Scientific Notebook No. 474: Documentation of Numerical Analyses for the Lab-Scale Heater Tests (11/06/2001 through 11/16/2001)

LABORATORY NOTEBOOK

CNWRA/SwRI

NOTEBOOK NO. ____________

ISSUED TO Ronald Green

ON ____________

DEPARTMENT ____________

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This notebook is to document numerical analyses of the lab-scale heater tests. The analyses were started in Notebook 209. This is a continuation.

The previous model was mostly re-formulated with smaller elements and greater resolution in the modified version.

The MBTRA Version 1.5 input file as currently appears is attached
on Spock/home/vgreen
~/1st/21st/1st66.dat

```
  Simulation of laboratory-scale dripping experiment - Bldg 51 CNWRA
 Nov 16, 2001
: lst66
: smaller model to fit in metra element dimension limitation
: This run statred with drip131 converted to DCM
: dcm-sm98 inc liq sat of matrix from 0.3 to 0.35
: lst03, repeat of dcm-sm98
: lst04, new dcm parameters, new bcon, removed top source
: lst06, added bottom bcon
: lst08, set areamodf=1e-2
: lst11, removed bottom bcon
: lst13, reset bcon q to 1 kg/d= 5.5989e-2 kg/m^2/s
: lst14, set areamodf=1e-4, crashed at 12 days
: lst15, set areamodf=1e-3
: lst17, new bottom bc
: lst18, reset infil rate at e-2 from e-3
: lst19, set areamodf=1e-1
: lst22, reset bottom bc to Dirichlet from Neuman
: lst23, set areamodf=1e-0
: lst24, set areamodf=1e-4
: lst26, set bottom bc mat sat 0.20
: lst27, set bot bc matr sat to 0.1, inc infil,areamodf = 1.0, top bc matr sat=0.65
: lst28, set areamodf=1e-4
: lst29, set top to source from bcon, same as from dcm-sm80 et al.
: lst30, lst29 died at 7.1 days, set volj from 0.05 to 0.002
: lst32, lst30 died at 198 days, removed bcon at bottom
: lst33, lst32 died at 5.7 days, reduced Kt at boundaries, revised init sat=dcm-sm80
: lst34, set areamodf=1.0
: lst36, modified drift V-G properties
: lst37, lst36 went 210, set areamodf=1.e-4
: lst38, lst37 died at 11 days, inc block size from 0.002 to 0.05
: lst39, sat at base too high, inc vol of bot, dec int sat
: lst40, areamodf set to 1.0
: lst41, set bottom int sat to .2
: lst42, areamodf=1e-4
: lst43, dec bot int sat to 0.1, inc vol to 5e0
: lst44, areamodf=1.0
: lst47, reduced k by 10x to 2e-18
: lst48, inc k by 100x to 2e-16
: lst49, inc size of bc to lower edge temp
: lst50, inc number of elements
: lst52, reading error in DCMXYZ corrected
: lst53, reduced size of edge elements
: lst56, inc size of bc, include drift properties
: lst57, new set of bc, std mass
: lst58, doubled heat output
: lst59, doubled heat output again
: lst60, dec int sat to 0.35, set bottom bc to 0.1 w/ vol = 1.0e-1
: lst61, reduced cp on bc, reduced heat to 2X
: lst62, heat back to 1X
: lst63, heat back to 4X, all bc to Kt=.05 w/C-m w/ cp=1e4
: lst64, inc Kt in interior to 0.5/1.0 from 0.4/0.7
: lst65, changed fract alpha to 1.3e-3 from 1.3e-1
: lst66, lowered heater by 0.1 to be consistent with exper.
:
RSTART  0
:                                   = 1 table look-up,; pref = ref. press.
:       XYZ                         = 0 correlations;   tref = ref. temp.
:       RADIAL                          ^
:       OTHER                           |
:
:grid  geometry  nx ny  nz ivplwr ipvtcal iout    pref tref  href
Grid   DCMXYZ    24 14  30    1       1     2     0        0    0     0
:
:       data taken from sandia report:Green et al. 1995, NUREG/CR-6348
:                                  :relative perm and pc
Pckr
:   i  type-curv swirm  rpmm(lamda)  alpham  swext  sgc   iecm
    1  Van-Gen   0.05   .3717        6.36e-7   0     0.0   0      ! matrix block
:
:   i  type-curv swrim unused  unused      p@0-sat sgc   iecm
:   2  linear    0.00  0.000        0.00    1.0     0.0   0      ! emplacement drift
```

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```
:   i  type-curv swrim unused  unused     p@0-sat sgc   iecm
    2  linear    0.01  0.800      1.0e-1   0.0     0.0  0     ! emplacement drift
:
:   i  type-curv swrim unused  unused     p@0-sat sgc   iecm
    3  linear    0.01  0.000      0.00     1.0     0.0  0     ! primary fracture
:
:   i  type-curv swirf  rpmf(lamda)  alphaf  swext  sgc  iecm
    4  Van-Gen  0.08   0.7619    1.3e-3    0.0    0.0   0    ! matrix fractures
0           :blank line
:
 Debug  1
 0
Thermal-prop
: no rho         cpr     ckdry  cksat     crp  crt    tau  cdiff    cexp  enbd
  1  1.600e+03 840.0    0.50   1.00      0    0      .5  2.13e-5  1.8   0. 0 !matrix
  2  1.600e+03 840.0   10.0   10.0       0    0      .5  2.13e-5  1.8   0. 0 !drift
skip
  3  1.600e+03 5.0e+7   0.50   1.00      0    0      .5  2.13e-5  1.8   0. 0 !side boundaries
  4  1.600e+03 1.0e+9   0.50   1.00      0    0      .5  2.13e-5  1.8   0. 0 !bottom boundary
  5  1.600e+03 5.0e+7   0.50   1.00      0    0      .5  2.13e-5  1.8   0. 0 !top boundary
  6  1.600e+03 5.0e+8   1.50   2.00      0    0      .5  2.13e-5  1.8   0. 0 !front bc near heater
: noskip
  3  1.600e+03 840.0    0.50   1.00      0    0      .5  2.13e-5  1.8   0. 0 !side boundaries
  4  1.600e+03 840.0    0.50   1.00      0    0      .5  2.13e-5  1.8   0. 0 !bottom boundary
  5  1.600e+03 840.0    0.50   1.00      0    0      .5  2.13e-5  1.8   0. 0 !top boundary
  6  1.600e+03 840.0    1.50   2.00      0    0      .5  2.13e-5  1.8   0. 0 !front bc near heater
noskip
  3  1.600e+03 1.0e4    0.05   0.05      0    0      .5  2.13e-5  1.8   0. 0 !side boundaries
  4  1.600e+03 1.0e4    0.05   0.05      0    0      .5  2.13e-5  1.8   0. 0 !bottom boundary
  5  1.600e+03 1.0e4    0.05   0.05      0    0      .5  2.13e-5  1.8   0. 0 !top boundary
  6  1.600e+03 1.0e4    0.05   0.05      0    0      .5  2.13e-5  1.8   0. 0 !front bc near heater
0
:     igrid   rw      re
DXYZ   0
: (dx(i),i=1,nx)
0.004 .008 .015 .015 .015 .015 .015 .03 .03 .03 !total for line 0.177
0.03 .03 .03 .03 .03 .03 .03 .03 .03 .03  !total for line 0.3
0.03 .03 .03 .015  !total for line 0.105
:total in x-direction is 0.582 plus .019 beyond edge elements, 24 elements
: (dy(j),j=1,ny)
0.02 .02 .02 .02 .02 .02 .02 .02 .02 .02  !total for line 0.2
0.02 .02 .02 .01  !total for line .07
:total in y-direction is 0.27 plus .03 beyond edge elements, 14 elements
: (dz(k),k=1,nz)
skip
0.03 .06 .06 .06 .06 .06 .06 .04 .02 .02  !total for line 0.51, and 0.54 from top
0.015 .015 .02 .03 .03 .02 .015 .015 .02 .02  !total for line 0.20
0.04 .06 .06 .06 .06 .06 .06 .03 !total for line 0.43 and 0.46 from bottom
noskip
: lowered heater by 0.1
0.03 .06 .06 .06 .06 .06 .06 .06 .04 .04  !total for line 0.53, and 0.56 from top
0.02 .02 .015 .015 .025 .03 .03 .025 .015 .015 !total for line 0.21
0.02 .02 .04 .04 .06 .06 .06 .06 .06 .03 !total for line 0.45 and 0.48 from bottom
:total z-direction is 1.19 plus .06 beyond end elements, 30 elements
:
PhiK
: i1 i2 j1 j2 k1 k2 ist ithrm vb  porf permxf permyf permzf pormm permm  istm ithrmm
  1  24  1 14  1  30 4   1 1.0e-2 1.00 1.e-10 1.e-10 1.e-10 0.42  2.e-16 1    1 ! matrix
:
skip
: following are new bc with more mass to have lower edge temps
  1  24 14 14    1 30 4   3 1.0e-2 1.00 1.e-10 1.e-10 1.e-10 0.42  2.e-17 1    3 ! front
 24  24  1 14    1 30 4   3 1.0e-2 1.00 1.e-10 1.e-10 1.e-10 0.42  2.e-17 1    3 ! side
  1   4 14 14   14 19 4   6 1.0e-2 1.00 1.e-10 1.e-10 1.e-10 0.42  2.e-17 1    6 ! front at heater
  1  24  1 14    1  1 4   5 1.0e-2 1.00 1.e-10 1.e-10 1.e-10 0.42  2.e-17 1    5 ! top
  1  24  1 14   30 30 4   4 5.0e-0 1.00 1.e-10 1.e-10 1.e-10 0.42  2.e-17 1    4 ! bottom
noskip
: skip
: following are new bc with standard mass for edge elements
  1  24 14 14    1 30 4   3      0. 1.00 1.e-10 1.e-10 1.e-10 0.42  2.e-17 1    3 ! front
 24  24  1 14    1 30 4   3      0. 1.00 1.e-10 1.e-10 1.e-10 0.42  2.e-17 1    3 ! side

: 1   4 14 14   14 19 4   6      0. 1.00 1.e-10 1.e-10 1.e-10 0.42  2.e-17 1    6 ! front at heater
  1  24  1 14    1  1 4   5      0. 1.00 1.e-10 1.e-10 1.e-10 0.42  2.e-17 1    5 ! top
  1  24  1 14   30 30 4   4 1.0e-1 1.00 1.e-10 1.e-10 1.e-10 0.42  2.e-17 1    4 ! bottom
: end of bc elements
: noskip
  1   3  1 14   14 14 2   2      0. 1.00 1.e-10 1.e-10 1.e-10 0.99  1.e-12 4    2 ! drift
  1   5  1 14   15 15 2   2      0. 1.00 1.e-10 1.e-10 1.e-10 0.99  1.e-12 4    2 ! drift
  1   6  1 14   16 16 2   2      0. 1.00 1.e-10 1.e-10 1.e-10 0.99  1.e-12 4    2 ! drift
  1   6  1 14   17 17 2   2      0. 1.00 1.e-10 1.e-10 1.e-10 0.99  1.e-12 4    2 ! drift
  1   5  1 14   18 18 2   2      0. 1.00 1.e-10 1.e-10 1.e-10 0.99  1.e-12 4    2 ! drift
  1   3  1 14   19 19 2   2      0. 1.00 1.e-10 1.e-10 1.e-10 0.99  1.e-12 4    2 ! drift
: noskip
  0
:
Init
:  i1  i2  j1  j2  k1  k2  p          t     sg    xg2 pm         tm    sgm xgm
    1  24  1   14   1  30  1.0315e5 20.0  0.65 0.   1.0315e5 20.0 .65  0. ! matrix
    1  24  1   14  30  30  1.0315e5 20.0  0.90 0.   1.0315e5 20.0 .90  0. ! bottom
skip
    1   3  1   14  14  14  1.0315e5 20.0  0.99 0.   1.0315e5 20.0 .99  0. ! drift
    1   5  1   14  15  15  1.0315e5 20.0  0.99 0.   1.0315e5 20.0 .99  0. ! drift
    1   6  1   14  16  16  1.0315e5 20.0  0.99 0.   1.0315e5 20.0 .99  0. ! drift
    1   6  1   14  17  17  1.0315e5 20.0  0.99 0.   1.0315e5 20.0 .99  0. ! drift
    1   5  1   14  18  18  1.0315e5 20.0  0.99 0.   1.0315e5 20.0 .99  0. ! drift
    1   3  1   14  19  19  1.0315e5 20.0  0.99 0.   1.0315e5 20.0 .99  0. ! drift
noskip
0
DCMPARA
: i1 i2 j1 j2 k1 k2   volf  areamodf  xlm   ylm    zlm
   1 24  1 14  1 30   0.050   1.0      .05   0.03   .05  1.000 ! matrix
0
:
```

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```
Recurrent
:         ns      fach        facm  (fach and facm are multipliers)
Source   2      4.00         1.
: this is for the heat source
:  is1 is2 js1 js2 ks1 ks2  istyp
    1   3   1  3   17  17   33
:0.0     0.0
1.e+4  3.51e+1
1.e+10 3.51e+1
0
: this for the water infiltration
:  is1 is2 js1 js2 ks1 ks2  istyp
    1   2   1  7    1   1   13
0.0     20.0   0.0
2.60e5 20.0   0.0
3.60e5 20.0  2.894e-6
1.486e7 20.0  2.894e-6
1.815e7 20.0  7.534e-7
1.e+10 20.0  7.534e-7
0
Output   C=-10 Q=-10   T=1   G=1   P=1
:
:      isolv  newtnmn  newtnmx  north  nitmax  level
Solve 4       2          12       4     100
:
:AUTO-step  DPMXE    DSMXE  DTMPMXE   DP2MXe TACCEL   IAUTODT  FAC1
AUTO-step   5.0E+4   0.03     5.0      1.e4  1.0e-3      0       0
:
:TOLR TOLP  TOLS  TOLT  TOLP2  TOLM  TOLA  TOLE rtwotol  rmxtol   smxtol
Tolr   1. 5.e-4  5.e-3  1.     1.e-3 1.e-3 1.e-3  1.e-12  1.e-12  1.e-12
:
:Limit dpmx    dsmx dtmpmx dp2mx dtmn dtmx icutmx
LIMIT  1.e5    .08    10.   1.e5 1.e-9 .8
:
:      target  dt    dpmx   dsmx   dp2mx   dtmpmx
:
:      print all at every target time
PLOTS 1 0 4
1 10 451 541

Time[d] 5.
Time[d] 10.
Time[d] 50.
Time[d] 110.
Time[d] 172.
Time[d] 210.
Ends
```

The major difference from earlier models of the 1st is that this model has 24 x 14 x 30 elements for 10,080 total elements, using 2 planes of symmetry (Z-plane in 2 ~~orientation~~) orientations. RJF 11/16/01

I have reviewed this SN and determined that it complies with QAP-001. To fully understand and replicate the work described herein, the qualified thermohydrologic modeler would need to refer to SN 209.

Gordon Wittmeyer 9/21/2004

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