       .15        1.
    7           .457       .05  5.105e-5      1.e7        1.
REFCO           1.e5       20.                                  -75.

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
   2   2       21010 0000020000400 03
                          -1.                          9.81
     1.e-9      1.e9
     1.e-5
                 .25
TIMES----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
    1    1
     1.e-9
INDOM----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8

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

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

ENDCY----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
SEED                                        0.9
```

Results for Gravity-Capillary Equilibrium (EOS9)

```
*reos9a* ... input file for demonstrating EOS9 capabilities

         OUTPUT DATA AFTER (    1,  1)-2-TIME STEPS

@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@

 TOTAL TIME     KCYC    ITER  ITERC    KON        DX1M
 0.10000E-08      1       1      1      2       0.00000E+00

@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@

ELEM.  INDEX   PRES        S(liq)      PCAP        K(rel)      DIFFUS.
               (PA)                    (PA)                    (m^2/s)

A11 1      1 0.10000E+06 0.97637E-01 -.68555E+06 0.00000E+00 0.00000E+00
A21 1      2 0.10000E+06 0.10422E+00 -.58761E+06 0.00000E+00 0.00000E+00
A31 1      3 0.10000E+06 0.11320E+00 -.48968E+06 0.00000E+00 0.00000E+00
A41 1      4 0.10000E+06 0.12620E+00 -.39174E+06 0.00000E+00 0.00000E+00
A51 1      5 0.10000E+06 0.14696E+00 -.29381E+06 0.00000E+00 0.00000E+00
A61 1      6 0.10000E+06 0.18592E+00 -.19587E+06 0.41660E-07 0.20638E-10
A71 1      7 0.10000E+06 0.28960E+00 -.97935E+05 0.31535E-04 0.45936E-08
A81 1      8 0.10000E+06 0.10000E+01 0.00000E+00 0.10000E+01 0.62661E+00
A91 1      9 0.19794E+06 0.10000E+01 0.00000E+00 0.10000E+01 0.62661E+00
AA1 1     10 0.29587E+06 0.10000E+01 0.00000E+00 0.10000E+01 0.62661E+00

@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@


             ELEM1  ELEM2  INDEX   FLO(LIQ.)   VEL(LIQ.)
                                    (KG/S)       (M/S)

             A11 1  A21 1      1  0.00000E+00  0.00000E+00
             A21 1  A31 1      2  0.00000E+00  0.00000E+00
             A31 1  A41 1      3  0.00000E+00  0.00000E+00
             A41 1  A51 1      4  0.00000E+00  0.00000E+00
             A51 1  A61 1      5  0.00000E+00  0.00000E+00
             A61 1  A71 1      6  0.14885E-17  0.14710E-19
             A71 1  A81 1      7 -0.45277E-18 -0.44744E-20
             A81 1  A91 1      8 -0.21755E-07 -0.62261E-10
             A91 1  AA1 1      9 -0.65268E-07 -0.18679E-09
```

```
...ITERATING...  AT [   2,  1] --- DELTEX = 0.100000E+10
       MAX. RES. = 0.186777E-01  AT ELEMENT AA1 1  EQUATION   1
A61 1(   2,  2) ST = 0.100000E+10 DT = 0.100000E+10 DX1= -.186552E-09
       DX2= 0.000000E+00 T =  20.000 P =        0. S = 0.185923E+00

*reos9a* ... input file for demonstrating EOS9 capabilities

         OUTPUT DATA AFTER (    2,  2)-2-TIME STEPS

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 TOTAL TIME     KCYC    ITER  ITERC    KON        DX1M
 0.10000E+10      2       2      3      2       0.86753E+01

@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@

ELEM.  INDEX   PRES        S(liq)      PCAP        K(rel)      DIFFUS.
               (PA)                    (PA)                    (m^2/s)

A11 1      1 0.10000E+06 0.97637E-01 -.68555E+06 0.00000E+00 0.00000E+00
A21 1      2 0.10000E+06 0.10422E+00 -.58761E+06 0.00000E+00 0.00000E+00
A31 1      3 0.10000E+06 0.11320E+00 -.48968E+06 0.00000E+00 0.00000E+00
A41 1      4 0.10000E+06 0.12620E+00 -.39174E+06 0.00000E+00 0.00000E+00
A51 1      5 0.10000E+06 0.14696E+00 -.29381E+06 0.00000E+00 0.00000E+00
A61 1      6 0.10000E+06 0.18592E+00 -.19587E+06 0.41660E-07 0.20638E-10
A71 1      7 0.10000E+06 0.28960E+00 -.97935E+05 0.31535E-04 0.45936E-08
A81 1      8 0.10000E+06 0.10000E+01 0.00000E+00 0.10000E+01 0.62661E+00
A91 1      9 0.19794E+06 0.10000E+01 0.00000E+00 0.10000E+01 0.62661E+00
AA1 1     10 0.29588E+06 0.10000E+01 0.00000E+00 0.10000E+01 0.62661E+00

@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@


             ELEM1  ELEM2  INDEX   FLO(LIQ.)   VEL(LIQ.)
                                    (KG/S)       (M/S)

             A11 1  A21 1      1  0.00000E+00  0.00000E+00
             A21 1  A31 1      2  0.00000E+00  0.00000E+00
             A31 1  A41 1      3  0.00000E+00  0.00000E+00
             A41 1  A51 1      4  0.00000E+00  0.00000E+00
             A51 1  A61 1      5  0.00000E+00  0.00000E+00
             A61 1  A71 1      6 -0.86113E-18 -0.13256E-19
             A71 1  A81 1      7 -0.17091E-13 -0.16890E-15
             A81 1  A91 1      8 -0.17287E-13 -0.49476E-16
             A91 1  AA1 1      9 -0.13806E-13 -0.39509E-16
```

Words to the Wise

- When running simulations for field problems, where site-specific features should be modeled, much of the work ends up dealing with geometry (gridding).
- Large grids make simulations run more slowly, generate larger data files, and make it harder to understand what is going on.
- Start with a simple, coarse grid, and “debug” the problem.
  - facilitates data preparation
  - runs more easily and faster
  - smaller input and output files
  - makes it easier to understand what's happening
  - facilitates checking and debugging
- Can put most other problem features in place.
- After model is running satisfactorily, proceed to desired gridding and grid resolution.
- Check on grid sensitivity.

TOUGH2 Training Course

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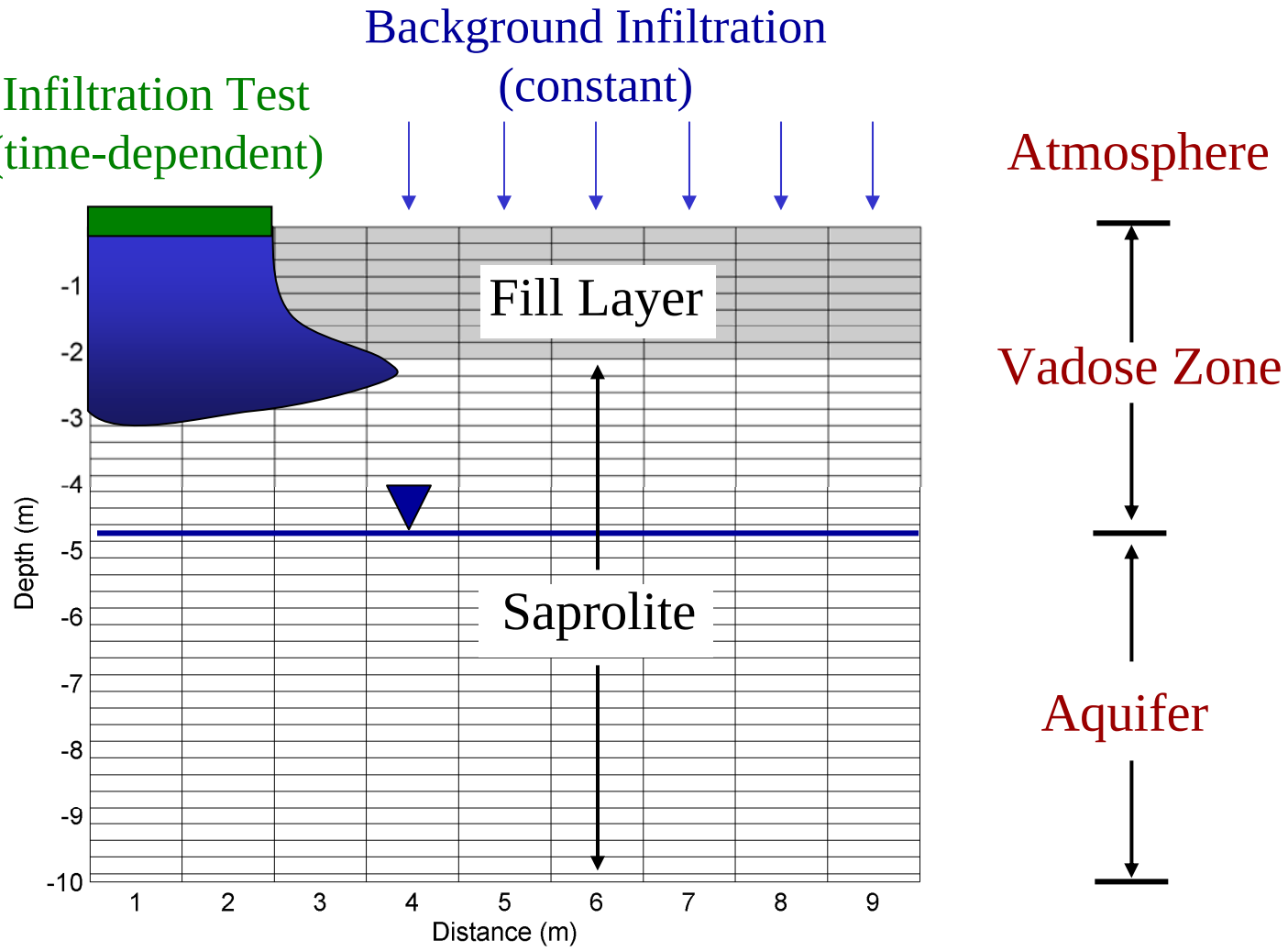
Sample Problem 2DVZ: Infiltration Test in the Vadose Zone

- Problem Description
- Part A: Mesh Generation
- Part B: Material Properties
- Part C: Boundary Conditions
- Part D: Background Infiltration
- Part E: Initial Conditions
- Part F: Steady-State Infiltration
- Part G: Infiltration Test
- Problem Variations (EOS3, ?)

Problem Description



Goals of Sample Problem

- Model the flow of water in the vadose zone (using EOS9)
- Create a 2-D mesh using MESHMAKER (ELEME and CONNE blocks)
- Assign rock properties in ELEME block to specify geological layers
- Assign boundary conditions (modifying ELEME block by hand and using free software available for TOUGH2)
- Add constant background infiltration (using GENER block)
- Get steady-state initial conditions (obtaining INCON block)
- Simulate infiltration test (using INCON and GENER blocks)
- Become familiarized with time-stepping and output parameters (PARAM block)
- Consider problem variations including extension to nonisothermal flow (using EOS3)

Part A: Mesh Generation

Part A involves generating the MESH file that contains the ELEME and CONNE blocks. The MESHMaker block is used for this purpose.

A.1 MESHMaker block (p. 160, 177-183 in manual)

- Open *PartA.txt*. Note that the first line is reserved for the title. See Figure 1. Textpad, WordPad and Notepad can be used for editing the text files. Caution: do not insert "tabs" into the files.
- First generate a 1-D Cartesian mesh in the Z-direction. Enter "XYZ" for the variable WORD (p. 160), and consult manual (p. 180). Specify a total of 42 elements, with a grid spacing of 1.0E-3, 0.25, 0.25, …., 0.25, 1.0E-3 m.
- (Hint: fill in values for the blank spaces marked by "?")

```
Input file for Part A of sample problem 2DVZ
MESHMAKER ----*----2----*----3----*----4----*----5----*----6----*----7----*----8
???                          Select XYZ for cartesian grid

NX       1 1.0000            Select dX and dY to yield cross section of column
NY       1 1.0000
NZ       1 ?                 Add (dummy) top boundary element
NZ      ?? 0.2500            Create uniform grid for 10 m long column
NZ       ? 1.0E-3            Add (dummy) bottom boundary element
                             Needs one empty line to terminate XYZ block
                             Needs another empty line to terminate MESHMAKER
ENDCY
```

Figure 1. MESHM block for *PartA.txt* of Sample problem 2DVZ.

A.2 Run TOUGH2 with *PartA.txt* as input file

- Open a DOS command prompt window:

  `START→Programs→Accessories→Command Prompt`

  (or double-click on *cmd.exe* in C:\TOUGH2)

- Change directory to location of input files, for example:

  `cd C:\TOUGH2\...\PartA`

  (or copy input files into directory C:\TOUGH2 and run code there)

- Run TOUGH2 with EOS9 by typing:

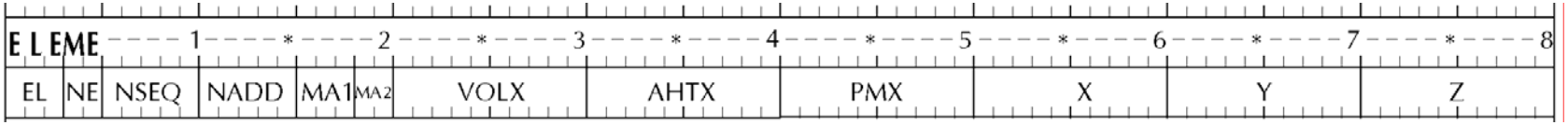
  `t2_eos9 < PartA.txt > PartA.out`

- Open the following output files:

  PartA.out, MESH

SIDE NOTE (Block ELEME)

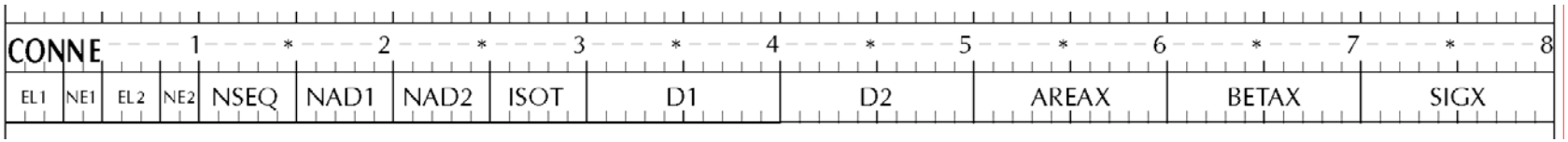
- Element name (format: AAAII, e.g., ELE99)
- Material type (5 character name or number of order in ROCKS block)
- Volume [m^3]
- Optional:
  - Interface area to heat-conducting, confining layer
  - X-, Y- and Z-coordinates




```
ELEME----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
A11 1          SOIL  0.100E-09 0.100E+01           0.500E+00 0.500E+00 -.500E-10
A21 1          FRACT 0.500E-01                     0.500E+00 0.500E+00 -.250E-01
A31 1              7 0.500E-01                     0.500E+00 0.500E+00 -.750E-01
.....
Name        Material   Volume    AHTX   (Perm Mod.)   X         Y         Z
```

SIDE NOTE (Block CONNE)

- A connection connects two elements
- Each element can have multiple connections
- Names of two elements (AAAII AAAII)
- Anisotropy index
- Nodal distances to common interface [m]
- Interface area [m^2]
- Cosine of angle between gravity and connection line




```
CONNE----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
A11 1A21 1                    3 0.500E-10 0.250E-01 0.100E+01 0.100E+01
A21 1A31 1                    3 0.250E-01 0.250E-01 0.100E+01 0.100E+01
A31 1A41 1                    3 0.250E-01 0.250E-01 0.100E+01 0.100E+01
...
Element 1 and 2            ISOT    D1        D2       AREAX      BETAX
```

Q-A.1.1: Open *PartA.out* and scroll down to “PARAMETERS FOR FLEXIBLE DIMENSIONING”. Are the maximum number of elements (`MNEL`) and maximum number of connections (`MNCON`) sufficiently large?

Q-A.1.2: Scroll down further. Do the grid increments appear as you expected?

Q-A.1.3: Open the MESH file. What are the minimum and maximum Z values?

Q-A.1.4: What are the nodal distances for the first connection (between elements “A11 1” and “A21 1”)? Why are they different?

➢ Now modify the `MESHMaker` block to create 10 grid blocks in the X-direction with 1.0 m spacing (in addition to the 42 elements already being created in the Z-direction. Make sure the alignment in the input file is correct.

Q-A.1.5: Open the `MESH` file and examine the naming sequence of the elements in the new 2-D mesh. Note that the elements have a certain naming convention with sequentially increasing letters and numbers. In this case, which elements correspond to the first column in the model (i.e., with X-coordinates equal to minimum value, and Z-coordinates spanning over total range)?

➢ Rename the output file `MESH` as *MESH_PartA* to be used later.

SIDE NOTE (Block ROCKS)

- Material name (5 characters, case sensitive)
- Hydrological properties
  - Porosity
  - Absolute permeability [m^2] in three (arbitrary) directions
  - Parameters of relative permeability and capillary pressure functions (overwrite defaults given in block RPCAP)
- Thermal properties
  - Rock grain density [kg/m^3]
  - Formation heat conductivity (wet) [W/m°C]
  - Rock grain specific heat [J/kg ° C]

```
Name     NAD     DROK        PORO     PER(1)     PER(2)     PER(3)       CWET      SPHT
ROCKS----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
SAND       0     2650.      .4000 1.000E-12 1.000E-12 1.000E-13       2.51       920.
GRAVE      0     2650.      .3000 1.000E-11 1.000E-11 1.000E-11       2.51       920.
BOUND      2     2650.      .9900 1.000E-12 1.000E-12 1.000E-12       2.51    100000.
                (additional parameters on this line, see Manual p. 161)
    3              0.3        0.1
    1              0.0        0.0        1.0
```

SIDE NOTE (Additional Properties)

- Additional, EOS-specific fluid properties and other parameters are given in blocks `SELEC` and `DIFFU` (see Manual)
- For EOS9 (Richards equation):
  - Special “domain” **`REFCO`** contains **reference water properties**.
  - If omitted, default values are assumed.

```
ROCKS----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
SAND            2650.     .4000 1.000E-12 1.000E-12 1.000E-13      2.51      920.
REFCO       1.013E05      15.0   999.213 1.135E-03 4.594E-10

              Press.     Temp.   Density Viscosity Compressibility
```

Part B: Material Properties

In Part B of this problem we specify 4 material properties in the model domain. Materials are created in the ROCKS block, and then assigned to the desired elements in the ELEME block.

B.1 ROCKS block

➢ Open *PartB.txt*. Note two materials called SAPRO and ATMOS.

Q-B.1.1: What are the porosity and permeability values of these materials? Is the permeability of SAPRO isotropic or anisotropic? What is the reason for material ATMOS?

➢ Create a third material called FILLI with a porosity of 0.3 and isotropic permeability of 5.0E-12. Use the same RELP and PCAP data as for SAPRO (see Figure 2).

➢ Create a fourth material called BOUND with all properties (all 4 lines) the same as material SAPRO (see Figure 2). Leave a blank line after to close the block!

```
Input file for Part B of sample problem 2DVZ
ROCKS----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
SAPRO    2    2500.0     .2000 1.000E-12 1.000E-12 1.000E-12       2.0     1000.

    7           0.30      0.20       1.0      0.05
    7           0.30      0.19    1.0e-3     5000.      1.00
ATMOS    2    2500.0      0.99 1.000E-12 1.000E-12 1.000E-12       2.0     1000.

    7           0.30      0.20       1.0      0.05
    8
FILLI    2    2500.0     .3000 5.000E-12 5.000E-12 5.000E-12       2.0     1000.

    7           0.30      0.20       1.0      0.05
    7           0.30      0.19    1.0e-3     5000.      1.00
BOUND    2    2500.0     .2000 1.000E-12 1.000E-12 1.000E-12       2.0     1000.

    7           0.30      0.20       1.0      0.05
    7           0.30      0.19    1.0e-3     5000.      1.00
(blank line)
```

Figure 2. ROCKS block in *PartB.txt* of Sample problem 2DVZ. SAPRO and ATMOS represent saprolite and the atmosphere, while FILLI is a 2 m-thick layer of fill material and BOUND is the lower boundary of the model.

SIDE NOTE (Free software available for TOUGH2)

Free Software (no support)

Module	Version	Description	Download		
			Executable (PC)	Source Code	Manual
EXT	1.0	Extracts data from TOUGH2 output file for visualization with TECPLOT	Ext.exe	Ext.zip	Instructions
AMESH	1.0	Generates irregular TOUGH+ mesh	—	AMESH.zip	AMESH User's Guide
T2CHK	1.0	Calculates equilibrium saturations and data for plotting characteristic curves.	T2CHK.exe	—	Instructions
MoveMesh	1.0	Moves coordinates of TOUGH2 mesh.	MoveMesh.exe	MoveMesh.f	See source code
StratMesh	1.0	Mesh generator for 3D grids with multiple hydrostratigraphic units of variable thickness.	—	StratMesh.f StratMesh.inp	See source code and sample input file
AddBound	1.0	Deletes elements on a specified domain or replaces them with a single boundary element.	AddBound.exe	AddBound.f	See source code
Perm2Mesh	1.0	Reads coordinates and log(permeability modifier) from a file and assigns them to TOUGH2 elements.	—	Perm2Mesh.f	See sou code
AssignRock	1.0	Assigns rock type name to all elements within a specified box.	AssignRock.exe	AssignRock.f	See sou code
DelMatrix	1.0	Deletes all elements with a permeability smaller than a cut-off value.	—	DelMatrix.f	See source code
CutCavity	1.0	Cuts cavities of various shapes into 2D and 3D models.	—	CutCylinder.f CutRect.f CutEllipsoid.f	See source code
EOS9EOS3	1.0	Converts EOS9-SAVE file to EOS3-INCON file.	Eos9Eos3.exe	EOS9EOS3.f	See source code
DeleteElements	1.0	Deletes elements and connections in specified domain.	DeleteElements.exe	DeleteElements.f	See source code

- *AssignRock.f* is a program that allows you to assign a rock type to all elements that fall within a user-specified coordinate range.
- Easier than modifying ELEME block by hand!
- Some people use their own scripts (e.g., in Matlab)

- http://www-esd.lbl.gov/TOUGHPLUS/licensing.html#free

B.2 ELEME and CONNE blocks

- *AssignRock.exe* is run by typing, "AssignRock", and then follow the prompt to enter: input mesh file name, output file name, X_{min}, X_{max}, Y_{min}, Y_{max}, Z_{min}, Z_{max}.
- Add three layers by running *AssignRock.exe* three times (first use input mesh file *MESH_PartA* with output file name *MESH_PartB1*, then use input mesh file *MESH_PartB1* with output file name *MESH_PartB2*, etc.)

  FILLI layer: $[Z_{min}, Z_{max}] = [-2, 0]$

  SAPRO layer: $[Z_{min}, Z_{max}] = [-9.95, -2]$

  BOUND layer: $[Z_{min}, Z_{max}] = [-10.01, -9.95]$

  For each use $[X_{min}, X_{max}] = [0, 10.1]$, and $[Y_{min}, Y_{max}] = [0, 1]$
- Check the final output file (e.g., *MESH_PartB3*) to ensure that the distribution of materials is correct (see Figure 3).

```
ELEME
A11 1          FILLI0.1000E-020.1000E+01          0.5000E+000.5000E+00-.5000E-03
A21 1          FILLI0.2500E+00                    0.5000E+000.5000E+00-.1260E+00
A31 1          FILLI0.2500E+00                    0.5000E+000.5000E+00-.3760E+00
A41 1          FILLI0.2500E+00                    0.5000E+000.5000E+00-.6260E+00
A51 1          FILLI0.2500E+00                    0.5000E+000.5000E+00-.8760E+00
A61 1          FILLI0.2500E+00                    0.5000E+000.5000E+00-.1126E+01
A71 1          FILLI0.2500E+00                    0.5000E+000.5000E+00-.1376E+01
A81 1          FILLI0.2500E+00                    0.5000E+000.5000E+00-.1626E+01
A91 1          FILLI0.2500E+00                    0.5000E+000.5000E+00-.1876E+01
AA1 1          SAPRO0.2500E+00                    0.5000E+000.5000E+00-.2126E+01
AB1 1          SAPRO0.2500E+00                    0.5000E+000.5000E+00-.2376E+01
AC1 1          SAPRO0.2500E+00                    0.5000E+000.5000E+00-.2626E+01
AD1 1          SAPRO0.2500E+00                    0.5000E+000.5000E+00-.2876E+01
AE1 1          SAPRO0.2500E+00                    0.5000E+000.5000E+00-.3126E+01
AF1 1          SAPRO0.2500E+00                    0.5000E+000.5000E+00-.3376E+01
AG1 1          SAPRO0.2500E+00                    0.5000E+000.5000E+00-.3626E+01
…
B51 1          SAPRO0.2500E+00                    0.5000E+000.5000E+00-.9626E+01
B61 1          SAPRO0.2500E+00                    0.5000E+000.5000E+00-.9876E+01
B71 1          BOUND0.1000E-020.1000E+01          0.5000E+000.5000E+00-.1000E+02
A11 2          FILLI0.1000E-020.1000E+01          0.1500E+010.5000E+00-.5000E-03
A21 2          FILLI0.2500E+00                    0.1500E+010.5000E+00-.1260E+00
…
B7110          BOUND0.1000E-020.1000E+01          0.9500E+010.5000E+00-.1000E+02
```

Figure 3. Preliminary ELEME block in *PartB.txt* of Sample problem 2DVZ. Atmosphere has not been added yet.

SIDE NOTE (Free software available for TOUGH2)

Free Software (no support)					
Module	Version	Description	Download		
			Executable (PC)	Source Code	Manual
EXT	1.0	Extracts data from TOUGH2 output file for visualization with TECPLOT	Ext.exe	Ext.zip	Instructions
AMESH	1.0	Generates irregular TOUGH+ mesh	—	AMESH.zip	AMESH User's Guide
T2CHK	1.0	Calculates equilibrium saturations and data for plotting characteristic curves.	T2CHK.exe	—	Instructions
MoveMesh	1.0	Moves coordinates of TOUGH2 mesh.	MoveMesh.exe	MoveMesh.f	See source code
StratMesh	1.0	Mesh generator for 3D grids with multiple hydrostratigraphic units of variable thickness.	—	StratMesh.f StratMesh.inp	See source code and sample input file
AddBound	1.0	Deletes elements on a specified domain or replaces them with a single boundary element.	AddBound.exe	AddBound.f	See source code
Perm2Mesh	1.0	Reads coordinates and log(permeability modifier) from a file and assigns them to TOUGH2 elements.	—	Perm2Mesh.f	See sou code
AssignRock	1.0	Assigns rock type name to all elements within a specified box.	AssignRock.exe	AssignRock.f	See sou code
DelMatrix	1.0	Deletes all elements with a permeability smaller than a cut-off value.	—	DelMatrix.f	See source code
CutCavity	1.0	Cuts cavities of various shapes into 2D and 3D models.	—	CutCylinder.f CutRect.f CutEllipsoid.f	See source code
EOS9EOS3	1.0	Converts EOS9-SAVE file to EOS3-INCON file.	Eos9Eos3.exe	EOS9EOS3.f	See source code
DeleteElements	1.0	Deletes elements and connections in specified domain.	DeleteElements.exe	DeleteElements.f	See source code

- *AddBound.f* allows you to replace a row or column of elements with a single element.
- Useful for connecting top of model to atmosphere or distributed source.

- http://www-esd.lbl.gov/TOUGHPLUS/licensing.html#free

- Use *AddBound.exe* to create an atmospheric layer and connect it to the top of the fill layer. Run the program by typing "AddBound", and then following the prompt to enter:
  - Input mesh file: *MESH_PartB3*
  - Output mesh file: *MESH_PartB4*
  - Boundary element name: 99999
  - Boundary rock type: ATMOS
  - Boundary element volume: 9 x 1 m x 0.25 m = 2.25 m^3
  - Nodal distance to boundary element: 1.0E-3
  - Domain shape: cube (=1)
  - $[X_{min}, X_{max}] = [0, 10.1]$
  - $[Y_{min}, Y_{max}] = [0, 1]$
  - $[Z_{min}, Z_{max}] = [-0.1, 0]$

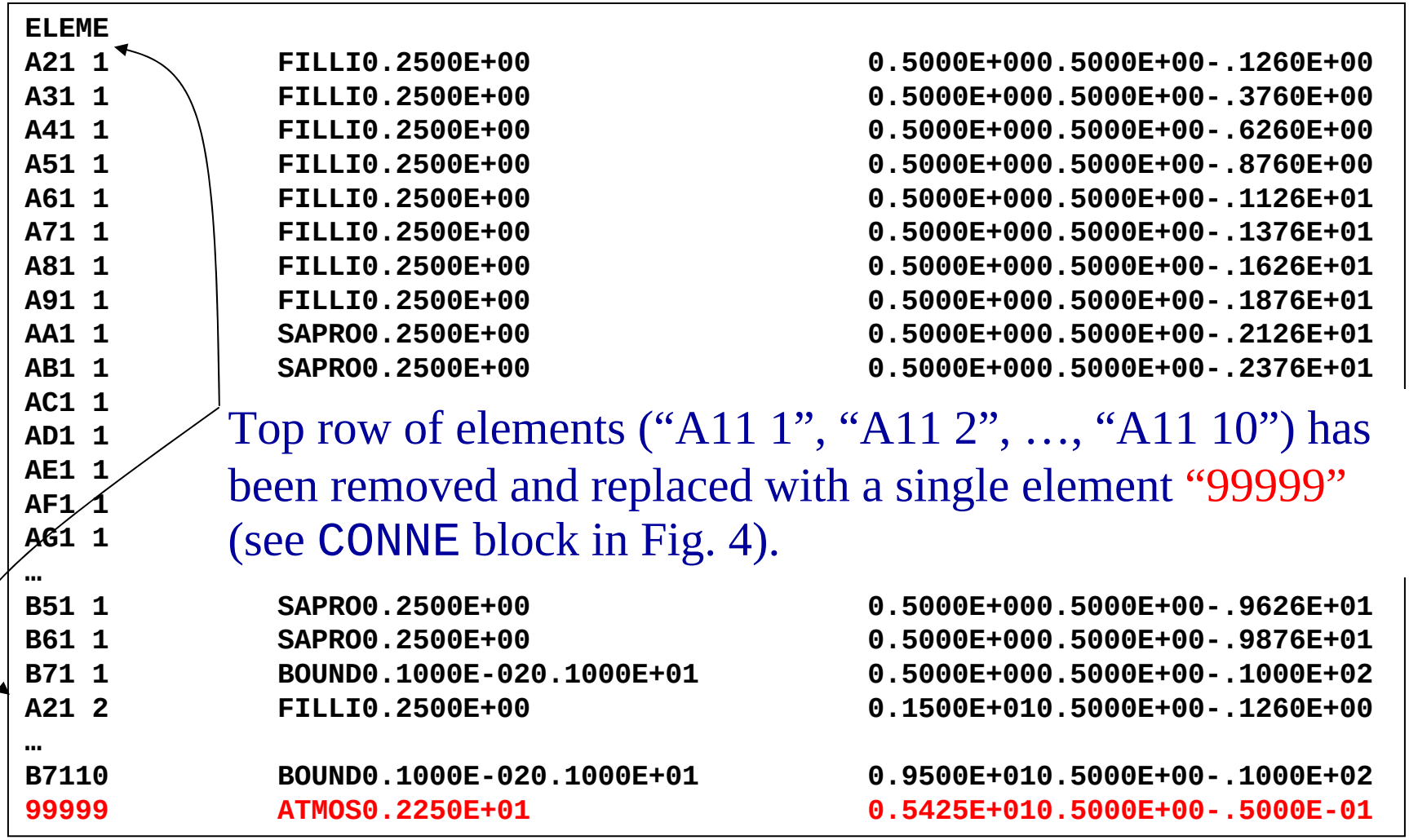
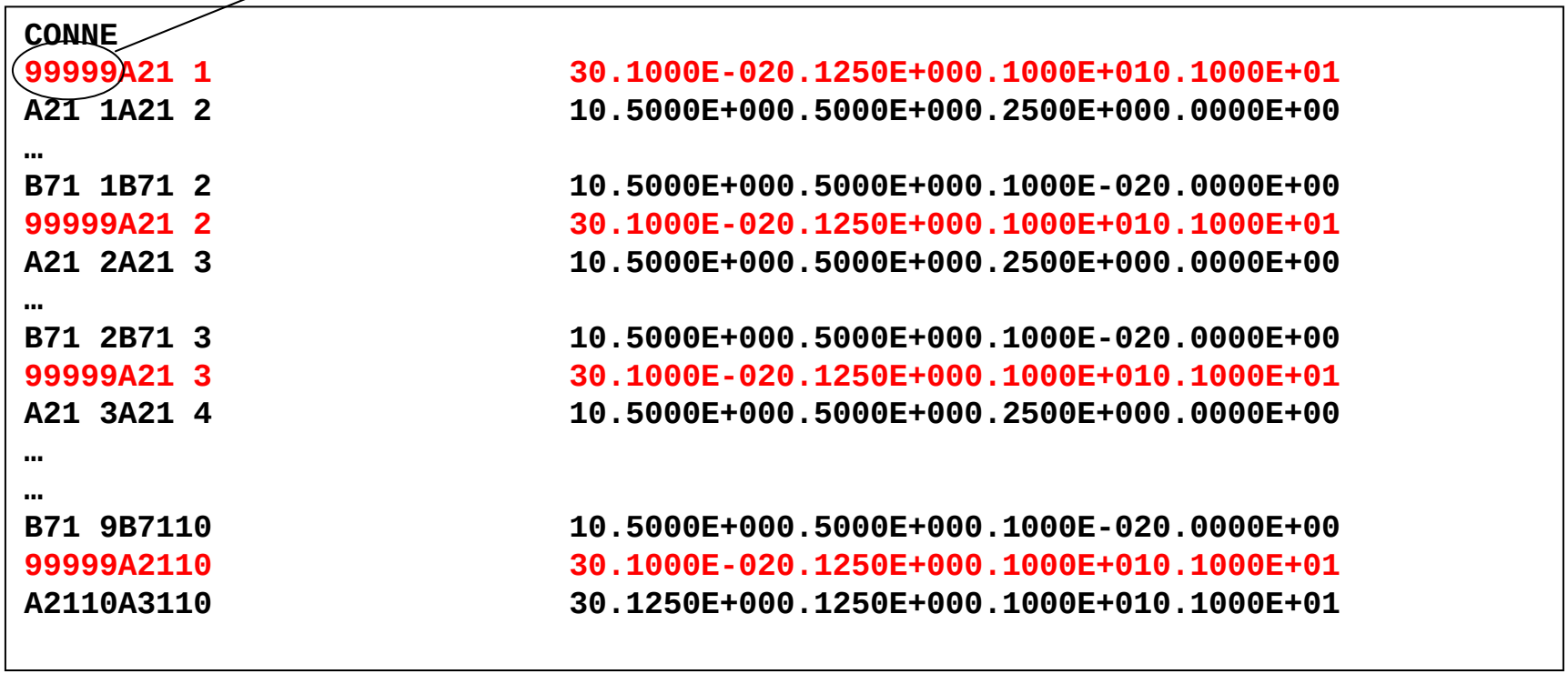


Figure 4. Final ELEME block in *PartB.txt* of Sample problem 2DVZ. The Atmosphere has been added.

Element “99999” is connected to “A21 1”, “A21 2”, …, “A21 10”



```
CONNE
99999A21 1                    30.1000E-020.1250E+000.1000E+010.1000E+01
A21 1A21 2                    10.5000E+000.5000E+000.2500E+000.0000E+00
…
B71 1B71 2                    10.5000E+000.5000E+000.1000E-020.0000E+00
99999A21 2                    30.1000E-020.1250E+000.1000E+010.1000E+01
A21 2A21 3                    10.5000E+000.5000E+000.2500E+000.0000E+00
…
B71 2B71 3                    10.5000E+000.5000E+000.1000E-020.0000E+00
99999A21 3                    30.1000E-020.1250E+000.1000E+010.1000E+01
A21 3A21 4                    10.5000E+000.5000E+000.2500E+000.0000E+00
…
…
B71 9B7110                    10.5000E+000.5000E+000.1000E-020.0000E+00
99999A2110                    30.1000E-020.1250E+000.1000E+010.1000E+01
A2110A3110                    30.1250E+000.1250E+000.1000E+010.1000E+01
```

Figure 5. Final CONNE block in *PartB.txt* of Sample problem 2DVZ. The Atmosphere has been added.

- Now we have a mesh to insert into the TOUGH2 input file. So copy contents of *MESH_PartB4* and paste into *PartB.txt* after the `INCON` block, leaving a blank line in between (Figure 6). Remove the lines of text following the "+++" at the end of the `CONNE` block that you just inserted.

```
----*----1 MOP: 123456789*123456789*1234 ---*----5----*----6----*----7----*----8
PARAM----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
   20001     1001000001000001004000040000
       0.0           1.000E-00                        9.81000
   1.0E-04
                 0.9
GENER----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8

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

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

ELEME
A21 1          FILLI0.2500E+00                    0.5000E+000.5000E+00-.1260E+00
A31 1          FILLI0.2500E+00                    0.5000E+000.5000E+00-.3760E+00
…
B6110          SAPRO0.2500E+00                    0.9500E+010.5000E+00-.9876E+01
B7110          BOUND0.1000E-020.1000E+01          0.9500E+010.5000E+00-.1000E+02
99999          ATMOS0.2250E+01                    0.5050E+010.5000E+00-.5000E-01

CONNE
99999A21 1                  30.1000E-020.1250E+000.1000E+010.1000E+01
A21 1A21 2                  10.5000E+000.5000E+000.2500E+000.0000E+00
…
B71 1B71 2                  10.5000E+000.5000E+000.1000E-020.0000E+00
99999A21 2                  30.1000E-020.1250E+000.1000E+010.1000E+01
…

ENDCY
```

Figure 6. Portion of input file for *PartB.txt* after contents of MESH file have been added (ELEME and CONNE blocks).

Part C: Boundary Conditions

The boundary conditions (BCs) can be specified in several ways by modifying the `ELEME` block (and by using the `GENER` block).

- Copy *PartB.txt* and paste/rename it *PartC.txt*. Modify this file accordingly in the following steps.

C.1 Vertical Boundaries

- For the vertical (side) boundaries of the model, we wish to have zero-flux BCs (Dirichlet), which is the default condition for boundary elements in TOUGH2, so nothing more needs to be done for these boundaries.

C.2 Bottom Boundary

- Specify a constant pressure (Neumann) BC at the bottom of the model by setting the element volumes to very large values (1E50); the corresponding primary variables will remain constant.
- Find all elements at the bottom of the model (material BOUND) and replace their volumes by 1.0E50.

```
ELEME----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
A21 1          FILLI0.2500E+00                      0.5000E+000.5000E+00-.1260E+00
...
B61 1          SAPRO0.2500E+00                      0.5000E+000.5000E+00-.9876E+01
B71 1          BOUND0.1000E-020.1000E+01            0.5000E+000.5000E+00-.1000E+02
```

```
ELEME----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
A31 1          FILLI0.2500E+00                      0.5000E+000.5000E+00-.3760E+00
...
B61 1          SAPRO0.2500E+00                      0.5000E+000.5000E+00-.9876E+01
B71 1          BOUND1.0000E+500.1000E+01            0.5000E+000.5000E+00-.1000E+02
```

- Text editor trick: go to the "edit" menu, choose "replace". Paste `BOUND0.1000E-02` into the "find" field, and type `BOUND1.0000E+50` into the "replace with" field…Be careful using "replace all"!

C.3 Top Boundary

- In Part D, we will specify a constant flux at the top of the model by adding a water source (using GENER block) in the fill layer.
- Run TOUGH2 by typing "t2_eos9 < *PartC.txt* > *PartC.out*".

SIDE NOTE (Inactive element concept). Dirichlet boundaries can also be specified using inactive elements (see p. 62 of manual), which reduces the number of unknowns by removing elements from the mass/heat balance equations. All elements occurring in the ELEME block after an element with a *zero or negative volume* are assumed to be inactive, while those before are active. Alternatively, one can insert a line with a fictitious element name (e.g., with "INA" in columns 1-3); the following elements are automatically taken to be inactive.

Depending on the order—by row or by column—of the elements, this feature may require reordering the ELEME block (i.e., putting the desired inactive boundary elements after the active elements).

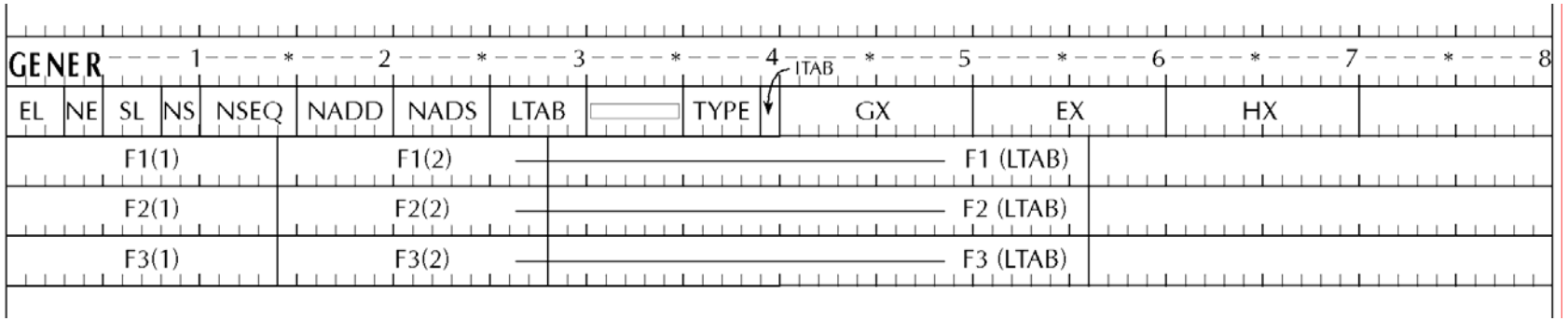
Part D: Background Infiltration

Background infiltration (steady-state flow in the vertical direction) is implemented by injecting water at a constant mass rate into each grid block at the top of the fill layer. The GENER block is used for this purpose (see manual starting on p. 174).

- Copy *PartC.txt* and paste/rename it *PartD.txt*.
- Next open *GENER_Info_PartD.txt* and paste contents into *PartD.txt*, after PARAM block and before ELEME block (leave blank line below).

- Modify the new GENER block in *PartD.txt* so that water is injected at a constant generation rate of 1.0E-6 kg/s.
  - TYPE ="WATE"
  - GX = 1.0E-6
- Add a source to the top row of the FILLI layer by specifying the code name of the first element [EL,NE]= "A21 1". Also enter the name of the source [SL,NS] = "INJ01".
- Add 9 additional sources using NSEQ, NADD, and NADS
  - Number of additional elements with same injection rate NSEQ = 9
  - Increment between code numbers in element names NADD = 1
  - Increment between code numbers in source names NADS = 1
- Check that the GENER block is consistent with Figure 7.
- Run TOUGH2 by typing "t2_eos9 < *PartD.txt* > *PartD.out*"

a)



b)

```
----*----1 MOP: 123456789*123456789*1234 ---*----5----*----6----*----7----*----8
PARAM----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
   20001     1001000001000020004000040000
       0.0           1.000E-00                        9.81000
   1.0E-04
                 0.9
GENER----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
A21 1INJ01    9    1    1    0     WATE 1.0000e-06

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

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

ELEME
A21 1          FILLI0.2500E+00                    0.5000E+000.5000E+00-.1260E+00
A31 1          FILLI0.2500E+00                    0.5000E+000.5000E+00-.3760E+00
```

Figure 7. GENER block a) format requirements and b) portion in input file *PartD.txt* used to simulate background infiltration.

Part E: Initial Conditions

In this step we calculate a 2-D profile for a steady-state system that contains an aquifer (water table at 5 m) and unsaturated zone above.

E.1 Primary Variables in EOS9 (p. 52 of manual)

- There is only one primary variable in EOS9 (see below)

Relevant T2 Blocks

MULTI

INCON
INDOM
PARAM
SAVE

Components	# 1: water
Parameter choices	
(NK, NEQ, NPH, NB) =	(1, 1, 1, 6) water, isothermal (default; no other choices available)
Primary Variables *†	
saturated conditions	
(P_{liq}) - (water pressure: $P_{liq} \geq P_{gas}$)	
unsaturated conditions	
(S_{liq}) - (water saturation: $0 < S_{liq} < 1$)	

* The first primary variable may be initialized as X1 < 0, in which case it will be taken to denote capillary pressure, and will be converted internally to S_{liq} in the initialization phase.

† Reference gas phase pressure, flow system temperature, and (optionally) thermophysical parameters of water density, viscosity, and compressibility may be specified through a fictitious ROCKS domain `'REFCO'`.

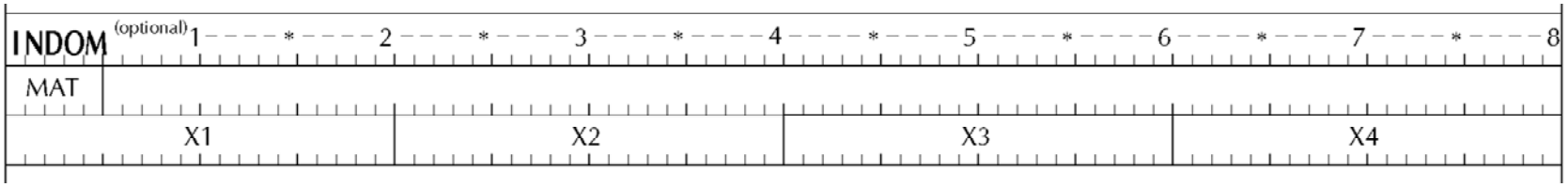
E.2 Set Pressure at Bottom of Model using `INDOM` Block

- Copy *PartD.txt* and paste/rename it *PartE.txt*.
- The `INDOM` block will be used to give initial conditions for the material (BOUND) at the lower boundary of the model (it will remain fixed since it is a Dirichlet boundary).
- Make the pressure at the bottom of the model (at 10 m depth) equal the pressure of a 5 m column of water above it by setting $P_{BOUND} = \rho g H + P_{atm} \sim 1000 \times 9.81 \times 5 + 1.013E5 = 0.1503E6$ Pa.
- Create an `INDOM` block after the `GENER` block by typing "`INDOM`" on one line, the material "BOUND" on the next line, and the value of P_{bound} of the following line. Leave a blank line above and below the new block (see Figure 8).

E.3 Default initial conditions in `PARAM` Block

Q-E.3.1: What are the default initial conditions in *PartE.txt* for the remaining materials (`PARAM.4`, p. 168)?

a)



b)

```
----*----1 MOP: 123456789*123456789*1234 ---*----5----*----6----*----7----*----8
PARAM----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
      20001     1001000000000200040000 4000
       0.0           1.000E-00                        9.81000
   1.0E-04
                  0.9      ← Default initial conditions
GENER----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
A21 1INJ01    9    1    1    0     WATE 1.0000e-04

INDOM----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
BOUND
          0.150300E6

ELEME
A21 1          FILLI0.2500E+00                    0.5000E+000.5000E+00-.1260E+00
A31 1          FILLI0.2500E+00                    0.5000E+000.5000E+00-.3760E+00
```

Figure 8. a) Format requirements for `INDOM` block, and b) specifying initial conditions with `INDOM` and `PARAM.4` for *PartE.txt*.

- Change `MOP(7)` to 0 to suppress output of input data.
- Run TOUGH2 by typing "t2_eos9 <*PartE.txt* >*PartE.out*"
- Examine the following output files: *PartE.out*, *SAVE*

```
*************************************************************************************************************************
*************************   EOS9: EQUATION OF STATE FOR SATURATED/UNSATURATED FLOW (RICHARDS EQUATION)   *************************
*************************      Special version with capability for random permeability modification      *************************
*************************************************************************************************************************

   ONLY AVAILABLE OPTION IS: (NK,NEQ,NPH,NB) = (1,1,1,6)
                          NK  =  1   - NUMBER OF FLUID COMPONENTS
                          NEQ =  1   - NUMBER OF EQUATIONS PER GRID BLOCK
                          NPH =  1   - NUMBER OF PHASES THAT CAN BE PRESENT
                          NB  =  6   - NUMBER OF SECONDARY PARAMETERS (OTHER THAN COMPONENT MASS FRACTIONS)

 DEFAULT REFERENCE CONDITIONS ARE (P,T) = ( .1013e6 Pascal, 15.0 deg-C)

 DEFAULT CONDITIONS ARE USED
 water density is d = 0.999213E+03 kg/m^3;      viscosity is vis = 0.113595E-02 Pa-s;      compressibility is cp = 0.463146E-09 1/Pa

 THE PRIMARY VARIABLE X1 IS PRESSURE FOR X1 > 0.101300E+06; IT IS LIQUID SATURATION FOR X1 < 1; IT IS Pcap for X1 < 0

 ********** VOLUME- AND MASS-BALANCES ***************************************************************************************

 ********** [KCYC,ITER] = [   0,  0] *****                                THE TIME IS  0.00000E+00 SECONDS, OR  0.00000E+00 DAYS


 PHASE VOLUMES IN PLACE
 GAS 0.24227500000000E+01 M**3;   LIQUID 0.20000000000000E+51 M**3

 LIQUID MASS IN PLACE 0.19984720647631E+54 KG

 *************************************************************************************************************************


 ...ITERATING...  AT [   1,  1] --- DELTEX = 0.100000E+01   MAX. RES. = 0.756175E-02  AT ELEMENT B61 1  EQUATION   1
 B61 1(   1,  2) ST = 0.100000E+01 DT = 0.100000E+01 DX1= 0.679957E-02 DX2= 0.000000E+00 T =  15.000 P =        1. S = 0.906800E+00

 WRITE FILE *SAVE* AFTER    1 TIME STEPS  ---  THE TIME IS 0.100000E+01 SECONDS
```

Figure 9. Excerpt from *PartE.out*.

Two-phase conditions ($S_a < 1$)

```
INCON -- INITIAL CONDITIONS FOR  411 ELEMENTS
A21 1           0.30000000E+00
 0.8999739435328E+00 0.0000000000000E+00
A31 1           0.30000000E+00
 0.8999999829750E+00 0.0000000000000E+00
A41 1           0.30000000E+00
 0.8999999999889E+00 0.0000000000000E+00
A51 1           0.30000000E+00
 0.9000000000000E+00 0.0000000000000E+00
A61 1           0.30000000E+00
 0.9000000000000E+00 0.0000000000000E+00
A71 1           0.30000000E+00
 0.9000000000000E+00 0.0000000000000E+00
A81 1           0.30000000E+00
 0.9000000000004E+00 0.0000000000000E+00
A91 1           0.30000000E+00
 0.9000000042222E+00 0.0000000000000E+00
AA1 1           0.20000000E+00
 0.9000451419297E+00 0.0000000000000E+00
AB1 1           0.20000000E+00
 0.9000000088535E+00 0.0000000000000E+00
AC1 1           0.20000000E+00
 0.9000000000017E+00 0.0000000000000E+00
AD1 1           0.20000000E+00
 0.9000000000000E+00 0.0000000000000E+00
AE1 1           0.20000000E+00
 0.9000000000000E+00 0.0000000000000E+00
AF1 1           0.20000000E+00
 0.9000000000000E+00 0.0000000000000E+00
AG1 1           0.20000000E+00
 0.9000000000000E+00 0.0000000000000E+00
AH1 1           0.20000000E+00
 0.9000000000000E+00 0.0000000000000E+00
AI1 1           0.20000000E+00
 0.9000000000000E+00 0.0000000000000E+00
AJ1 1           0.20000000E+00
 0.9000000000000E+00 0.0000000000000E+00
AK1 1           0.20000000E+00
 0.9000000000000E+00 0.0000000000000E+00
AL1 1           0.20000000E+00
 0.9000000000000E+00 0.0000000000000E+00
```

```
…
AM1 1           0.20000000E+00
 0.9000000000000E+00 0.0000000000000E+00
AN1 1           0.20000000E+00
 0.9000000000000E+00 0.0000000000000E+00
AO1 1           0.20000000E+00
 0.9000000000000E+00 0.0000000000000E+00
AP1 1           0.20000000E+00
 0.9000000000000E+00 0.0000000000000E+00
AQ1 1           0.20000000E+00
 0.9000000000000E+00 0.0000000000000E+00
AR1 1           0.20000000E+00
 0.9000000000000E+00 0.0000000000000E+00
AS1 1           0.20000000E+00
 0.9000000000000E+00 0.0000000000000E+00
AT1 1           0.20000000E+00
 0.9000000000000E+00 0.0000000000000E+00
AU1 1           0.20000000E+00
 0.9000000000000E+00 0.0000000000000E+00
AV1 1           0.20000000E+00
 0.9000000000000E+00 0.0000000000000E+00
AW1 1           0.20000000E+00
 0.9000000000000E+00 0.0000000000000E+00
AX1 1           0.20000000E+00
 0.9000000000000E+00 0.0000000000000E+00
AY1 1           0.20000000E+00
 0.9000000000000E+00 0.0000000000000E+00
AZ1 1           0.20000000E+00
 0.9000000000000E+00 0.0000000000000E+00
B11 1           0.20000000E+00
 0.9000000000000E+00 0.0000000000000E+00
B21 1           0.20000000E+00
 0.9000000000000E+00 0.0000000000000E+00
B31 1           0.20000000E+00
 0.9000000000000E+00 0.0000000000000E+00
B41 1           0.20000000E+00
 0.9000000000054E+00 0.0000000000000E+00
B51 1           0.20000000E+00
 0.9000001908931E+00 0.0000000000000E+00
B61 1           0.20000000E+00
 0.9067995705262E+00 0.0000000000000E+00
B71 1           0.20000000E+00
 0.1503000000000E+06 0.0000000000000E+00
```

Pressure at lower boundary (S_a=1)

Figure 10. Excerpt from *SAVE* for *PartE.txt* after 1 time step

- Figure 9 shows that the total liquid mass in place is a large number (~0.2E+54 kg) due to the large volume specified for BOUND.
- There is a special switch in TOUGH2 to remove a material from being counted in the material balance: Change SPHT of block ROCKS for BOUND to $>10^4$ for this purpose (p. 161 in manual).
- Make this change and run the code again. The new total liquid mass in place should be ~0.2E+05 kg.

```
Input file for Part E of sample problem 2DVZ
ROCKS----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
… (Several lines omitted)
FILLI    2    2500.0     .3000 5.000E-12 5.000E-12 5.000E-12       2.0     1000.

    7           0.30      0.20       1.0      0.05
    7           0.30      0.19    1.0e-3     5000.      1.00
BOUND    2    2500.0     .2000 1.000E-12 1.000E-12 1.000E-12       2.0     1.0E5
    7           0.30      0.20       1.0      0.05
    7           0.30      0.19    1.0e-3     5000.      1.00
(blank line!)
…
```

Removes BOUND from material balance

Part F: Steady State

In this step we run the code to steady state to obtain the initial conditions for the ponded infiltration simulation. The parameters that need to be modified for time step control are given in the PARAM block (see side note 2 pages below). Steady-state conditions are achieved (approximately) when the primary variables no longer change with increasingly large time steps. For this to occur, the maximum number of time steps to be calculated (MCYC) must be a large number and the maximum time step (DELTMX) must also be large so that the code does not terminate before reaching steady state.

- Copy and paste/rename *PartE.txt* as *PartF.txt*.
- Increase MCYC to 1000 in PARAM.2 (p. 156) so that the code can run to steady state. Check that DELTMX is blank or large.
- Run TOUGH2 by typing "t2_eos9 < *PartF.txt* > *PartF.out*.
- Examine the output files *PartE.out*, *SAVE*.

SIDE NOTE (Simulation Time)

Variable	Description	Default
TSTART	Starting time of simulation	0
TIMAX	Simulated end time	∞
MCYC	Maximum number of time steps	-
DELTEN	Initial time step size	-
DELTMX	Upper limit for time step size	∞

```
----*----1 MOP: 123456789*123456789*1234 ---*----5----*----6----*----7----*----8
PARAM----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
   2 MCYC     1001000000000020004000040000
    TSTART     TIMAX    DELTEN    DELTMX             9.81000
   1.0E-04
                 0.9
```

```
----*----1 MOP: 123456789*123456789*1234 ---*----5----*----6----*----7----*----8
PARAM----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
   21000     1001000000000020004000040000
       0.0           1.000E-00                    9.81000
   1.0E-04
                 0.9
```

Q-F.1.1: What was the maximum simulation time and the time step at the last iteration? (Open *PartF.out* and scroll down to the last occurrence of "OUTPUT DATA")

Q-F.1.2: What message in the output file indicated that steady state was reached?

Q-F.1.3: Is the water table at the correct depth?

- See Figures 11 and 12.
- Rename the *SAVE* file as *SAVE_PartF*, and delete the line starting with "+++" and the lines below.

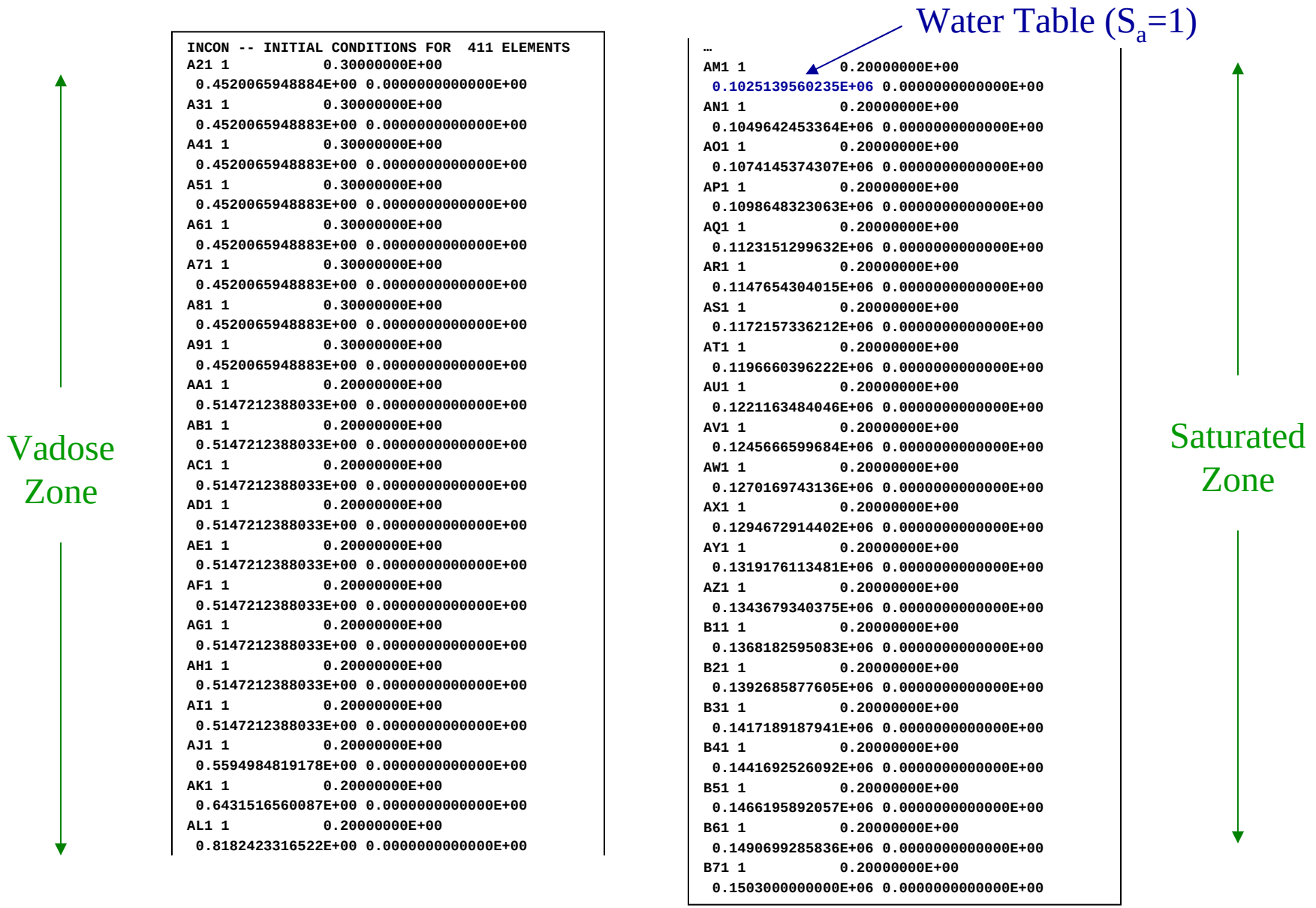


Figure 11. Excerpt from *SAVE* for *PartF.txt* for steady state.

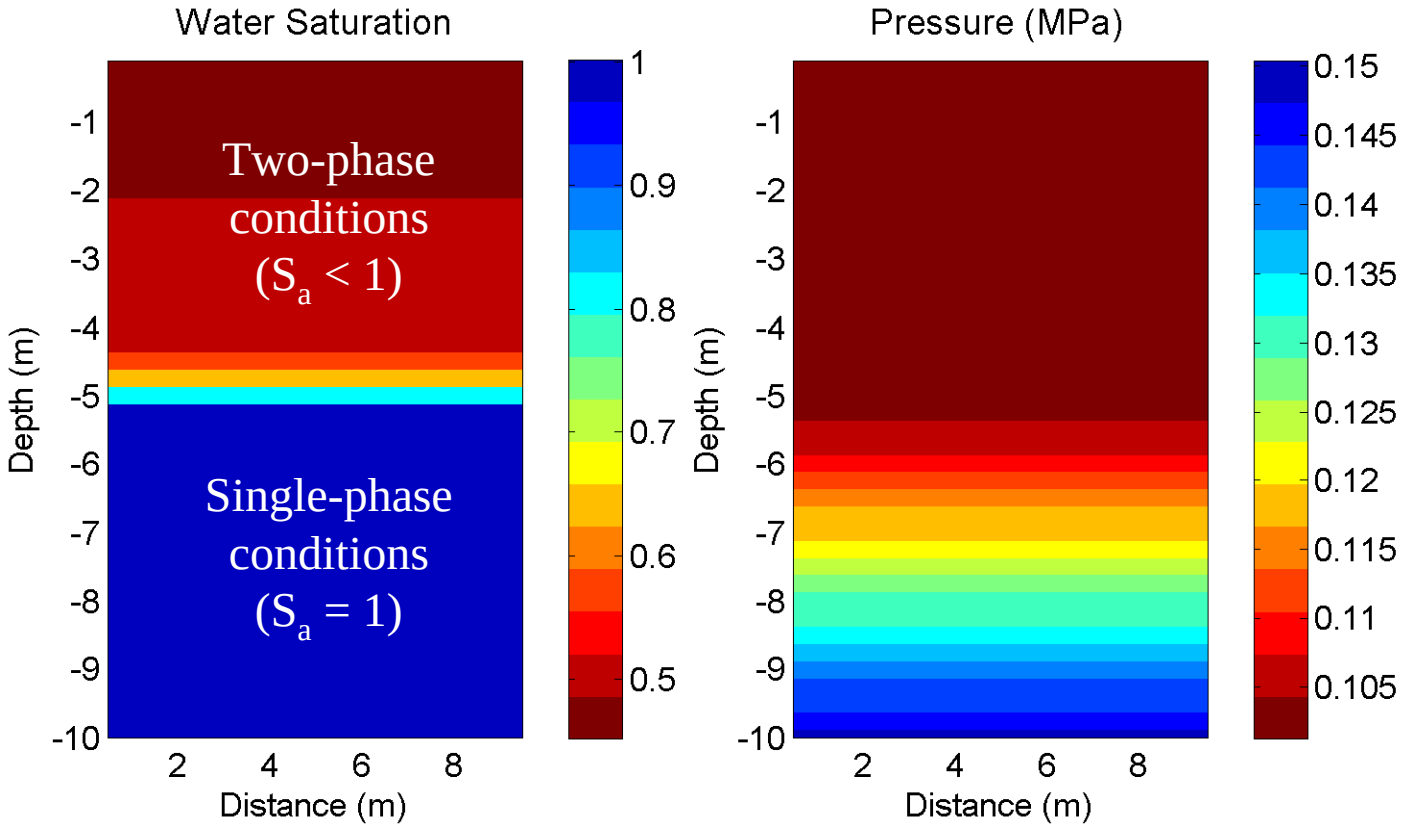


Figure 12. Steady-state profile in *PartF.txt*

SIDE NOTE (What makes TOUGH2 stop?)

- Reached one of the user–specified stopping criteria:
  - Maximum number of time steps
  - Maximum simulation time
- Convergence failures:
  - Wrong initialization of primary variables
  - Too many (>10) consecutive time steps converging within a single Newton-Raphson iteration →
    - Steady state is reached
    - Time step is too small (check `DELTEN`, `DELTMX`, `TIMES` block)
    - Newton-Raphson error criterion is too loose (reduce `RE1`)
  - Convergence failure followed by convergence within a single Newton-Raphson iteration →
    - May indicate steady state!
    - Serious convergence difficulty (usually phase changes)
  - More than 25 time-step reductions

Part G: Infiltration Test

In this step we will 1) use the initial conditions simulated in Part F, and 2) add constant-rate infiltration by specifying another source in the GENER block. The *SAVE* file generated at the end of the previous step contains the output corresponding to the steady-state distribution for this problem, which will serve as the initial conditions.

- Copy *PartF.txt* and paste/rename as *PartG.txt*.
- Replace the INCON block in *PartG.txt* with the contents of the SAVE file created in the last step (*SAVE_PartF.txt*). Also remove the INDOM block (or just change keyword to xNDOM).
- Now add the new GENER block and a TIMES block from the file *GENER_TIMES_Info_PartG.txt*. The GENER block includes an additional time-dependent source for an infiltration test. The TIMES block creates output at certain times. See Figure 13.

Q-G.1.1: Explain the time-dependent infiltration source (its strength, duration, elements to which it is applied, etc.)?

```
GENER----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
A21 1INJ01    9    1    1    0     WATE 1.0000e-06
A21 1INF01    1    1    1    3     COM11
         0.0e0         8.64E4         1.0e10
    1.0000e-02            0.0            0.0
           0.0            0.0            0.0

TIMES----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
6
       0.0   21600.0   43200.0   86400.0  172800.0 5529600.0
```

Figure 13. New GENER and TIMES blocks used in Part G (from *GENER_TIMES_Info_PartG.txt*) to initiate an infiltration test, and to print output at given times, respectively.

- Note that `ITAB` should be non-zero when reading data from a table, even if the problem is non-isothermal.
- Increase `MCYC` to 1000 in `PARAM.2` (p. 156) to allow the code to run to steady state.
- Make sure `MOP(12)` is set to 2. This option uses the "step function" option in handling generation rates (see P. 164 of manual).
- Change `TSTART` to 0.0, and enter the total simulation time of 64 days (5529600.0 sec).
- Run TOUGH2 by typing "t2_eos9 < *PartG.txt* > *PartG.out*"
- Examine the output files *PartG.out*, and see Figures 14 and 15.

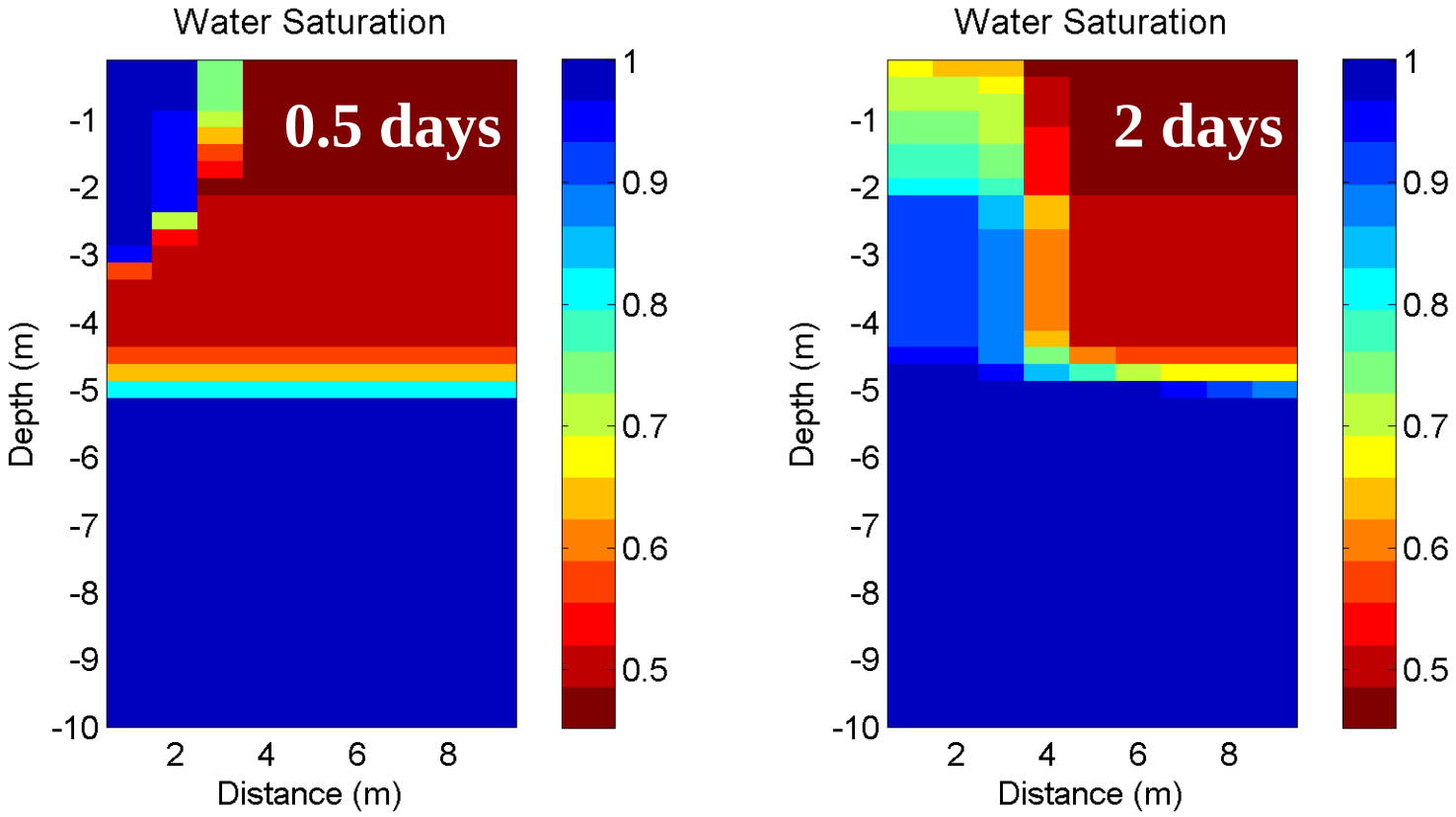


Figure 14. Water saturation distribution after start of infiltration test (duration of 1 day) at two times for EOS9.

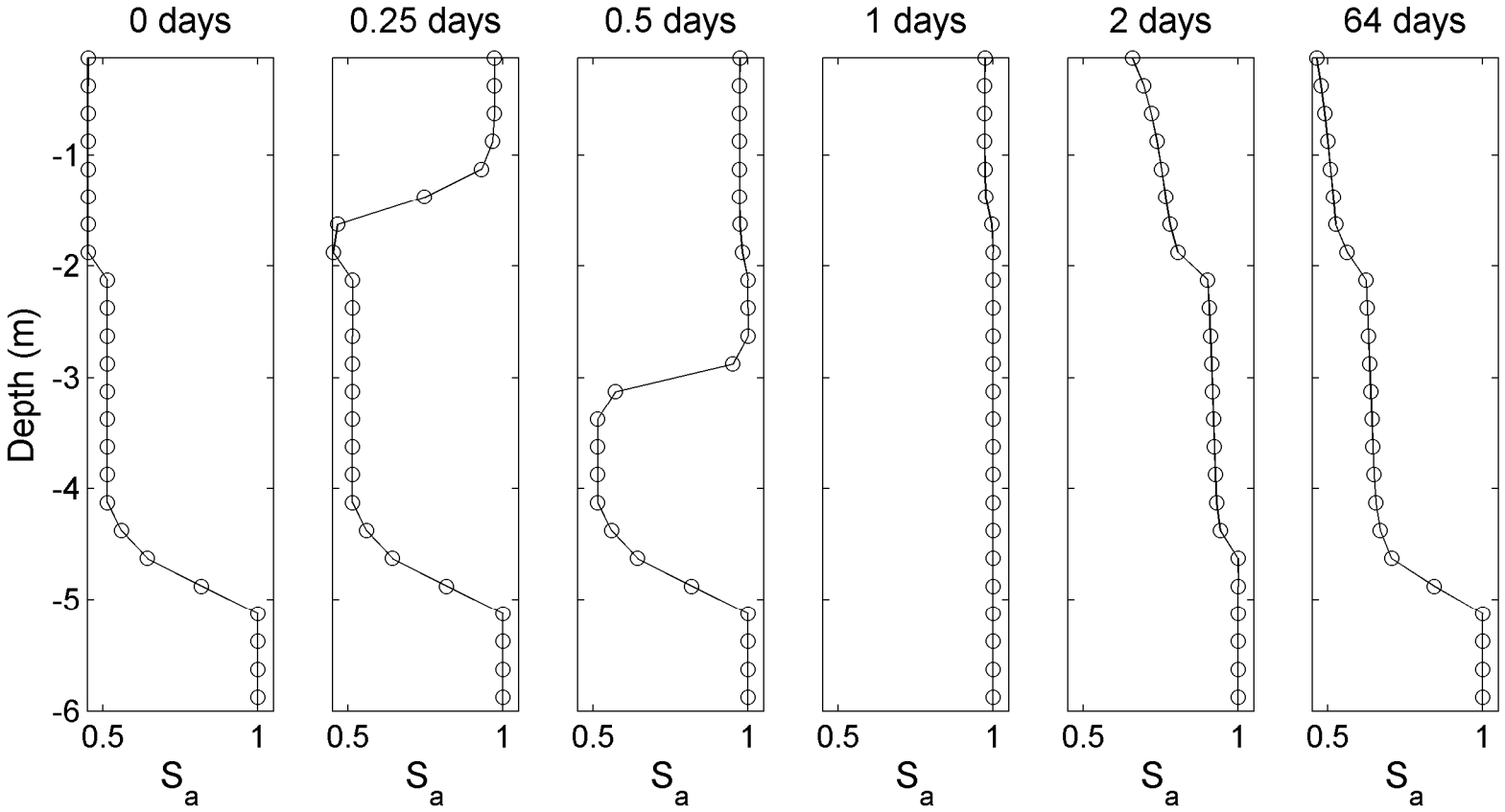


Figure 15. Water saturation profile at x=0 obtained for increasing times after start of infiltration test for EOS9.

SIDE NOTE (Output Options)

Variable	Description	Default
KDATA	Specify amount of printout	-
MCYPR	Printout occurs for every multiple of MCYPR steps	1
MOP(1)	Create printout for non-convergent iterations	no
MOP(7)	Printout of input data (recommended)	no
MOP(2-6)	Additional printout from various subroutines	no
	Additional printout times to be specified in block TIMES	

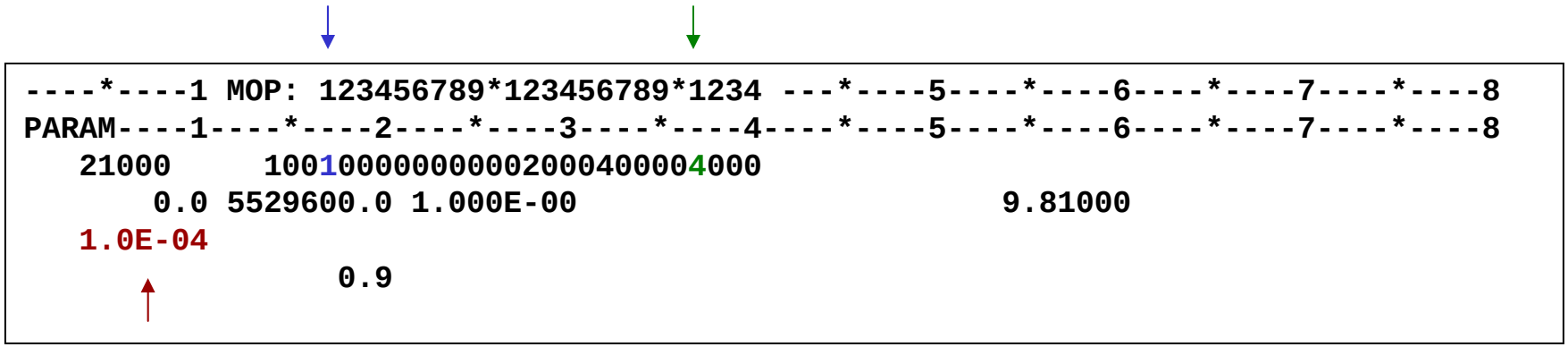
```
----*----1 MOP: 123456789*123456789*1234 ---*----5----*----6----*----7----*----8
PARAM----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
   21000     100100000100002000400004000
       0.0 5529600.0 1.000E-00                        9.81000
   1.0E-04
                  0.9
```

SIDE NOTE (Newton-Raphson and Linear Eqn. Solver)

Variable	Description	Default
RE1	Relative error convergence criterion	1.0E-5
MOP(1)	Create printout for non-convergent iterations	no
MOP(21)	Select linear equation solver	3

Check block SOLVR for additional options

Check file *LINEQ* for linear equation solver data



Problem Variation: Conversion from EOS9 to EOS3

After developing a TOUGH2 problem using EOS9, one may wish to incorporate temperature variations (i.e., make it nonisothermal) or to account for the movement of both water and gas. The TOUGH2 input file(s) can be modified accordingly to make this possible.

- Copy *PartG.txt* and rename it *PartH.txt*

Primary Variables for EOS3 (p. 36 of manual)

- The primary variables for each grid block change depending on whether single- or two-phase conditions are present.
- Using values between 0 and 1 for the second primary variable implies aqueous phase conditions in a grid block (X is the primary variable). Whereas, using a value > 10 (and < 11), implies two-phase conditions (where the primary variable is S_g+ 10).

Relevant T2 Blocks

MULTI

INCON
INDOM
PARAM
SAVE

Components	# 1: water # 2: air
Parameter choices	
(NK, NEQ, NPH, NB) =	(2, 3, 2, 6) water and air, nonisothermal (default) (2, 2, 2, 6) water and air, isothermal molecular diffusion can be modeled by setting NB = 8
Primary Variables *	
single-phase conditions	
(P, X, T) - (pressure, air mass fraction, temperature)	
two-phase conditions	
(P_g, S_g + 10, T) - (gas phase pressure, gas saturation plus 10, temperature)	

* By setting MOP(19) = 1, initialization can be made with TOUGH-style variables (P, T, X) for single-phase, (P_g, S_g, T) for two-phase.

- Add MULTI for isothermal case (NK=2, NEQ=2, NPH=2, NB=6)
- The relative permeability and capillary pressure functions for the ATMOS material should allow for transfer or air but not water.
- Give the atmospheric grid block “99999” a Dirichlet boundary condition with pressure equal to atmospheric and constant high gas saturation (e.g., Sa = 0.1 or Sg = 0.9).
- Specify initial conditions using `INDOM` instead of `INCON` (hint: delete contents of `INCON` block without deleting keyword); set default initial conditions in `PARAM` block with gas saturation equal to zero (2nd primary variable equal to X = 0).
- To obtain steady-state profile, remove the source was used for the infiltration test in the `GENER` block (INF01-INF02); leave `TIMAX` blank so that steady state can be reached.
- To simulate infiltration test, copy *SAVE* file from steady-state run to `INCON` block, reinsert infiltration test source, and run.

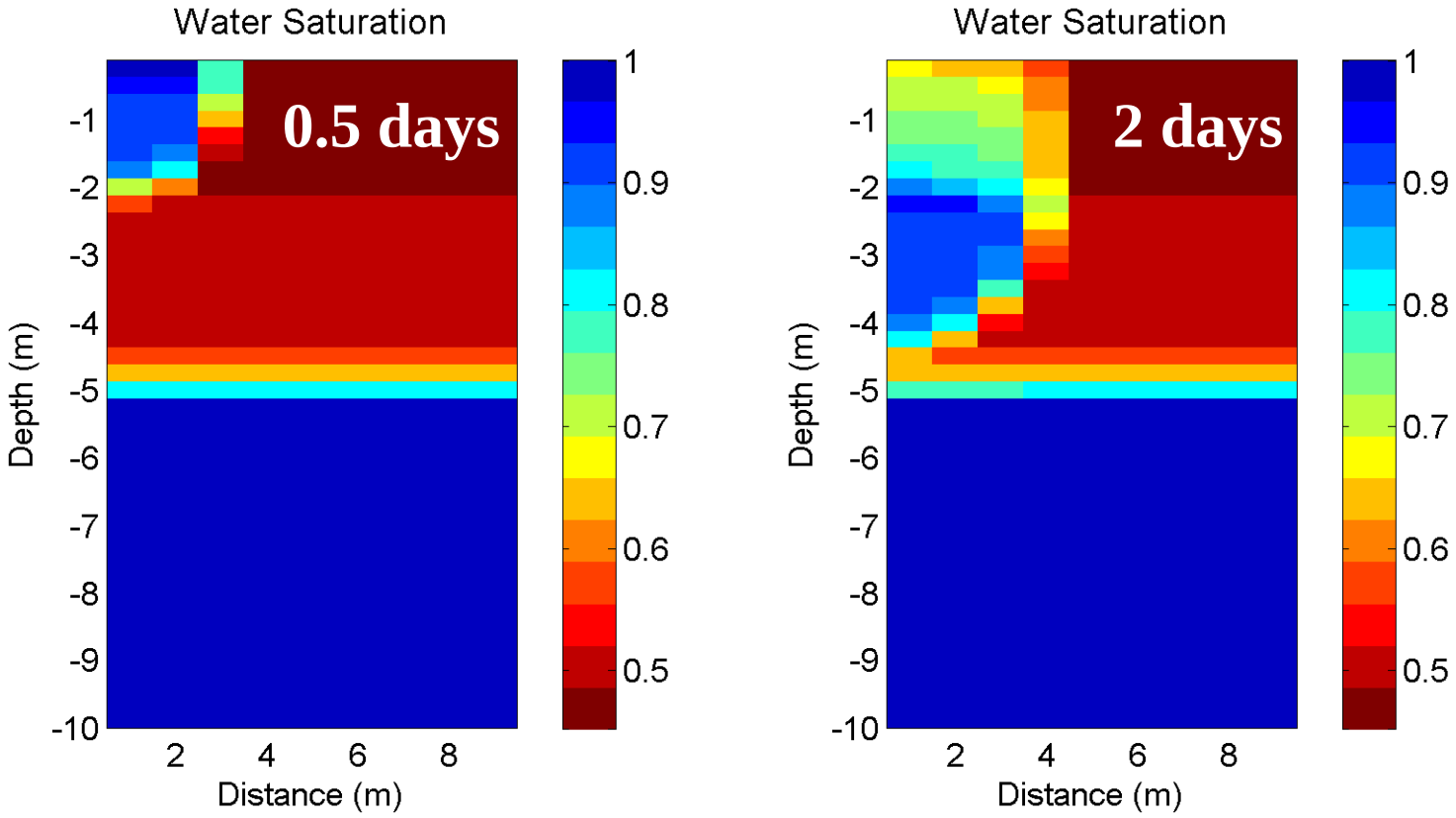


Figure 16. Water saturation distribution after start of infiltration test (duration of 1 day) at two times for EOS 3.

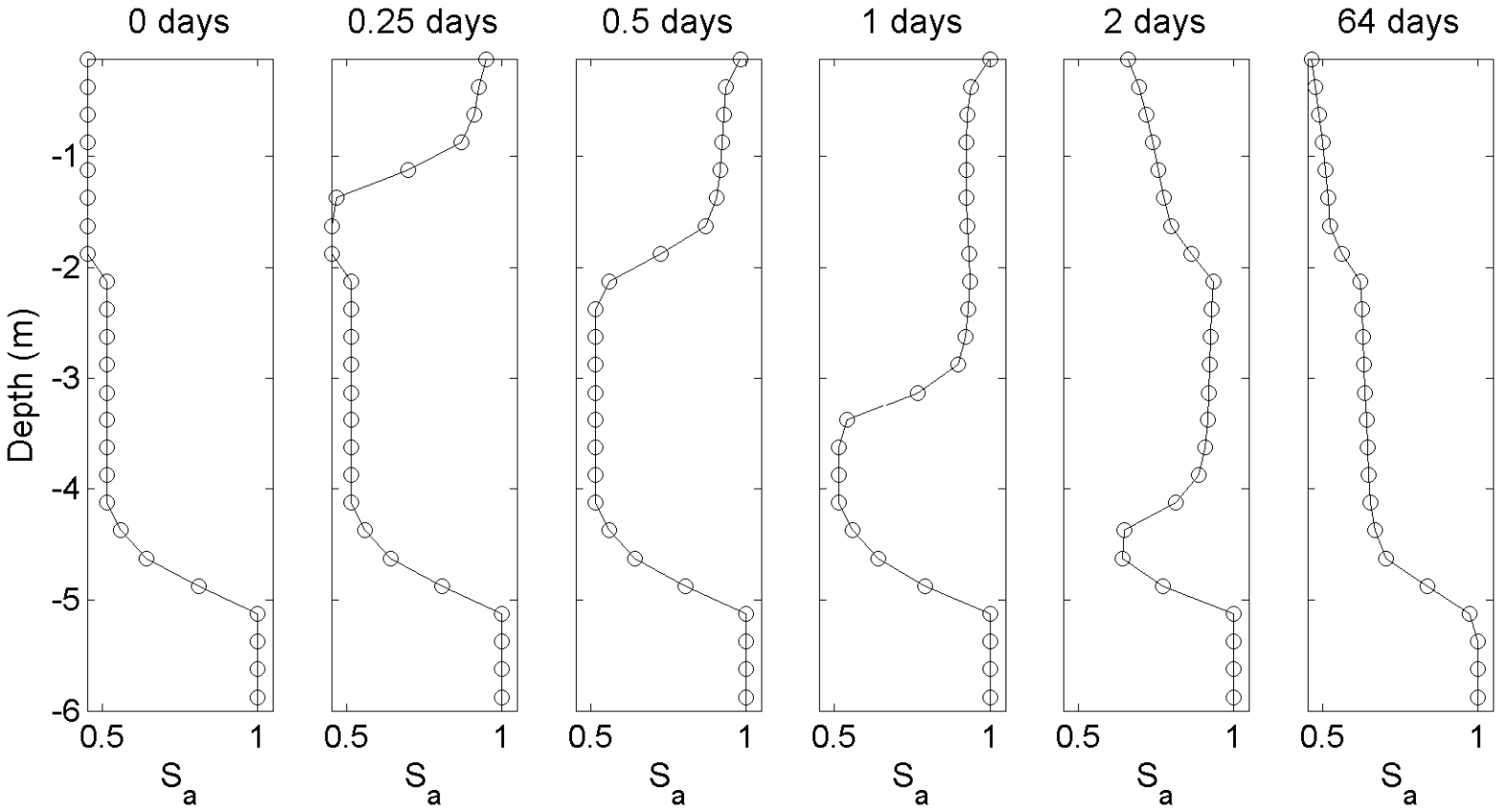


Figure 17. Water saturation profile at x=0 for increasing times after start of infiltration test for EOS3.