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CNWRA
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Initial Entries

Project: Thermal Effects on Flow Key Technical Issue. (KTI)
- 3D Drift Scale parametric Study.

Objective: Develop a 3D model of an emplacement drift using the METRA code to conduct a parametric study to identify key parameters affecting thermal-hydrologic regime in the immediate vicinity of the host rock surrounding the drift.

Charge # 20-5708-661

Project Staff: Mitcko Ahola
Rui Chen
Ron Green.

Computer Code: METRA Version Number 0.09.00 (Ver_BETA)

Multi-Component Unsaturated Fluid Flow Simulator
Developed by Mohan Seth (4/95)
Collaborated with Peter Lichtner
Sun Version.

Computer Platform: Sun Sparc 20 (sneezy).

The 3D model was generated utilizing the major geologic/hydrologic formations (i.e. TCw, PTn, TSw, TSv, CHnv, and CHnz.) The upper surface (z=0 m) was assumed to be the ground surface. The lower surface (z=684 m) was the water table where the saturation was set to 1.0.

M.A.
2/24/97

The upper surface (z=0) incorporated a fluid flux of (0.3 mm/yr) based on estimates from in situ data. Only 1/4 symmetry was modeled (i.e. symmetry planes in x-direction were midway between drifts and drift centerline, symmetry planes in the y-direction were midway between the canisters and the canister center.

For an 83 MTU/acre heat load, the drift spacing was taken to be 22.5 m and the canister spacing was 19.0 m.

The mesh dimensions were
- z-direction - 684 m - 43 elements
- x-direction - 11. m - 19 elements
- y-direction - 9.5 m - 10 elements

Number of elements = 43x19x10 = 8170.

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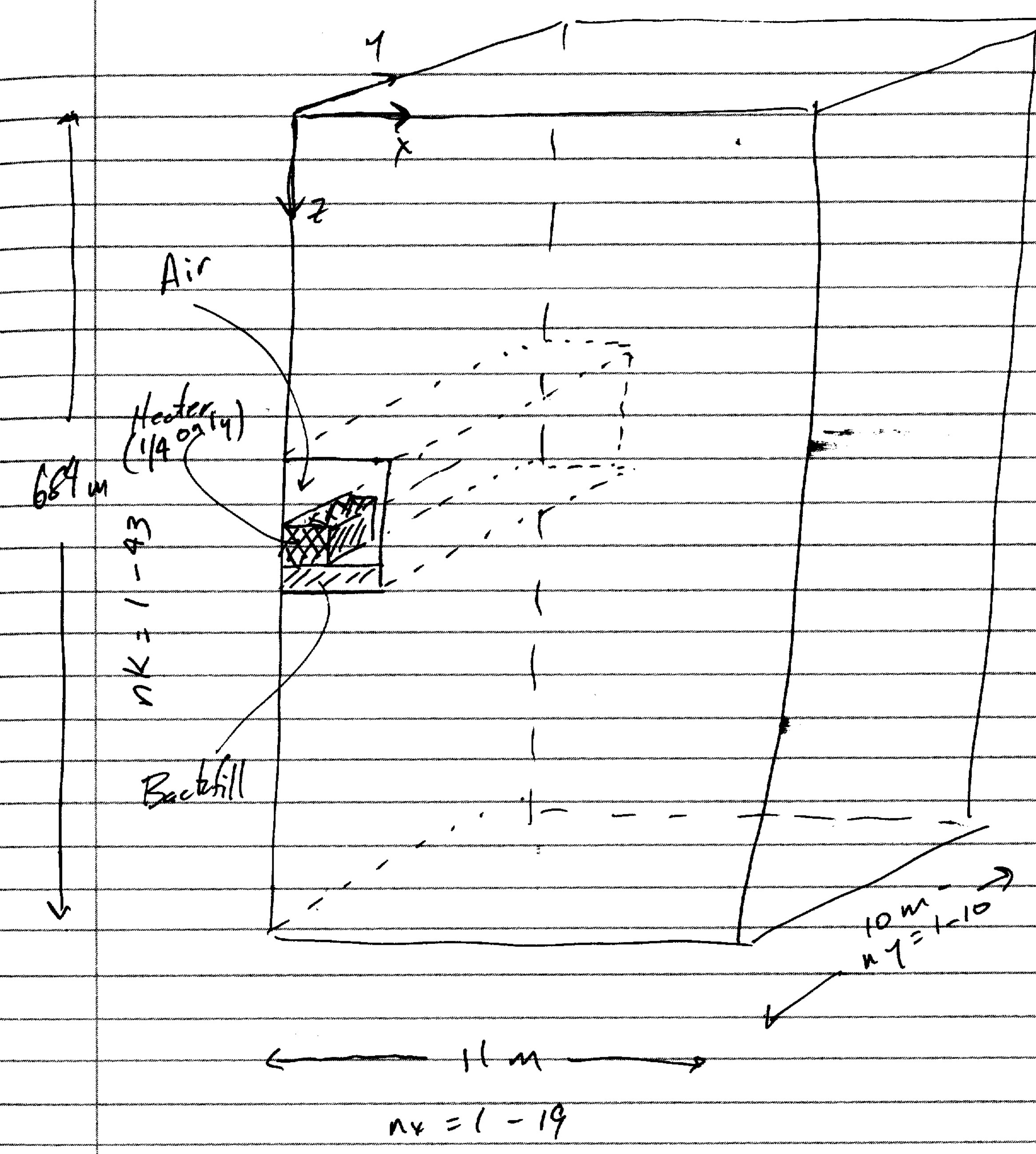
3/24/97



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3/24/97

Prior to excavating the drift and activating the heater, it was necessary to establish the initial conditions (i.e, pressure, liquid and gas saturations etc.). This was done in the absence of the drift and heater (i.e. drift assigned properties of Tsw_2 unit). The initial state was based on a 0.3 mm fluid flux at ground surface, water table or fully saturated at the base, 5 distinct hydrologic units with different Van Genuchten moisture retention parameters. The initial guess at liquid saturation was 0.25 (25%). The input data file was titled init-3d.dat. and attached on the following pages.

MA.
3/24/97


```
3D Metra file for initial steady state saturations in near field tunnel region
              March 12, 1997

::::::::::
: THE DRIFT SPACING OF THIS MODEL IS 22 m
: Canister spacing is 19.0 m
: xyz-multiple layer model of Yucca Mountain with repository heat source
: and air in the drift (no heat applied for steady state run)
: added 0.3 mm/yr infiltration using boundary condition command
: set upper element to large heat capacity
::::::::::
:
RSTART  0            : Designates the frequency of writing restart files (0 - every time step?)
:
:      XYZ                    = 1 table look-up.; pref = ref. press.
:      RADIAL                 = 0 correlations;   tref = ref temp.
:      OTHER
:
: ******************
:  Define Grids
: ******************
: nx = number of grid blocks in x direction
: ny = number of grid blocks in y direction
: nz = number of grid blocks in z direction
: ivplwr = lower or don't lower vapor-pressure of H2O due to capillarity (1 - lower, 0 - do not lower)
: ipvtab = index for calculating water pvt properties (0 - use correlations for water prop. 1 - construct tables)
: idir = whether D4-ordered direct method will be used (0 - not to be used, 1 - may be used)
: pref = Reference pressure for pore compressibility
: tref = Reference temperature for pore compressibility
: href = Reference depth of grid block
:
:grid  geometry  nx   ny   nz   ivplwr ipvtab  idir    pref tref  href
Grid   XYZ       19   10   43   1      1       1       0    0
:
: **********************************
:  Assigning elements to be monitored
: **********************************
: Waste Package, Drift Roof, Drift Sidewall, Pillar
Monitor 4371 3611 4379 3782 4550
:
: **************
:  Debug options
: **************
debug 1
0
:
: *********************************************************************
:  Define relative permeability and capillary pressure characteristics
: *********************************************************************
: i = sequential number of material types
: type = the characteristic curves (Van-Gen, Linear, tabular, and corey)
: swirm = irreducible liquid saturation for the matrix
: rpmm = Van Genuchten parameter for matrix
: alpham = Van Genuchten parameter for matrix
: swext = liquid saturation below which the capillary pressure is calculated based
:         on the slope dPcw/dSw evaluated at SWEXT.
: sgc = residual (immobile) gas saturation, fraction
: iecm = Equivalent Continuum Model (ECM) formulation (0 do not invoke, 1 invoke, 2 ECM with tables)
: swirf = residual liquid saturation for fracture, fraction
: alphaf = parameter in Van-Genuchten equation for fracture (1/Pa)
: phim = matrix porosity (fraction)
```

```
: phif = fracture porosity (fraction)
: permm = intinsic matrix permeability (m^2)
: permf = intrinsic fracture permeability
:
Pckr                          :relative perm and pc keyword
:   i  type-curv   swirm   rpmm(lamda) alpham     swext  sgc      iecm
:                  swirf   rpmf(lamda) alphaf     phim        phif    permm     permf
: (TCw)
    1  Van Gen     0.002   0.3600      8.4e-7     0.0    0.0      1
                   0.040   0.7636      1.305e-5   0.087       1.8e-3  9.7e-19   3.9e-12
: (PTn)
    2  Van-Gen     0.100   0.8500      1.53e-6    0.0    0.0      1
                   0.040   0.7636      1.305e-5   0.421       1.8e-3  3.9e-14   3.9e-13
: (TSw)
    3  Van-Gen     0.080   0.4400      5.8e-7     0.0    0.0      1
                   0.040   0.7636      1.305e-5   0.139       1.8e-3  1.9e-18   3.9e-12
: (TSv)
    4  Van-Gen     0.080   0.4438      5.8e-7     0.0    0.0      1
                   0.040   0.7636      1.305e-5   0.065       1.8e-3  1.9e-18   3.9e-12
: (CHnv)
    5  Van-Gen     0.041   0.7400      1.63e-6    0.0    0.0      1
                   0.040   0.7636      1.305e-5   0.331       1.8e-3  2.7e-14   3.9e-13
: (CHn2)
    6  Van-Gen     0.110   0.3800      3.13e-7    0.0    0.0      1
                   0.040   0.7636      1.305e-5   0.306       1.8e-3  2.0e-18   3.9e-12
:
: ******************
:  Backfill material
: ******************
    7  Van-Gen     0.01    0.7000      1.11e-5    0.0    0.0      1
                   0.04    0.7636      1.305e-5   0.50        1.8e-3  3.9e-14   3.9e-12
:
: ********************
: Metal Waste Package
: ********************
    8  Van-Gen     0.01    0.4400      5.80e-7    0.0    0.0      1
                   0.01    0.7636      1.305e-5   0.1            0.1  3.9e-99   3.9e-99
:
: *****
:  Air
: *****
    9  Van-Gen     0.01    0.4400      5.80e-7    0.0    0.0      1
                   0.01    0.7636      1.305e-5   0.99999 0.99999     3.9e-99   3.9e-99
:
0            : blank line to end pckr data
:
: ***************
:  Debug options
: ***************
Debug  1
0
:
: ********************
:  Thermal properties
: ********************
: no = sequential number of data set
: rho = rock density (kg/m^3)
: cpr = rock specific heat (J/kg-K)
: ckdry = thermal conductivity of dry rock (J/s/m-K)
: cksat = thermal conductivity of liquid saturated rock (J/s/m-K)
```



```
: crp = pore compressibility with pressure at constant T (1/Pa)
: crt = absolute value of pore compressibility with pressure at constant T (1/Pa)
: tau = tortuosity for binary diffusion
: cdiff = vapor-dir diffusion coefficient, (m^2/s)
: cexp = exponent for binary diffusion
: enbd = enhanced binary diffusion coefficient
:
Thermal-prop
: no rho        cpr    ckdry  cksat   crp  crt   tau  cdiff    cexp  enbd
  1  2.580e+03 728.0   1.69   2.23    0    0    .5   2.13e-5  1.8   0.
  2  2.580e+03 422.    0.61   0.81    0    0    .5   2.13e-5  1.8   0.
  3  2.580e+03 840.0   2.10   2.78    0    0    .5   2.13e-5  1.8   0.
  4  2.580e+03 948.    1.28   1.69    0    0    .5   2.13e-5  1.8   0.
  5  2.580e+03 488.0   0.84   1.11    0    0    .5   2.13e-5  1.8   0.
  6  2.580e+03 526.    1.42   1.88    0    0    .5   2.13e-5  1.8   0.
  7  2.580e+03 9e+50   1.69   2.23    0    0    .5   2.13e-5  1.8   0.
:
: ******************
:  Backfill material
: ******************
:
  8  2.580e+03 840.0   0.60   0.79    0    0    .5   2.13e-5  1.8   0.
:
: ******************
: Metal Waste Package
: ******************
:
  9 7.800e+03 450.0    50.0   50.0    0    0    .5   2.13e-5  1.8   0.
:
: *****
:  Air
: *****
:
 10 1.2        57.4    20.0   20.0    0    0    .5   2.13e-5  1.8   0.
:
0
: ****************************
:  Define size of grid-blocks
: ****************************
: igrid = grid-type (0 - block centered, 1 - point-distributed, 2 - boundary node at the surface corresp. to CTOUGH)
: dx = block sizes in x-direction
: dy = block sizes in y-direction
: dz = block sizes in z-direction
:
DXYZ   0
: (dx(i),i=1,nx)
0.25 0.25 0.25 0.25 0.375 0.375 0.375 0.375 0.5 0.5
0.5  0.5  0.5  0.75 0.75  1.0   1.0   1.0   1.5
: .25 .25 .375 .375 0.5 0.625 0.625 1. 1. 1.
: 1. 1. 0.625 0.625 0.5 .375 .375 .25 .25
: (dy(j),j=1,ny)
0.5 0.5 0.5 0.75 0.75 1.0 1.0 1.5 1.5 1.5
: (dz(k),k=1,nz)
: element 1-6 TCw
: element 7-10 PTn
: element 11-20 TSw above the opening
: element 21-22 backfill above the heater
: element 23-26 heater
: element 27-28 backfill below the heater
: element 29-35 TSw below the opneing
```

```
: element 36 TSv
: element 37-39 CHnv
: element 40-43 CHnz
16.00  16.00  16.00  16.00  16.00  15.00  14.00  13.00  13.00  13.00
15.00  20.00  34.00  30.00  30.00  30.00  17.00  10.00   5.00   2.50
  .75    .75    .50    .50    .50    .50    .75    .75   2.50   5.00
10.00  20.00  30.00  30.00  30.00   8.00  20.00  30.00  31.00  30.00
30.00  30.00  31.00
:
: ***************************************************************************
:  Rock porosity/permeability, depth and capillary pressure characteristics
: ***************************************************************************
: i j k = region to defined the property data
: ist = sequential curve number
: ithrm = thermal properties data set number read-in by THERmal
: vb = block volume (m^3)
: por = porosity
: permx = absolute rock permeability in x direction (m^2)
: permy = absolute rock permeability in y direction (m^2)
: permz = absolute rock permeability in z direction (m^2)
: porm = matrix porosity
: permm = matrix permeability
PhiK
: i1 i2 j1 j2 k1 k2 iist ithrm vb  por permx permy  permz  pormm permm
:   1 19  1 10  1  1   1   1   0         : Top boundary with high specific heat
   1 19  1 10  1  6   1   1   0.        : TCw
   1 19  1 10  7 10   2   2   0.        : PTn
   1 19  1 10 11 20   3   3   0.        : TSw
   1  8  1 10 21 22   3   3   0.        : AIR above the heater
   9 19  1 10 21 22   3   3   0.        : TSw right of opening
   1  4  1  5 23 26   3   3   0.        : heater
   1  4  6 10 23 26   3   3   0.        : Air behind heater
   5  8  1 10 23 26   3   3   0.        : AIR right of heater
   9 19  1 10 23 26   3   3   0.        : TSw right of the opening
   1  8  1 10 27 28   3   3   0.        : backfill below the heater (pedestal)
   9 19  1 10 27 28   3   3   0.        : TSw right of opening
   1 19  1 10 29 35   3   3   0.        : TSw below the opening
   1 19  1 10 36 36   4   4   0.        : TSv
   1 19  1 10 37 39   5   5   0.        : CHnv
   1 19  1 10 40 43   6   6   0.        : CHnz
:   1 19  1 10 43 43   6   6   6.3e7
   0
:
: *****************************************************************
:  Initial pres, saturation, temp. and mole fractions of gas phase
: *****************************************************************
: i j k = region for property data
: p = pressure for the defined region (Pa)
: T = temperature for the defined region (C)
: sg = gas phase satuation for the defined region (fraction)
: xa = mole fraction of air in the defined region
: sgm = matrix gas phase saturation for the defined region (ignored if ECM is not used)
:
Init
: i1  i2  j1  j2  k1  k2      p          t       sg       xg2      sgm
  1   19  1   10  1   43    1.01325e5  27.00   0.75      0.0      0.75
0
:
:
: ********************************
```



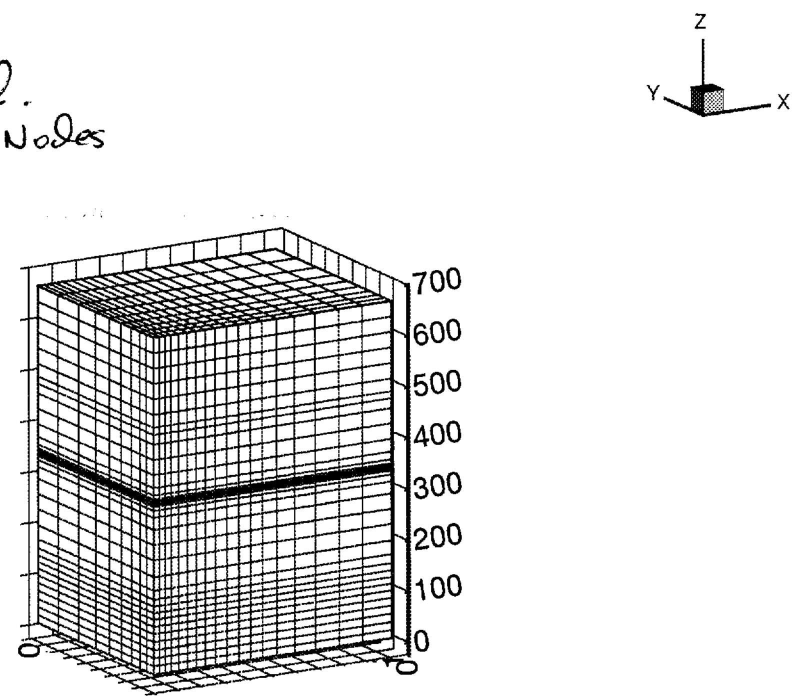
```
:  End of initialization data
: ****************************
Recurrent-data
:
: ***************
:  Output options
: ***************
: A = all the important arrays in tabular form
: C = output of convergence summary
: P = output of pressure array
: T = output of temperature array
: G = output of gas saturation array
: V = output of all directional velocity arrays
: B = boundary condition fluxes summary (not available)
: Q = source/sink summary (not available)
: L = output of liquid saturation
: Y = output of mole fraction of air in the gas phase
Output   A=1   C=1
:
: ********************************
:  Specify linear equation solver
: ********************************
: isolv = solver selection (1-Thomas Algorithm for 1d, 2-D4 method for 2d, 3-Watsolv with GMRES, 4-Watsolv with CGSTAB)
: newtnmn = minimum number of Newtonian iterations before a check on convergence is made
: newtnmx = maximum number of Newtonian iteration for convergence.
: north = Maximum number of vectors for orthogonolization for Watsolv
: nitmax = number of inner iterations for Watsolv
: level = degree of fill in incomplete LU factorization for Watsolv
:     isolv  newtnmn  newtnmx  north  nitmax  level
Solve  3      2        8        4      75       2
:
: ********************
:  Boundary Conditions
: ********************
: nbc = sequential number of boundary conditions
: itype = type of boundary conditions (1-Dirichlet, 2-Neumann, 3-velocity flux in meters/yr)
: iface = surface at which the boundary condition is imposed
: i j = region on the designated face where the conditions are imposed
: qbc = flux rate (if itype=2, kg/m^2/s)
: pbc = pressure at the designated surface with reference to the adjacent block center (Pa)
: tbc = temperature at the designated surface (C)
: sgbc = gas phase saturation at the designated surface
: xabc = mole fraction of air at the surface (for single phase and SGBC=1 or 0)
:     nbc
Bcon  2
: ityp fac    i1 i2 j1 j2
   2  TOP    1  19  1 10
: time     qflx        p       T      sg
   0.     9.513e-9   0.     13.0     0.
   1.e20  9.513e-9   0.     13.0     0.
   0
: ityp fac       i1 i2 j1  j2
   1  BOTTOM    1  19  1  10
: time   qflx     p          T      sg
   0.    0.   1.01325e5   27.0  0.001
   1.e20 0.   1.01325e5   27.0  0.001
   0
:
: **********************************
:  Define auto time step calculation
```

```
: ***********************************
: DPMXE = estimated maximum pressure change in any grid-block during a time step (.10e5 Pa)
: DSMXE = estimated maximum saturation change in any grid-block during a time step (.04)
: DTMPMXE = estimated maximum temperature change in any grid-block during a time step (5 C)
: DP2MXE = estimated maximum air-phase pressure change in any grid-block during a time step (.1e5 Pa)
: TACCEL = acceleration parameter for automatic time-step size calculation
: IAUTODT =
: FAC1 =
:
:AUTO-step  DPMXE    DSMXE  DTMPMXE   DP2MXe
AUTO-step   1.0E+4   0.03    5.0       1.e4
:
: *******************************************************
:  Overrides or modifies the tolerances for convergence
: *******************************************************
: TOLP = pressure tolerance (10 Pa)
: TOLS = saturation tolerance (0.0001)
: TOLT = temperature tolerance (.001)
: TOLP2 =  air partial pressure tolerance (10 Pa)
: TOLM = tolerance on mass residual (0.001)
: TOLA = tolerance on air residual (.001)
: TOLE = tolerance on energy residual (.001)
: Residual (L2) = max abs for total mass, error and energy equations
: RTWOMAX = rtwotol (initial residual norm)
: RMXTOL = absolute value of residual
: SMXTOL = max of (dx, dx/x)
:
:TOLR TOLP         TOLS  TOLT  TOLP2  TOLM   TOLA    TOLE
Tolr  10. 1.e-4  1.e-3  1.e+1 1.e-5   1.e-3  1.e-3   1.e-15    1.e-15    1.e-15
:
: ********************************************************************************
:  Set limit for the maximum change in the primary variables during a time step
: ********************************************************************************
: DPMX = maximum change in pressure over a time step in any block (.5e5 Pa)
: DSMX = maximum change in saturation over a time step (.10)
: DTMPMX = maximum change in temperature over a time step
: DPAMX = maximum change in partial air pressure over a step
: DTMN = minimum time step size allowed
: DTMX = maximum time step size allowed
: ICUTMX = maximum number of time-step cuts allowed during a time step
:
:Limit  dpmx    dsmx  dtmpmx  dpamx      dtmn     dtmx   icutmx
LIMIT  1.e5      .08      10.  1.e5  3.171e-8    1.e5
:
: SKIP                          : skip the heating part for obtaining the initial conditions
:
: ******************************************************************
:  Assigns a set of tables for sources and sinks as a function of time
: ******************************************************************
: NS = total number of sources and sinks
: FACH = scale factor of energy
: FACM = scale factor of mass
: is1, is2
: js1, js2
: ks1, ks2
: istyp = index for type of source/sink (1-mass rate specified, 2-not used, 3-heat rate with no mass specified
: TIMEQ = time in seconds
: QHT = temperature (if istyp=1), heat rate (if istyp=3)
: QMT = mass rate (if istyp=1), 0 (if istyp=3)
: source  NS    FACE      FACM
```

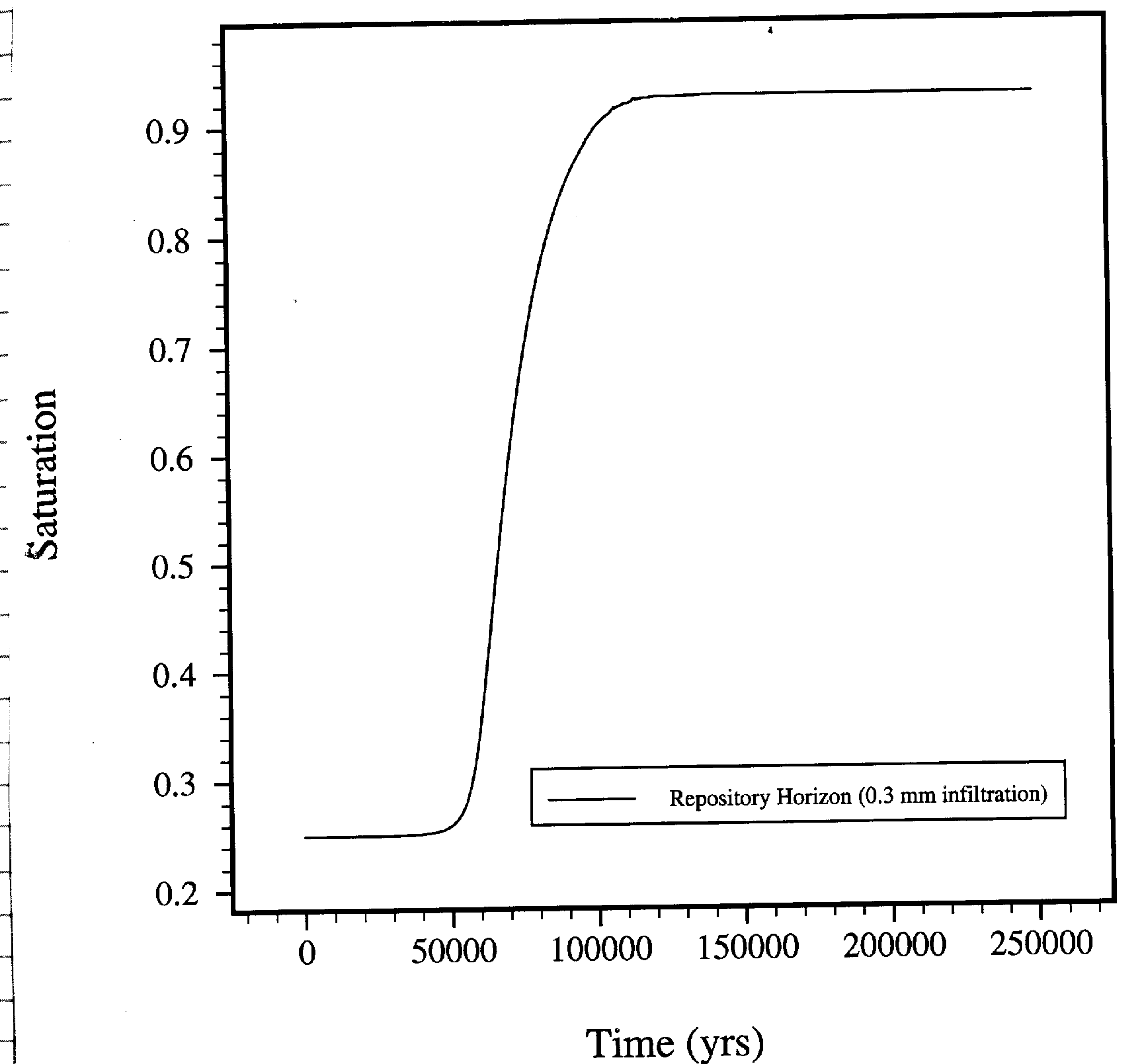


```
:Source   6      2.2      1.0    : water sources along the top surface & heater sources
:
: sources at the top boundary surface
:
: timeq(sec)   T/qht (C/(J/s))    qmt (kg/s) 80APD
:  is1  is2  js1 js2 ks1 ks2 istype
:    1    4    1   1   1   1    11
:0. 13.0  2.378e-9
:0
:
:    5   8   1   1  1  1  11
:0. 13.0  3.576e-9
:0
:
:    9   13   1   1  1  1  11
:0. 13.0  4.757e-9
:0
:
:    14   15   1   1  1  1  11
:0. 13.0  7.135e-9
:0
:
:    16   18   1   1  1  1  11
:0. 13.0  9.513e-9
:0
:
:   19   19   1   1  1  1  11
:0. 13.0  1.427e-8
:0
:
:       print all at every target time
rstart 1 0
PLOTS 1 5 4371 3611 4379 3782 4550
:Steady[y]  1.e-6  1.e-5  1.e-8
:      target  dt    dpmx   dsmx   dp2mx   dtmpmx
Time[y]  10.
Time[y]  1000.
Time[y]  10000.
Time[y]  100000.
Time[y]  250000.
:NONSKIP
Ends
```

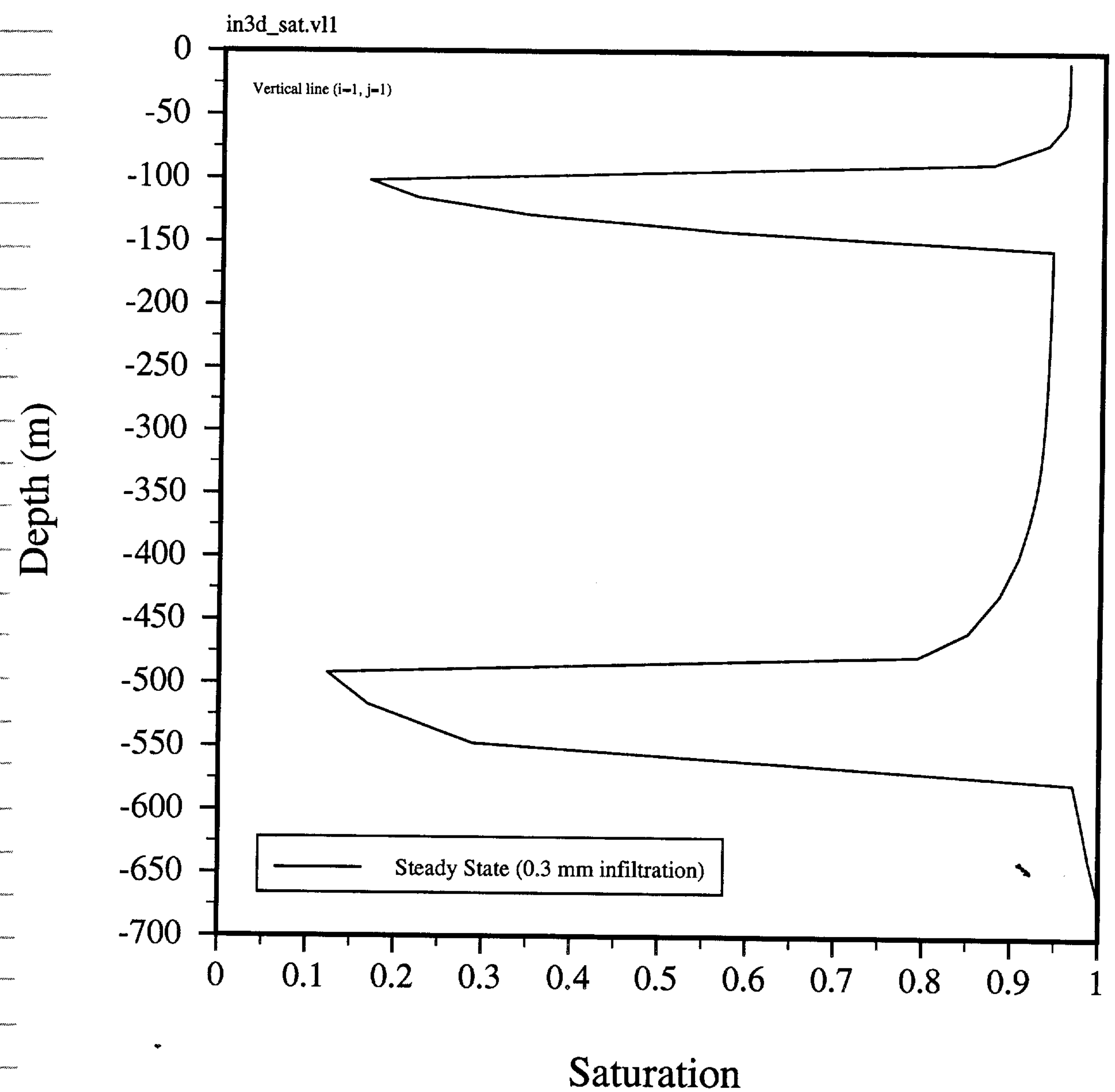
3D-Model.
19 x 10 x 43 Nodes
i j k



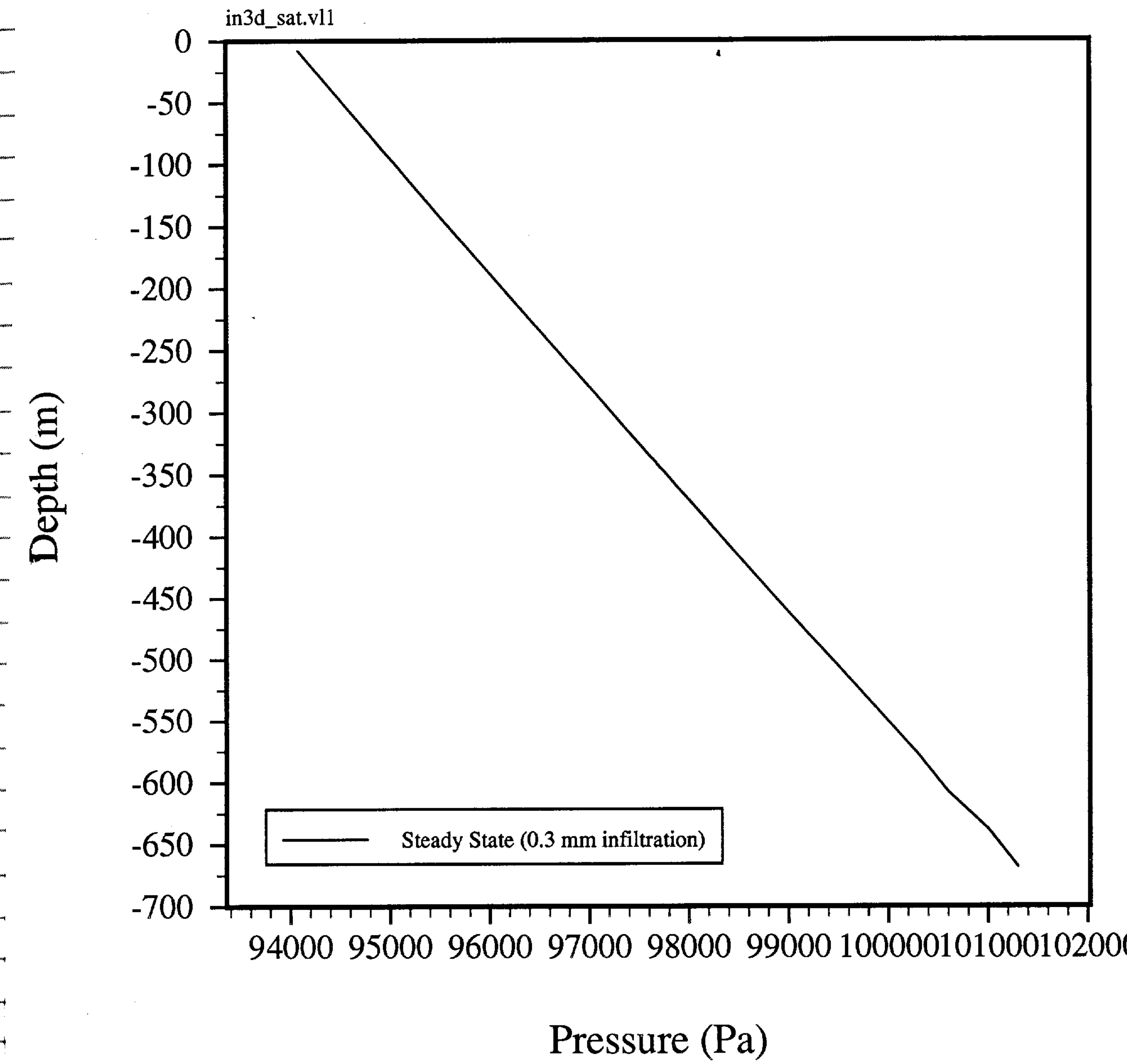
MA



Time history of node at repository horizon showing length of time necessary to reach steady state convergence.

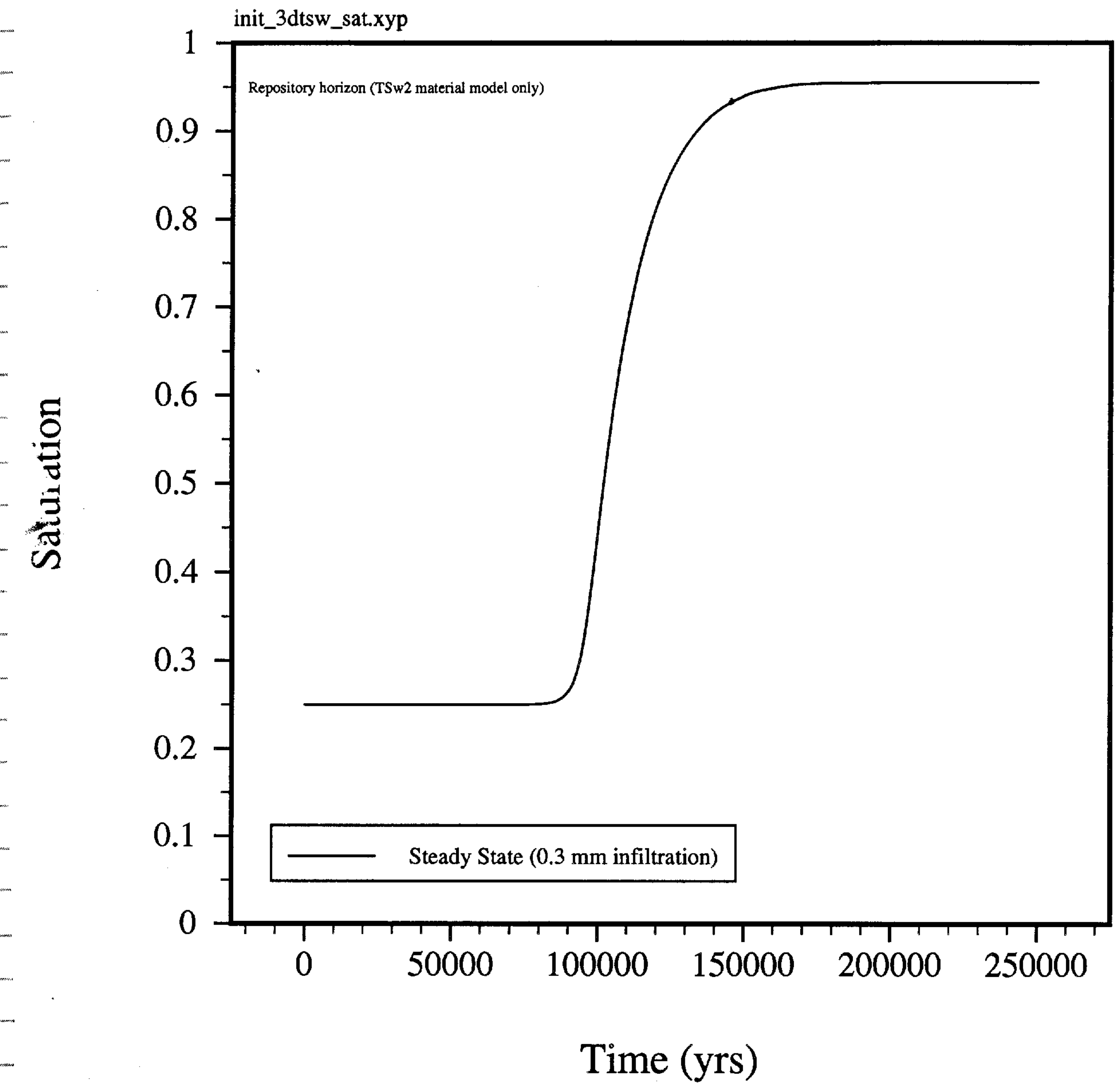


Profile of steady-state saturation with depth based on 0.3 mm infiltration, and various Van Genuchten Parameters for the different units.

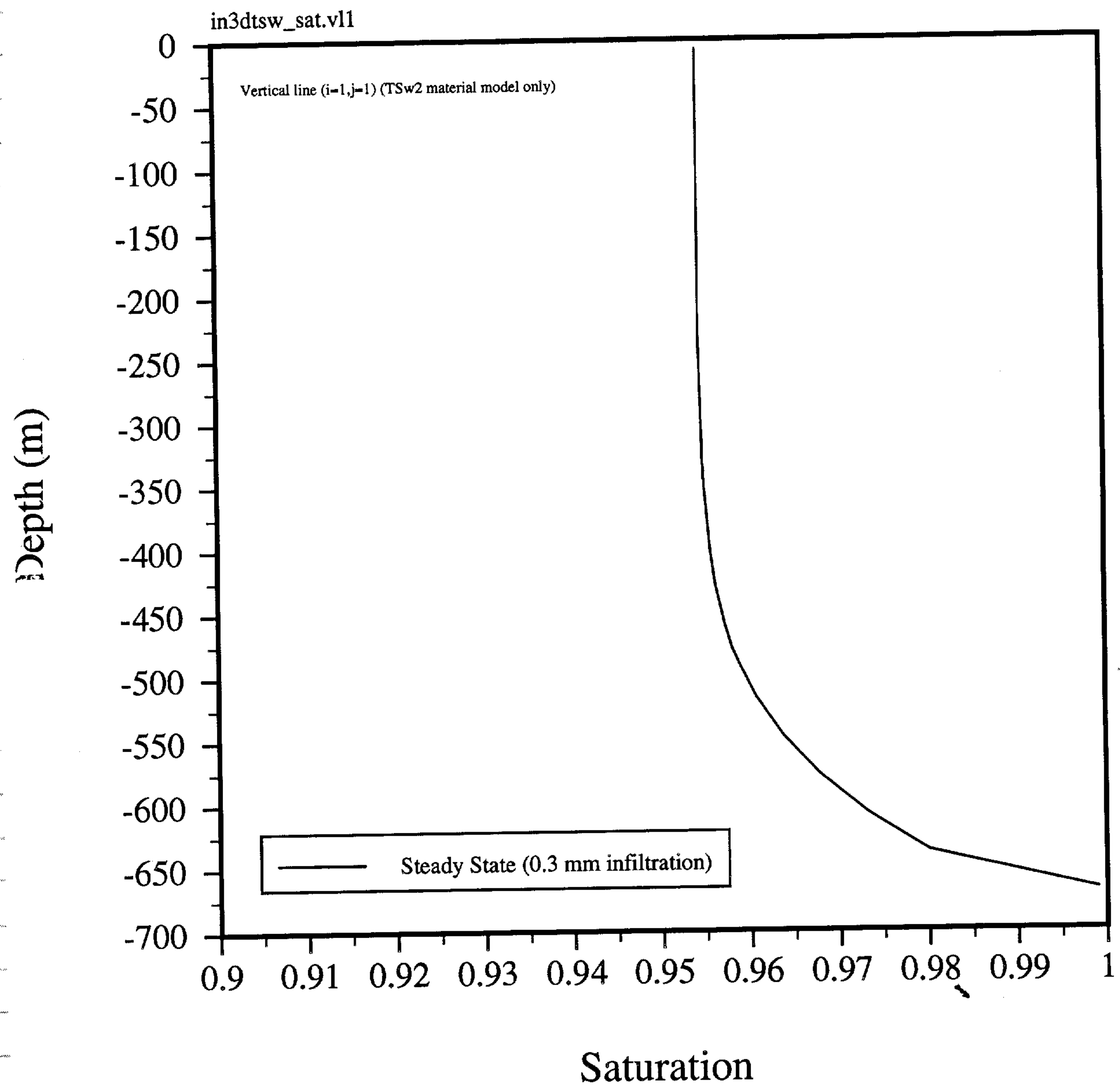


Profile of gas pressure with depth for steady-state solution. w/o heat.

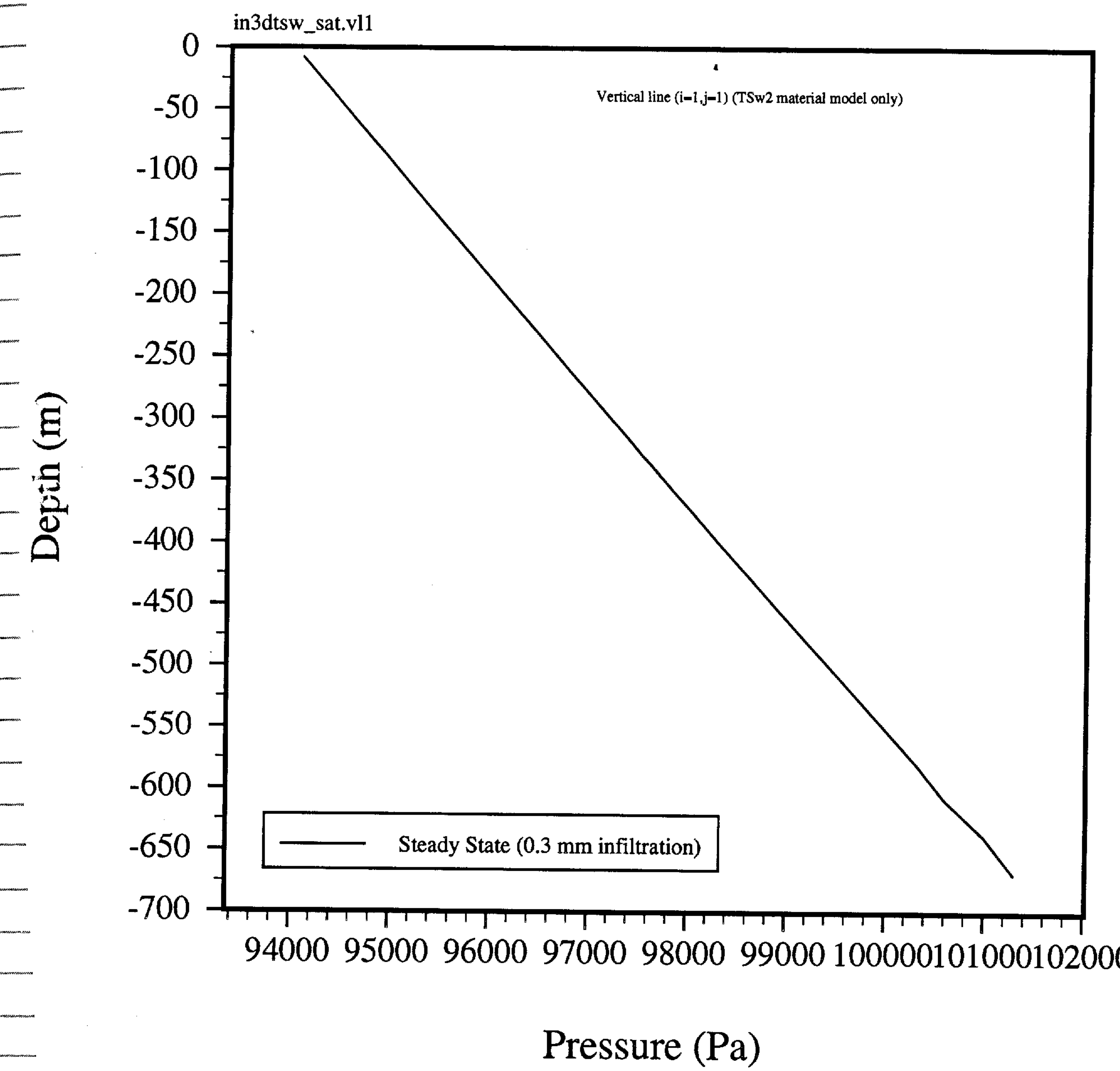
An attempt was made to utilize the initial steady state run (with multiple layers in the TH run with the heater (83 MTU/acre). However, although the problem ran, a very small timestep resulted in which running out the problem to 100-1000 yrs became impractical. Based on this, it was decided to simplify the problem for the time being incorporating only one material (TSw2) throughout. The following plots show the initial steady state run w/o heat for the one material model.



Time history of node at repository horizon for initial steady state run.

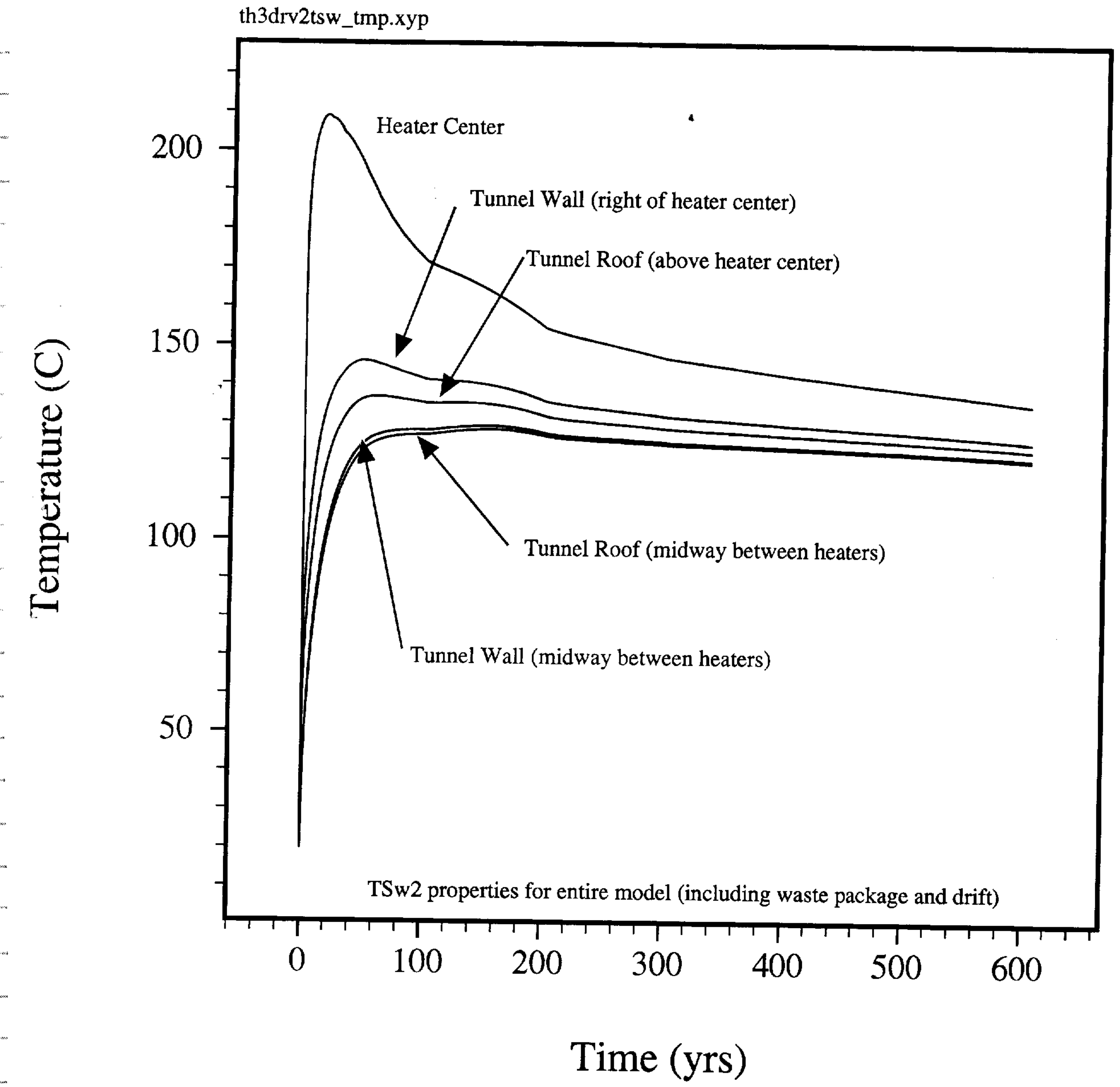


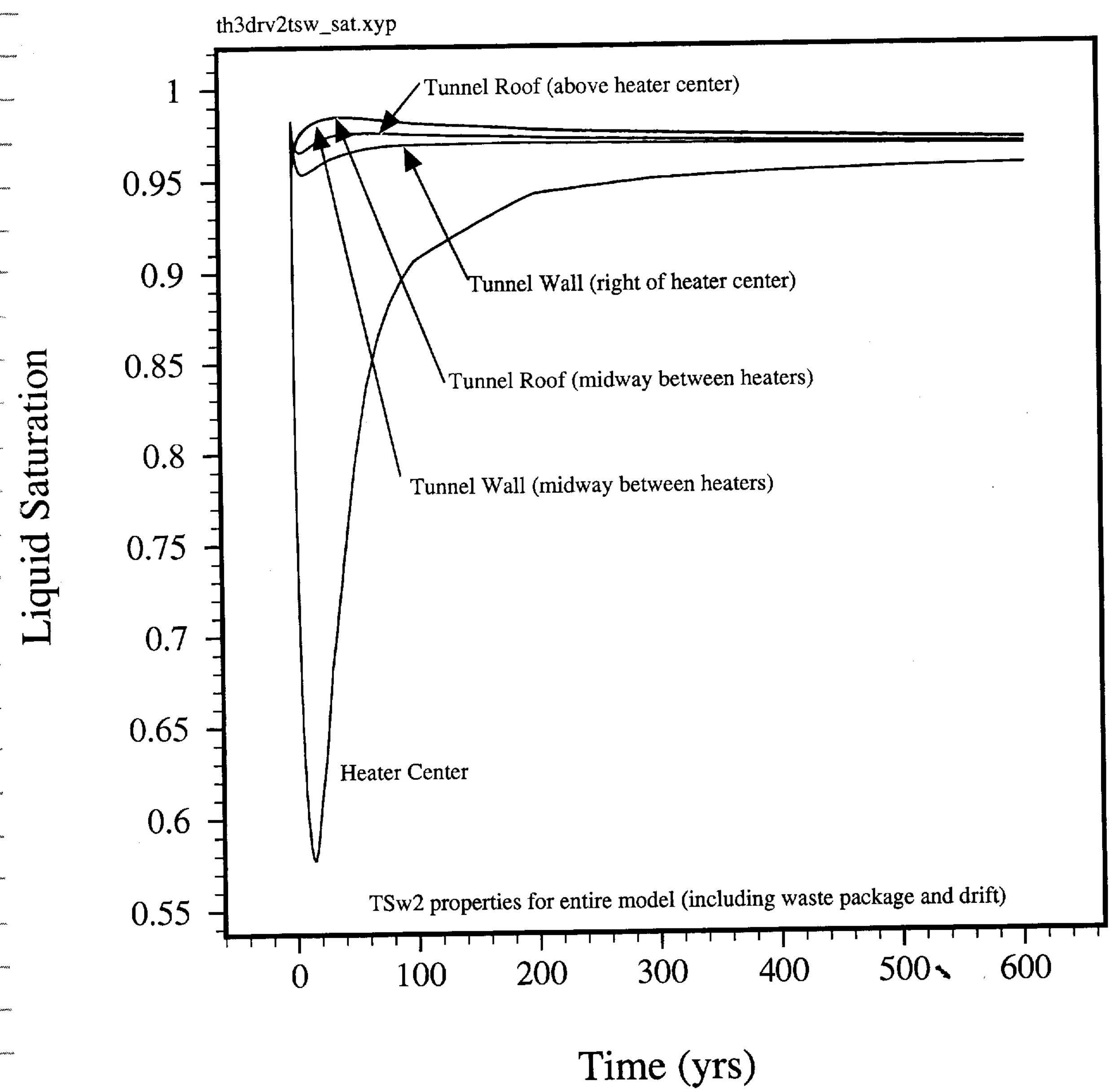
Final saturation profile with depth for the initial steady state run (TSw2 material throughout depth).

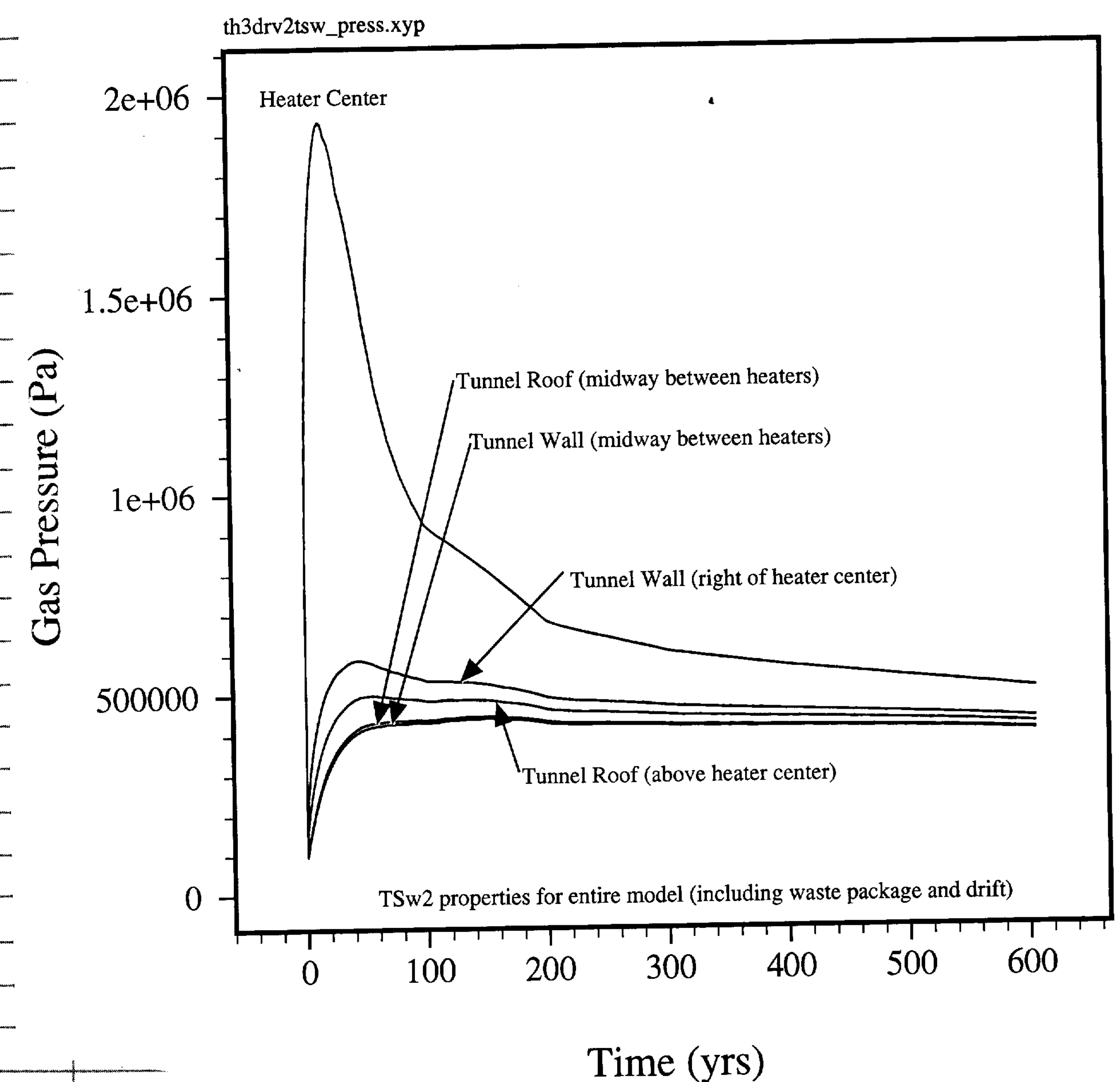


Final gas pressure profile with depth for initial steady state run

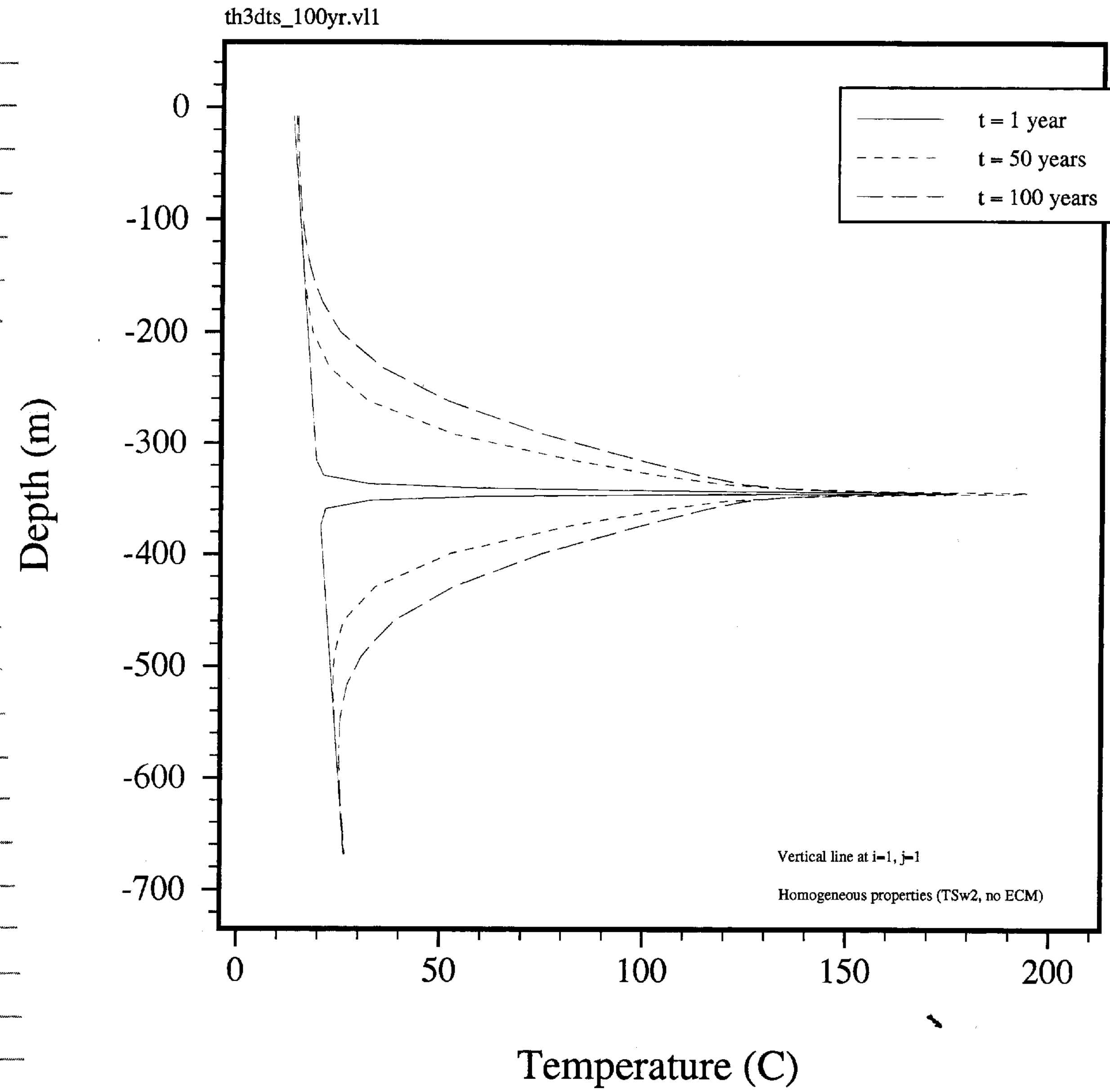
The next step was to use the previous initial state data for the thermal run. Using Metra Version 0.96 (Jan, 1997), the thermal run was attempted to 10,000 yrs. The run was initiated on a Friday and terminated by keyboard Monday morning after reaching only 600 yrs of thermal simulation. Maximum timestep reached about (0.22 yrs) or ≈ 80 days during the run using the Watsolv-4 solver. Results are presented in the following pages. Note that in the TH run (file name th3drv2tsw.dat), the drift was not simulated. The drift and heater were assumed to have material properties of TSw2 material. Note that the ECM option was not utilized in this run.

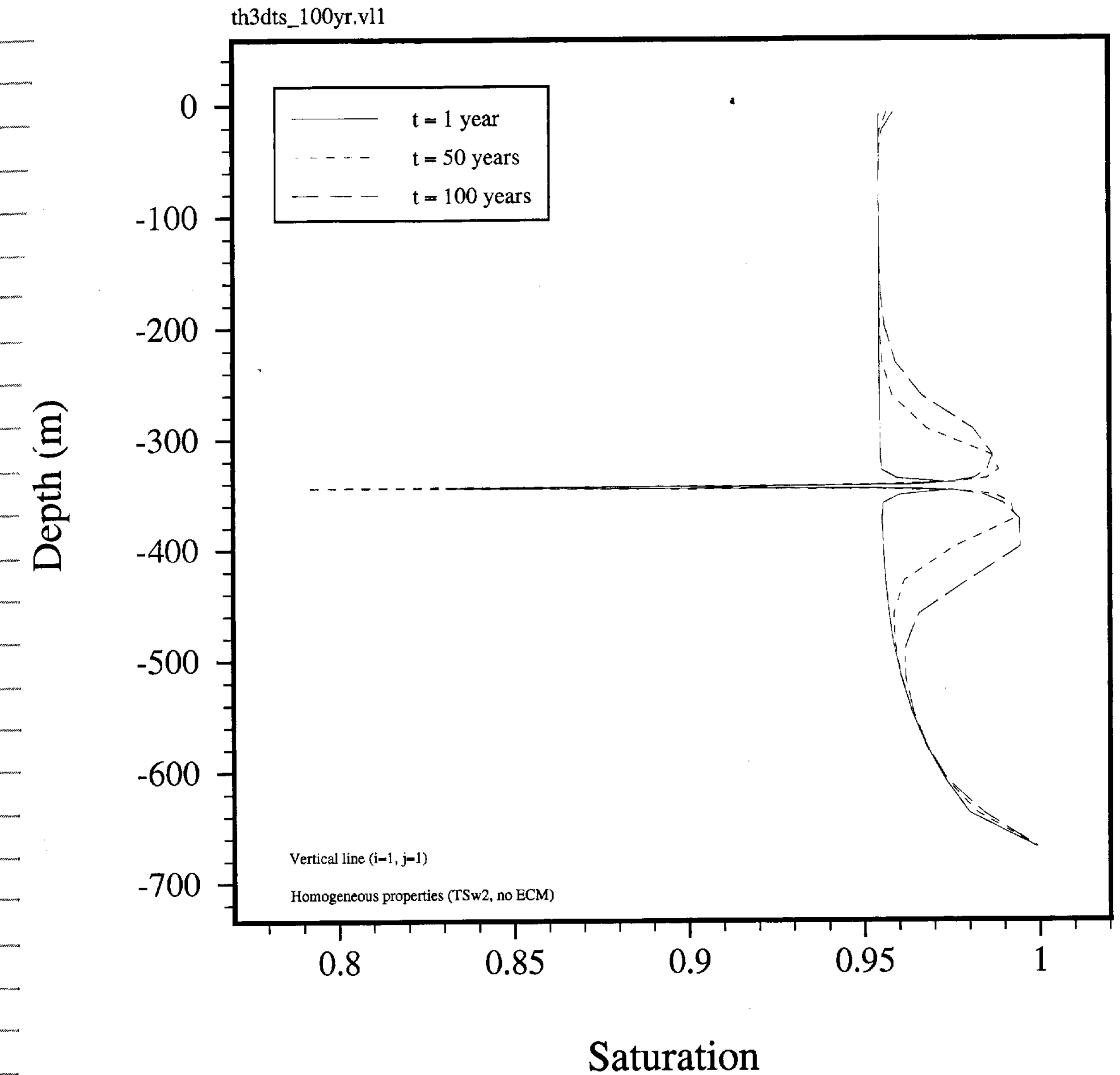


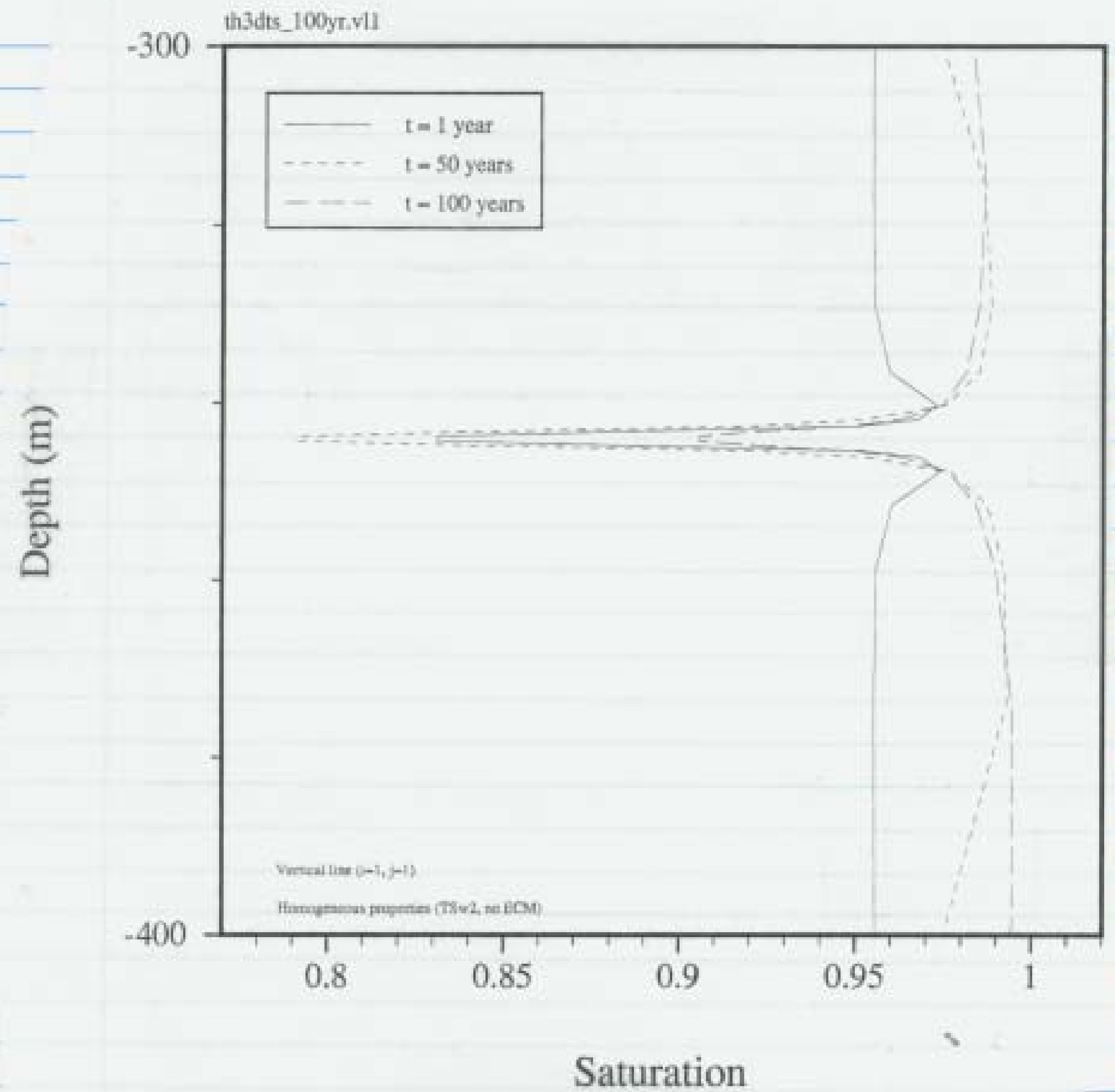




High gas pressure interpreted to be unrealistic. Most likely due to the fact that the ECM option was not implemented, only the matrix flow was


th3dts_100yr.vl1
t = 1 year
t = 50 years
t = 100 years
Vertical line at i=1, j=1
Homogeneous properties (TSw2, no ECM)
Depth (m)
Temperature (C)
0
-100
-200
-300
-400
-500
-600
-700
0
50
100
150
200


th3dts_100yr.vl1
t = 1 year
t = 50 years
t = 100 years
Vertical line (i=1, j=1)
Homogeneous properties (TSw2, no ECM)
Depth (m)
Saturation
0
-100
-200
-300
-400
-500
-600
-700
0.8
0.85
0.9
0.95
1



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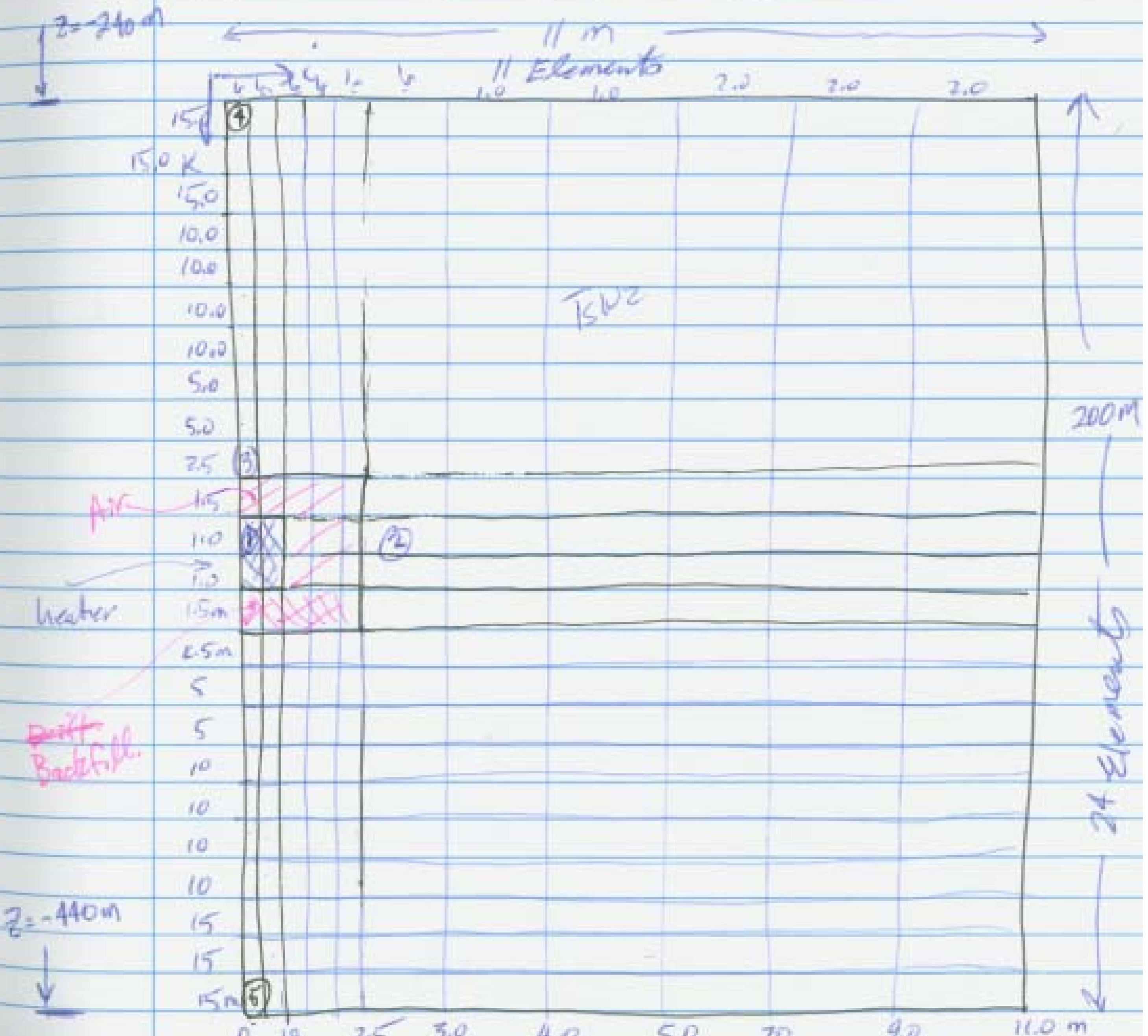
Because of the long run times for the 3D run (i.e., th3drv2tsw.dat) which had 19 x 10 x 43 elements in the i, j, and K direction (8170 total), it was decided that a reduced 3D model was necessary. The new 3D submodel contained 11 x 7 x 24 elements in the i, j, and K direction (1848 total.) The model is sketched below.



⑥ i=1, j=7, k=10 ⇒ m = 1 + (6)(11) + (9)(11)(7) ⇒ m = 760

Monitoring Points

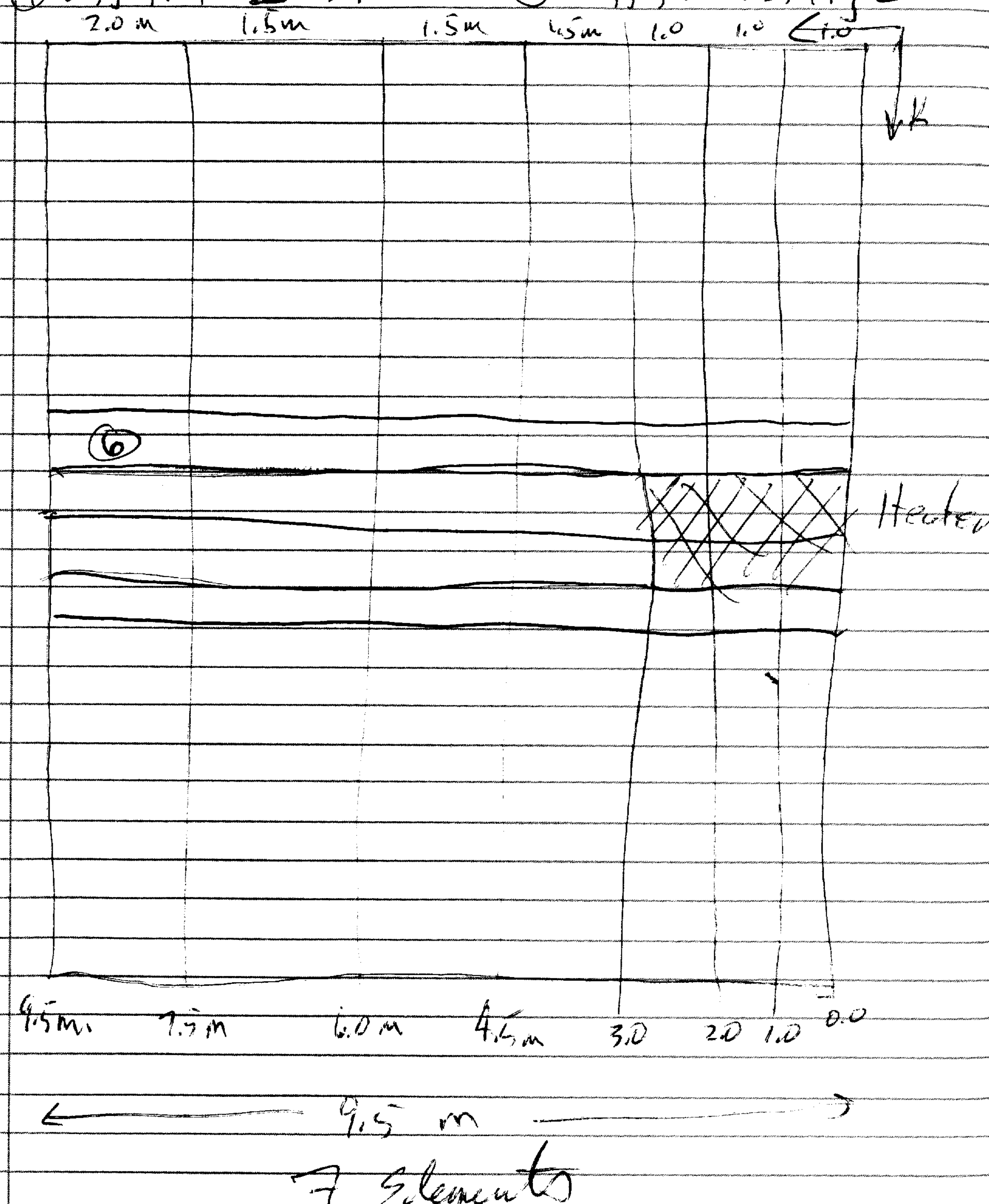
① i=1, j=1, k=12 ⇒ Elem. 848

② Elem ⇒ 853

③ Element 694 (i=j=1, k=10)

based on $m = i + (j-1)nx + (k-1)\,nx\,ny$ where nx = 11, ny = 7

④ i=1, j=1, k=1 ⇒ 1   ⑤ i=1, j=1, k=24 ⇒ 1792



Before heating, initial steady-state hydrologic run was necessary for the 3D submodel. Initial conditions were

p = 1.0135 e5 Pa air pressure

t = 27 °C

Sg (gas saturation) = 0.75

Sgm (matrix gas sat) = 0.75

Fluid flux of 0.3 mm/yr (9.513e-9 kg/m²·s) was reapplied at top boundary of 3D submodel. The bottom boundary was no longer at the water table (i.e., z = -662 m, Sl = 1.0, Sg = 0.0). As a result, the liquid saturation (Sl) was fixed at the value at the same depth from the large 3D model as read from the figure on page 18. Thus, at a depth of ≈ -450 m the large 3D model had a liquid saturation of ≈ 0.96 at steady state, which was used as the boundary condition in the 3D submodel.

Run ① The 3D initial hydrologic steady state run was then repeated for the submodel (w/o heat) which extended only 100 m above and below the heater

- fluid flux 0.3 mm/yr applied at top bd.
- liquid saturation applied at 96% at bottom boundary MA

Datafile C3_1.DAT MA

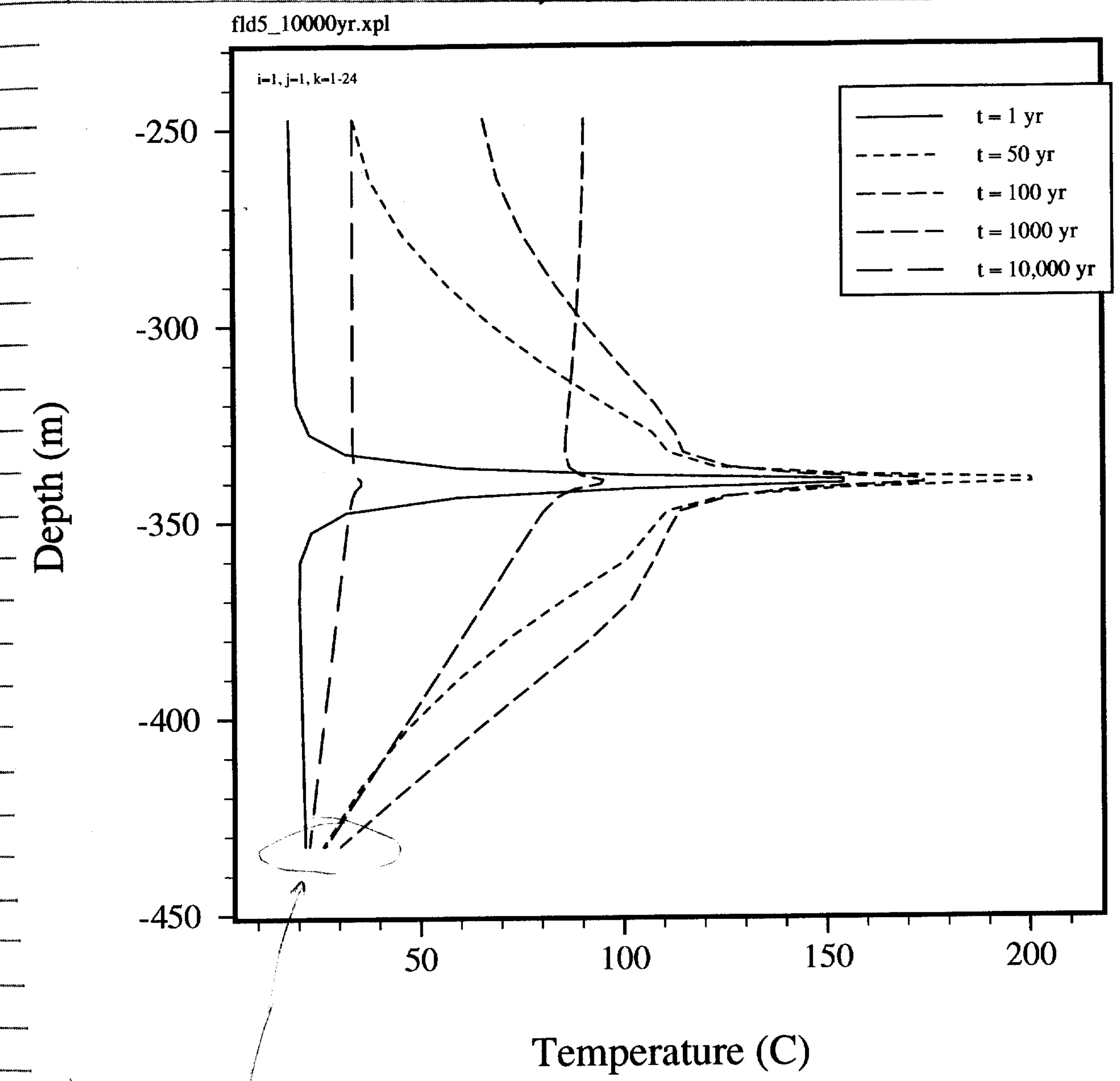
Run carried out to t = 0.25e6 yrs at which time steady state conditions reached. The cut & paste file was edited to include the initial temperature gradient of 0.02 °C/m. ~~Top boundary~~ in which at top (z = -240 m) the initial temp was 17.8 °C while at the bottom (z = -440 m) the initial temp was 21.8 °C.

Run (2) Thermal runs were then initiated. The first 3D TH run [Data File C3-TH1.DAT] was conducted at 1/3 the heat load. TSw2 properties (both hydrologic and thermal) were assumed throughout model. The gas saturation (initial) was adjusted to 99% in the heater region [i.e, i=1-2, j=1-3, k=12-13] via editing the initial condition cut & paste file [c3-in.int]. Run was completed out to t = 10,000 yrs in approx 3½ hrs on foxtrot (Sun Ultra Sparc).

Run (3) The next thermal run utilized the full heat load [i.e, 83 MTU/acre]. Again TSw2 material properties (both hydrologic and thermal) were assumed throughout. Gas saturation initialized to 99% in heater region. Initial conditions file C3-in.int. Run completed OK to 10,000 yrs in approx. 12 hrs.
Data File = C3-TH2.DAT

The following are temperature and saturation plots with depth at various time periods.

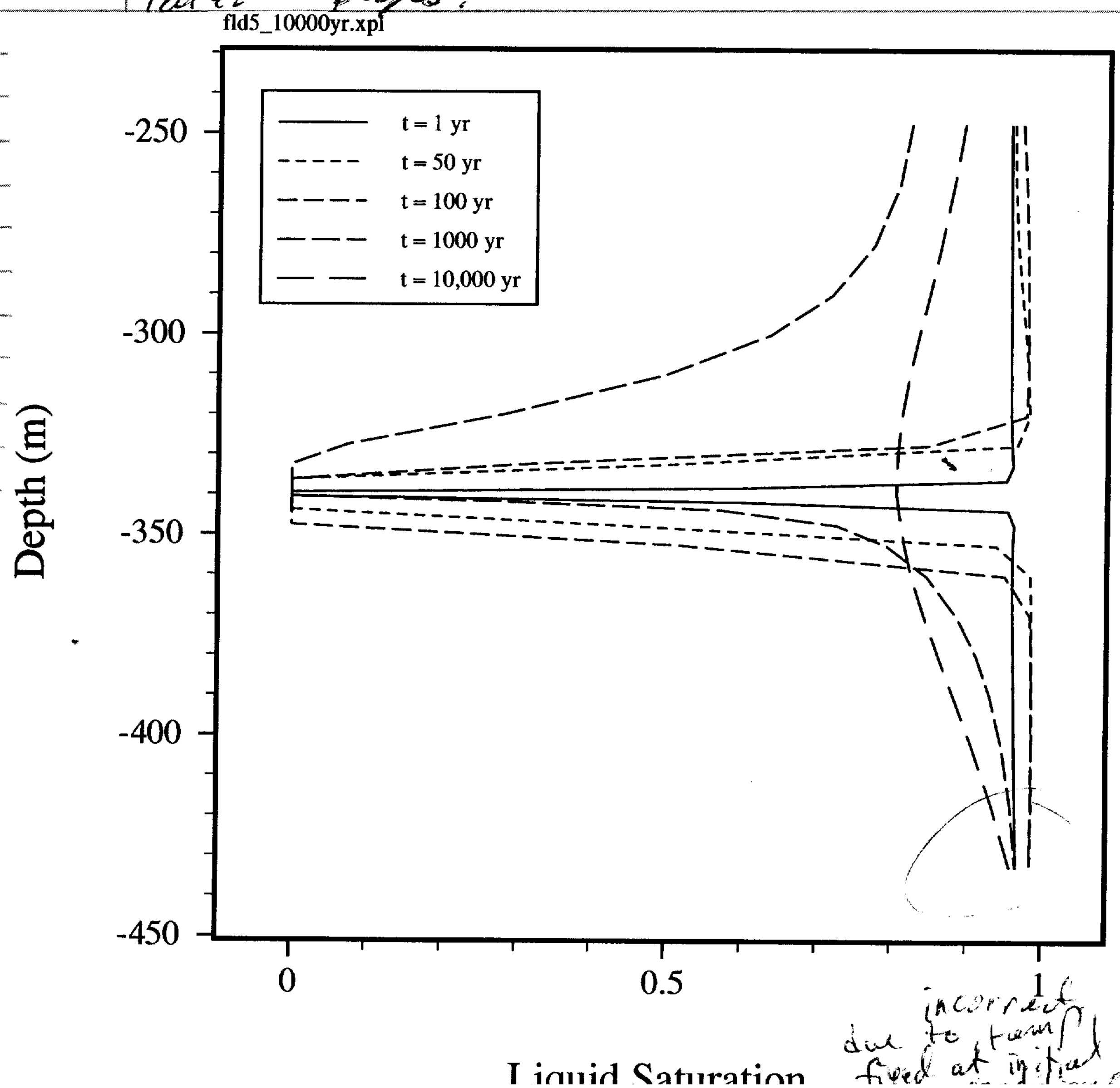
C3-TH2.DAT



Note: Boundary condition ~~condition~~ along bottom currently fixed at initial conditions T = 21.8 °C, Sl = 90%, and results in increasing error at long times. Compare with temp plot for large 3D model at t = 100 yrs on page 24. Also, since fluid flux is applied to top boundary top boundary temp cannot be controlled (assume adiabatic b.d.)

However, top boundary temperature does increase, and is only slightly hotter (≈15°C) than that on page 24 at same depth z = -240 m at t = 100 yrs.

It was decided that although the large 3D model takes a long time to run, it would be rerun and temp and saturation values stored at same depths as boundaries in 3D submodel for use as time varying boundary conditions in submodel. This will be discussed on later pages.



The fixed ~~cooler~~ temp at bottom boundary also incorrectly affects the dryout zone at bottom of model in the C3-th2.dat run.

Run (4) The next thermal run improved somewhat on the Run (3) in that the thermal properties of all the different materials were included in the 3D submodel i.e., Tsw2 (TopoPah Springs unit), Air in drift, Waste Package, and backfill in the floor. Also, the initial gas saturation was set to 99% in the entire drift (i=1-5, j=1-7 K=11-14) and not just in the heated region. New initial conditions cut and paste file = C3ain.int. [compare to C3-ini.int]

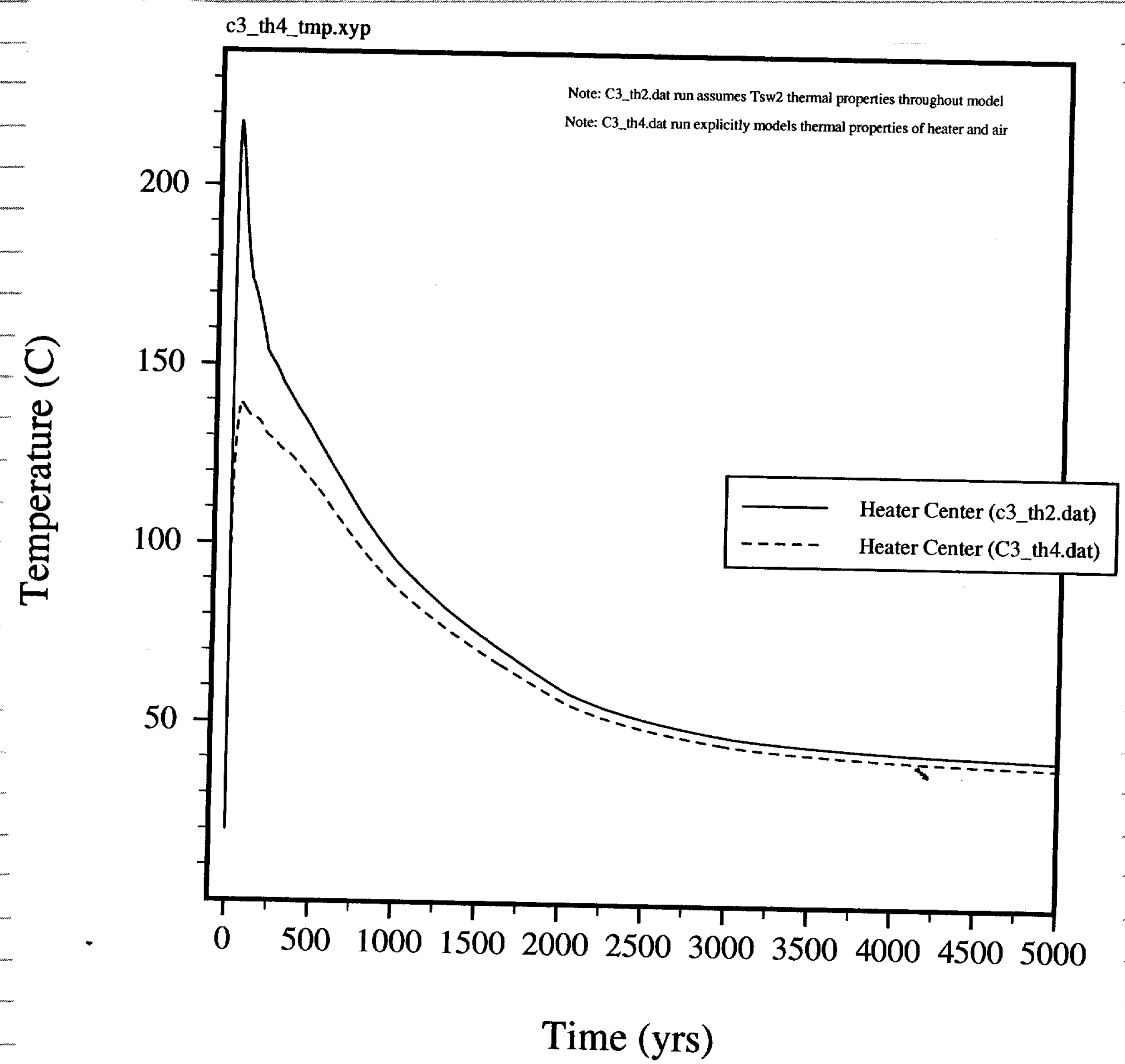
Data file = C3-TH4.DAT. Run completed to 10,000 yrs in ≈ 12 hours on Sun Ultra Sparc. Although, b.c. were applied the same as in run (3) and still need improvement.

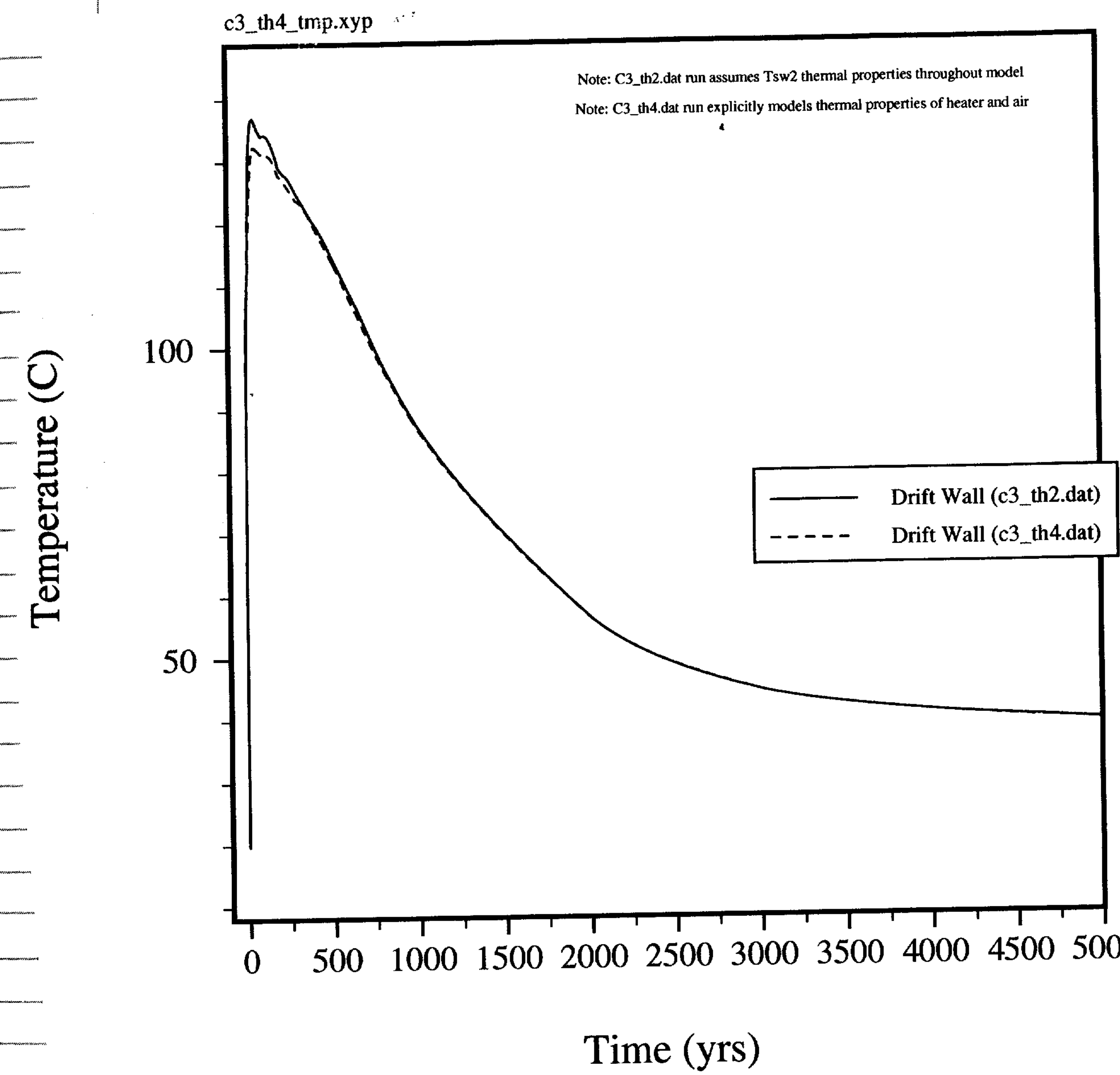
Thermal Properties.

	ρ (Kg/m³)	C_p (J/kg·C)	K_{dry}	K_{sat} (W/m·C)
Tsw2	2580.0	840.0	2.10	2.75
Air	1.2	57.4	20.0	20.0
Waste Package	7800.0	450.0	50.0	50.0
Backfill	2580.0	840.0	0.60	0.79

Comparing temperatures with time at the heater center and also at the right drift wall monitoring pts (1) and (2) [see pg 27] we see that when the thermal properties are included, the canister temp peaks at only 140°C vs 215°C. However, after the peak temperatures agree well. Also, at the drift wall

the temps agree well regardless of the thermal properties of heater and air.





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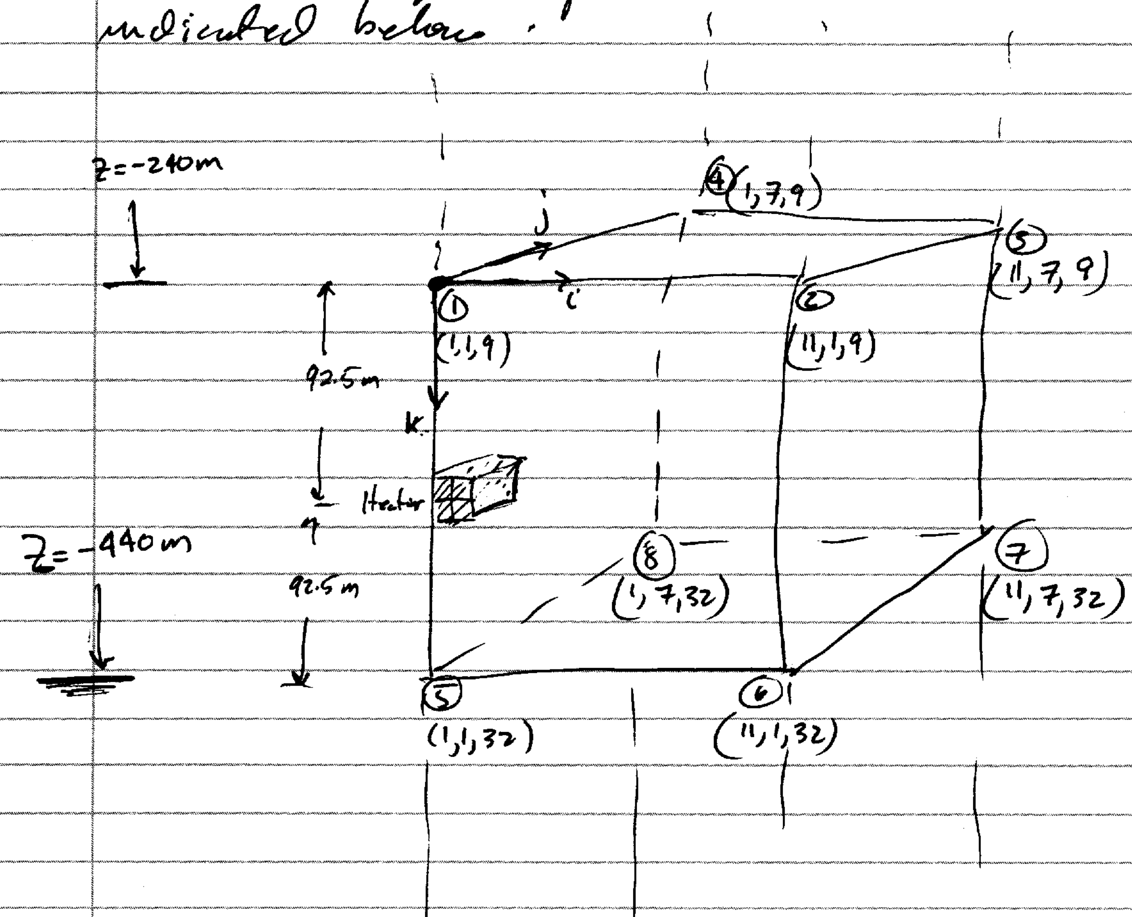
(5) The next 3D submodel run [Data File: C3-TH5.DAT] included the hydrologic properties for both the TSw2 rock as well as the air within the drift. The porosity of air was set to 99.9% and the permeability to 1.e-20 m^2 (several orders of magnitude lower than the rock) to simulate a capillary barrier to flow. The backfill and heater were assumed to have same hydrologic properties as air. Note: 3D Meta run appears highly sensitive to changes or contrasts in hydrologic properties, and as a result difficulties were incurred in trying to include a low porosity / low permeable waste package, high porosity / low permeable air, and high porosity / high permeable backfill. As a result, only 2 hydrologic materials (air & TSw2) were simulated for this run. All thermal properties were however, included (ie, TSw2, air, waste package, and backfill). The air thermal conductivity was, however, reduced from 20 W/m·K to 10 W/m·K, since this was determined more representative. Run time was longer than for that using datafile C3-TH4.dat (≈ 24 hrs verses 12 hours). Reduction of the air thermal conductivity increased the waste package peak temperature ≈ 10°C to ≈ 190°C. The next step is to ~~revise~~ incorporate time varying temperature and saturation boundaries at the top and bottom of the 3D submodel.

(6.) In order to incorporate time varying boundary conditions into the 3D submodel, a full scale 3D model run out to 10,000 yrs was required in which the time varying temperatures and saturations were stored at the upper and lower horizons (i.e., Z = -240 m, and Z = -440 m) for incorporation as b.c.'s into the submodel. Attempts to run the original full scale 3D model (as discussed on pages 20-26) out to 10,000 yrs failed. As a result, it was decided to the coarser submodel and simply extend this model to the upper ground surface and lower water table boundaries. The submodel increased in size from 11x7x24 (1848 elements) to 11x7x40 (3080 elements), which was still considerably less than the 19x10x43 (8170 Elem.) of the original full-scale 3D model. The new revised full-scale 3D model included vertical extensions (240 m, or 8 elements) onto the 3D submodel. The datafile was titled C3BIG_1.DAT. This model had to be again run to hydrologic steady state without heat to establish initial conditions (i.e., run to 250,000 yrs). A cut and paste file at this time was created [C3BIG.INT] which was read into a second run with the heater turned on. Again the top boundary included a flux of 0.3 mm/yr and const. temp b.c. of 13°C. The lower boundary was fixed at a temp. of 27°C with liquid saturation close to unity.

Temperatures and saturations were stored at the horizons of the 3D submodel as indicated below.



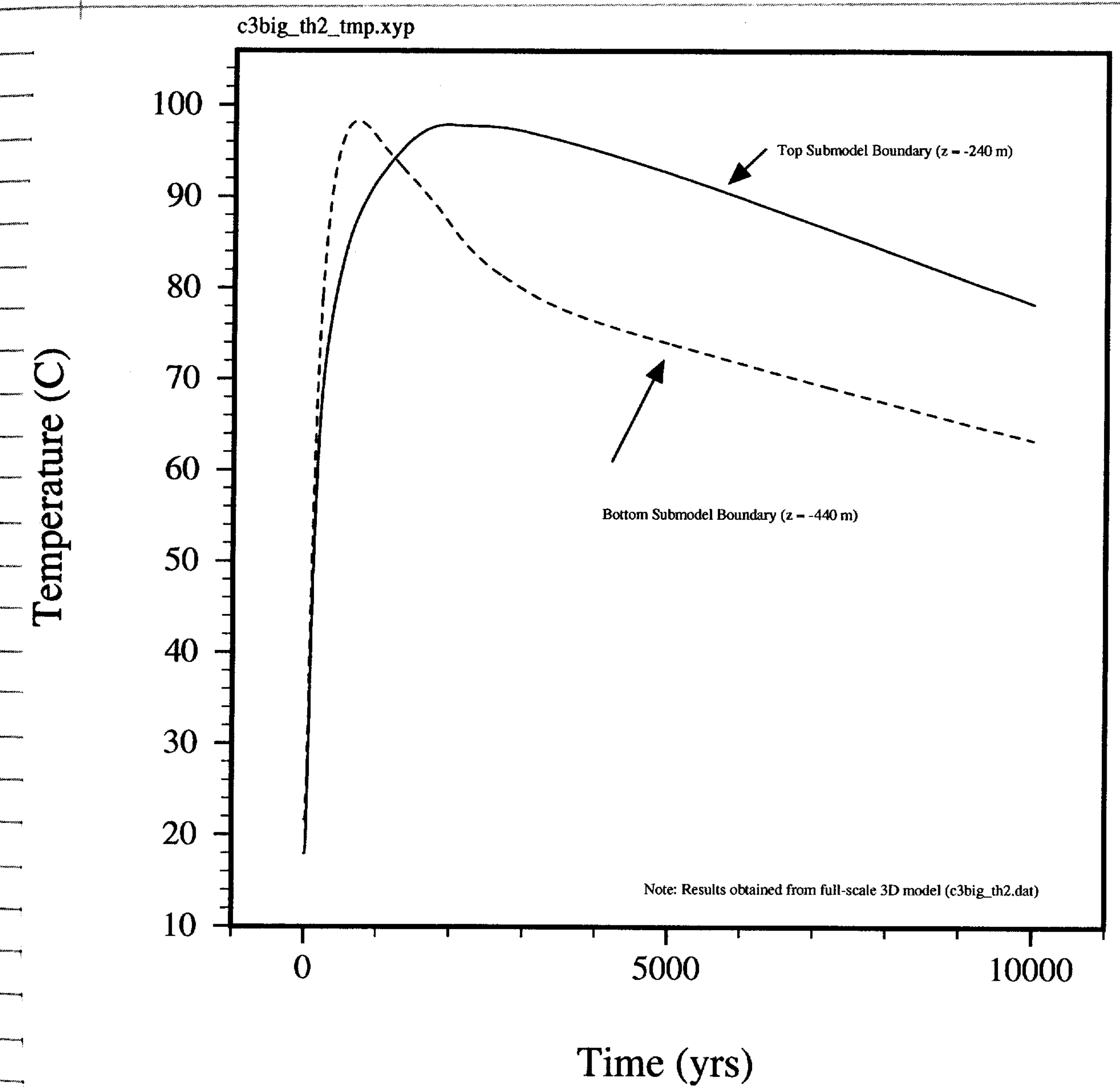
Monitoring Pt. (m)   nx = 11, ny = 7, nk = 40

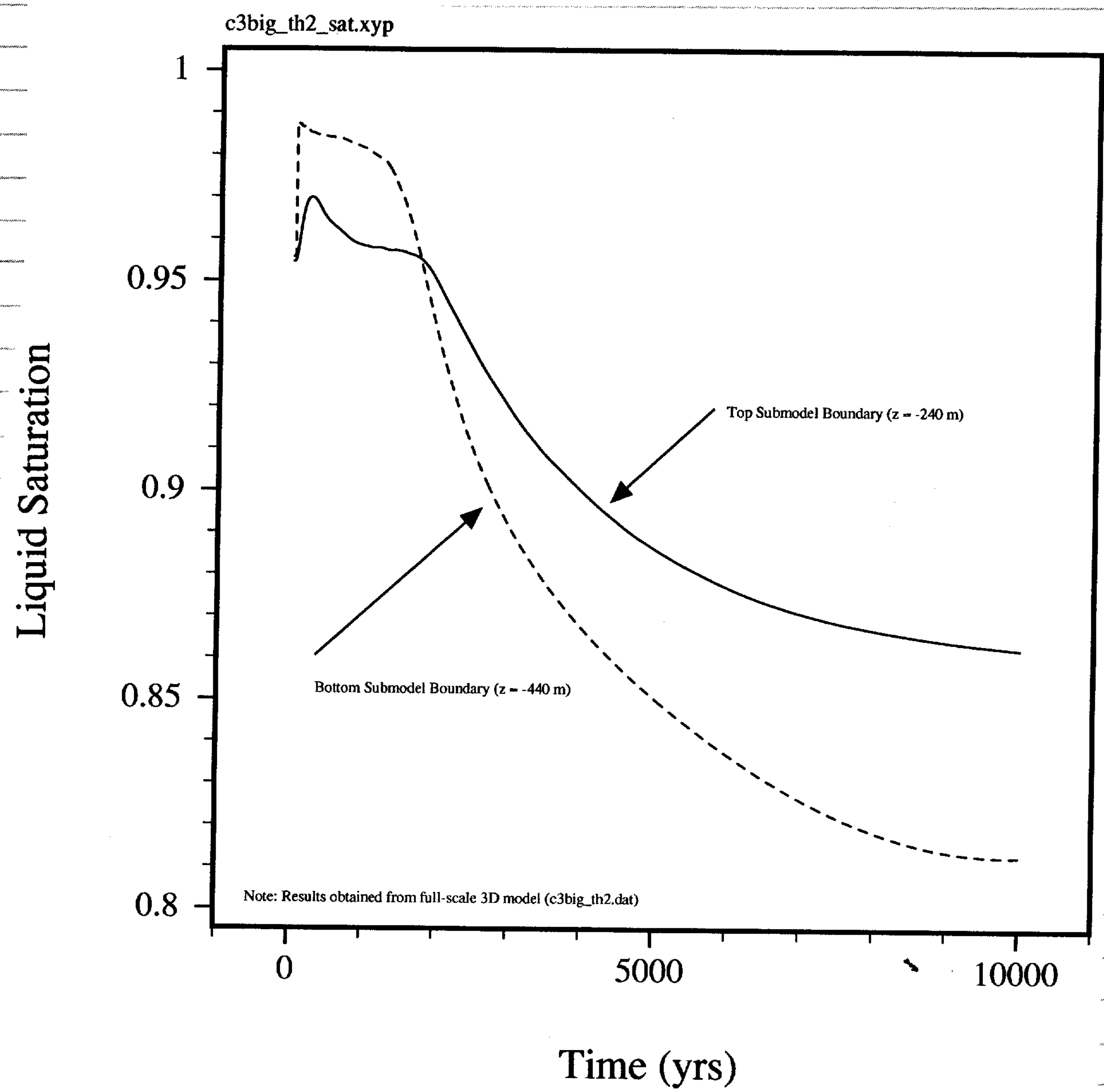
$m = i + (j-1)nx + (k-1)nx\,ny$

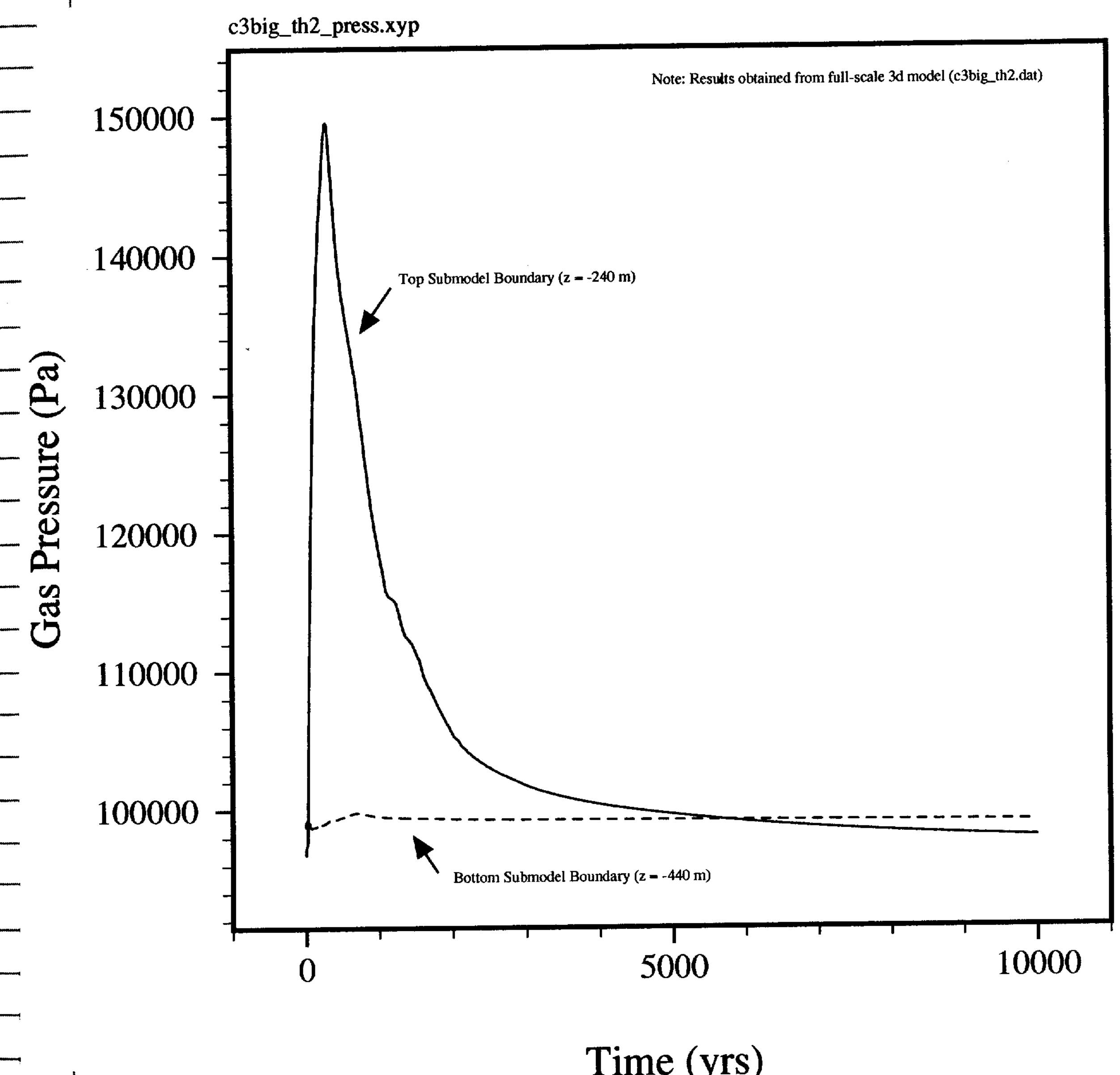
Pt. ① m = 617
② m = 627
③ m = 693
④ m = 683

⑤ m = 2388
⑥ m = 2398
⑦ m = 2464
⑧ m = 2454

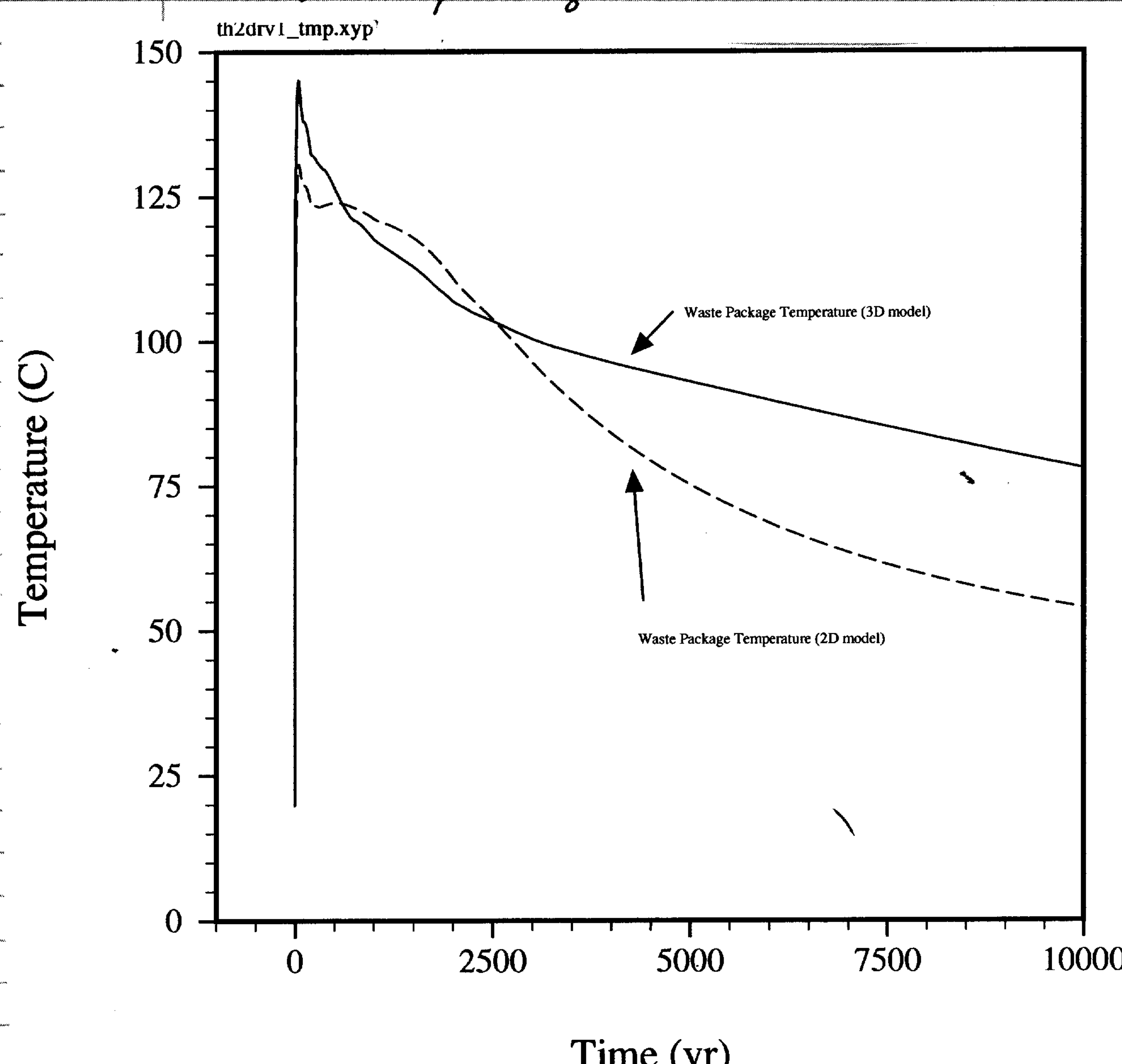
The temperatures and saturations are averaged at the 4 upper monitoring pts (i.e., 1-4) as well as the 4 lower plane monitoring pts (5-8). The average time varying values are then read in as boundary conditions for the smaller 3D submodel analyses. The temperature, liquid saturation, and pressure b.c. inputs are plotted below.

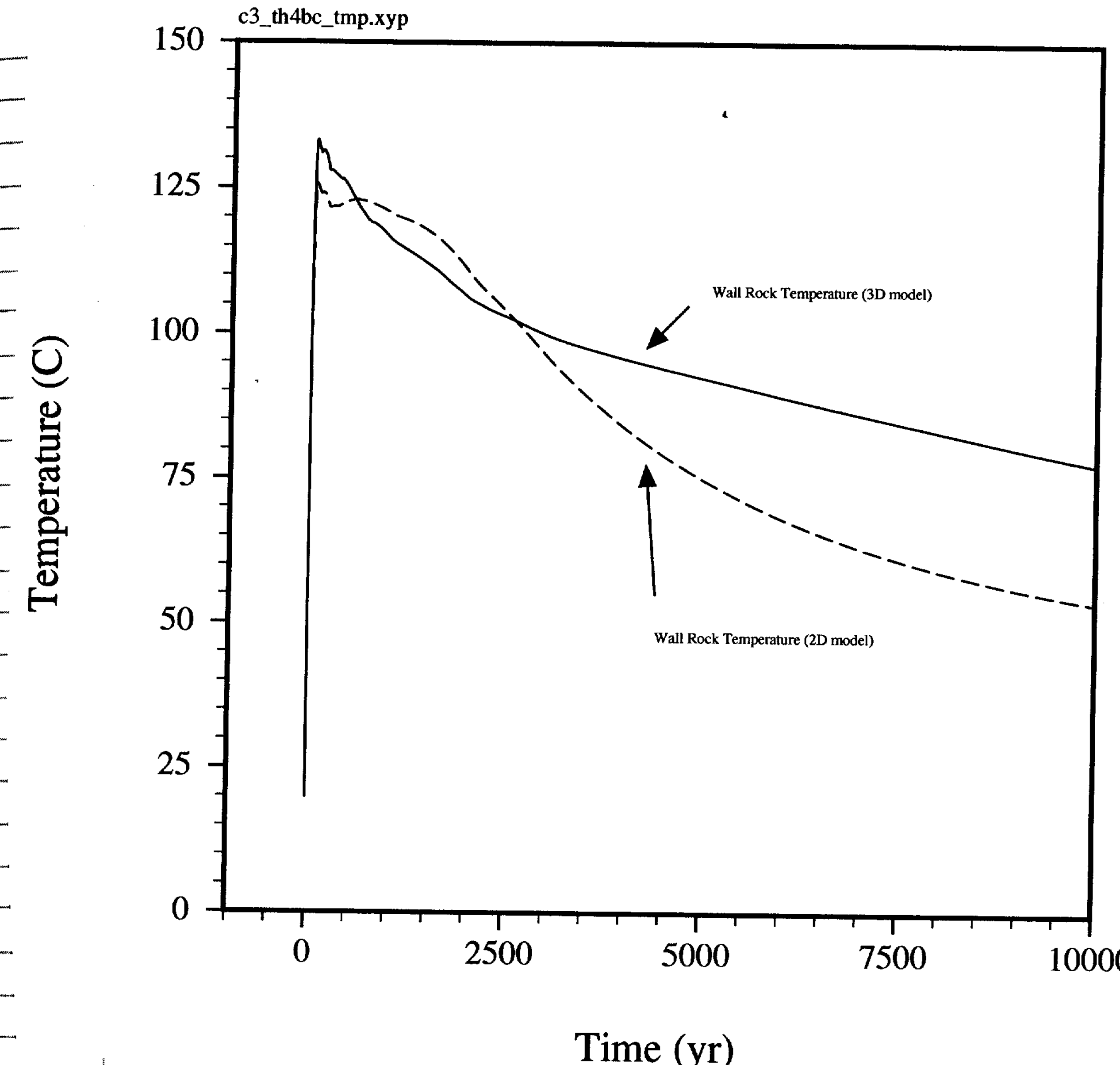



c3big_th2_sat.xyp
Liquid Saturation
1
0.95
0.9
0.85
0.8
0
5000
10000
Time (yrs)
Top Submodel Boundary (z = -240 m)
Bottom Submodel Boundary (z = -440 m)
Note: Results obtained from full-scale 3D model (c3big_th2.dat)


c3big_th2_press.xyp
Note: Results obtained from full-scale 3d model (c3big_th2.dat)
Gas Pressure (Pa)
150000
140000
130000
120000
110000
100000
0
5000
10000
Time (yrs)
Top Submodel Boundary (z = -240 m)
Bottom Submodel Boundary (z = -440 m)

Run #4 described on page 33 with the 3D submodel was rerun incorporating the new time varying top and bottom boundary conditions. (Note: only 50 data pts could be incorporated in to the BCON command). The new data file was labeled c3-th4bc.dat. Run completed ok overnight. The following 2 figures show comparisons between the 3D and 2D model results for temps variation with time at the waste package and wall of tunnel.





The following plots show comparisons between the 2D and 3D models at times 100, 1000, and 10,000 yrs. The 3D model data file was c3-th4bc.dat. Again, the 2D model incorporated all hydrologic units (PTn, TSw2, etc) as well as all thermal and hydrologic properties of the air, waste package and backfill. The 3D submodel included all thermal properties of TSw2, air backfill, and waste package, except hydrologic properties set to TSw2 throughout, although the gas saturation within drift was set to 99.9%. As a result after 10000 yrs, the 3D model shows the saturation increasing within drift during cool down period, simply because the capillary barrier with air in drift is not simulated.

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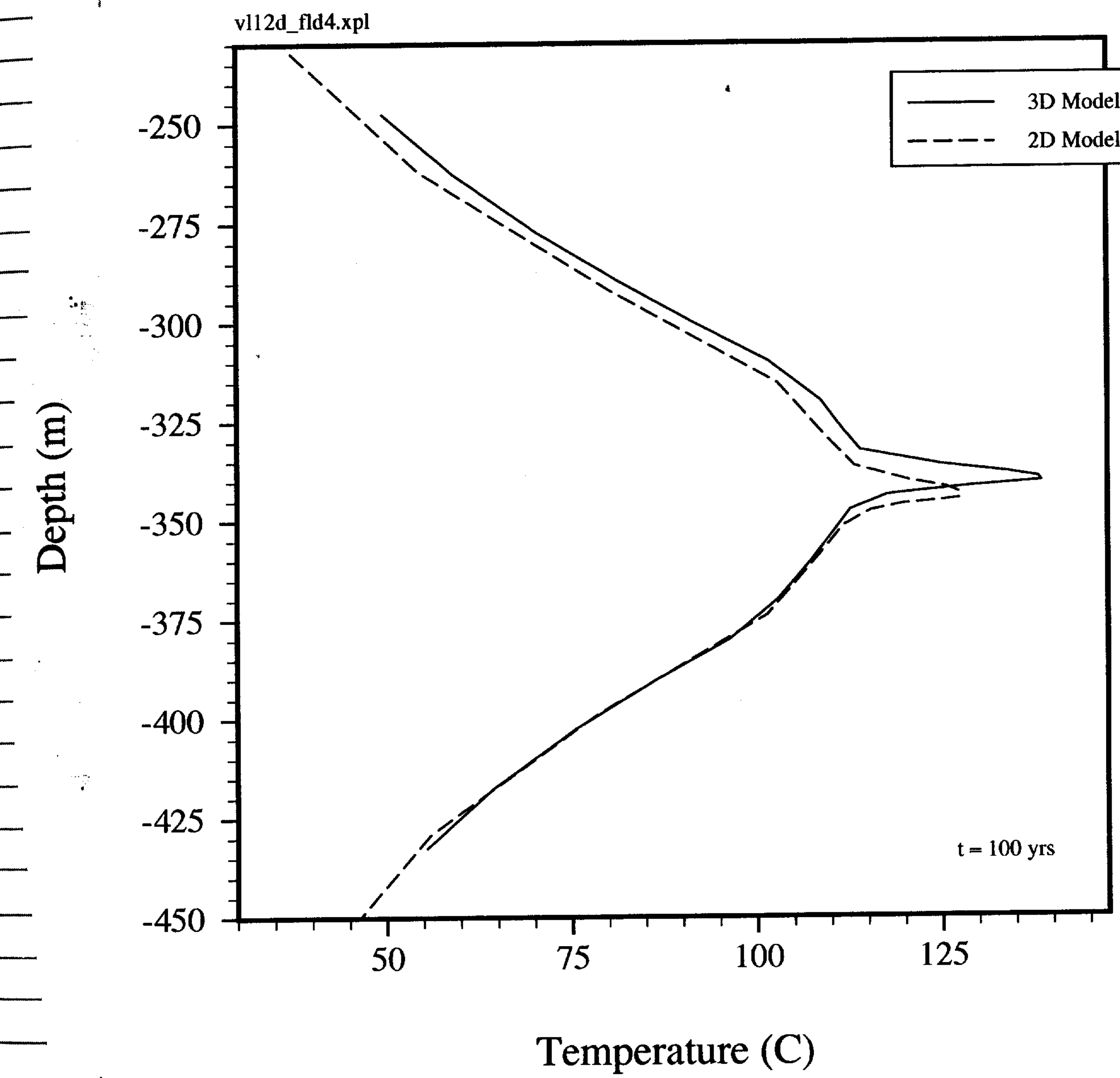
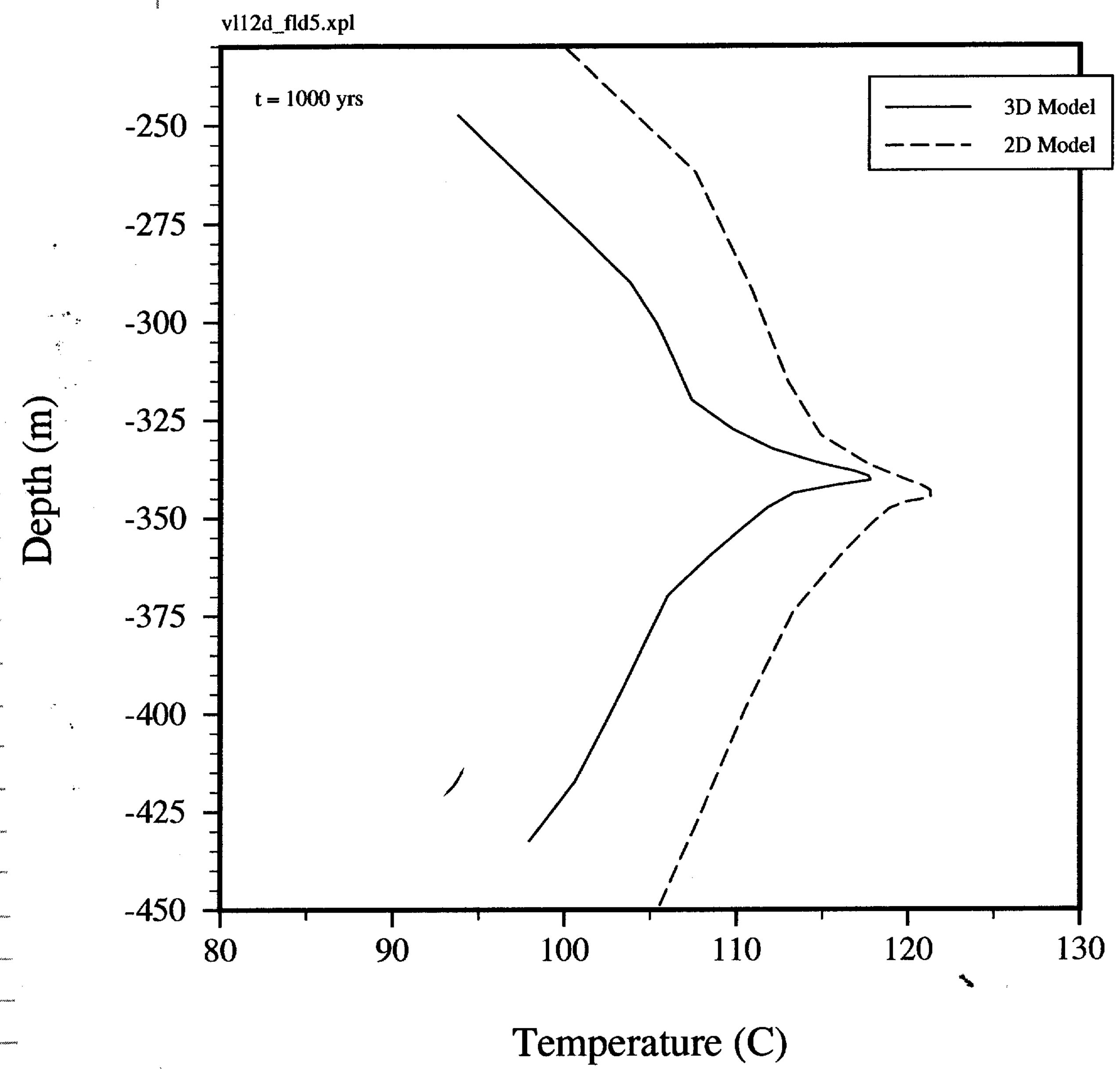
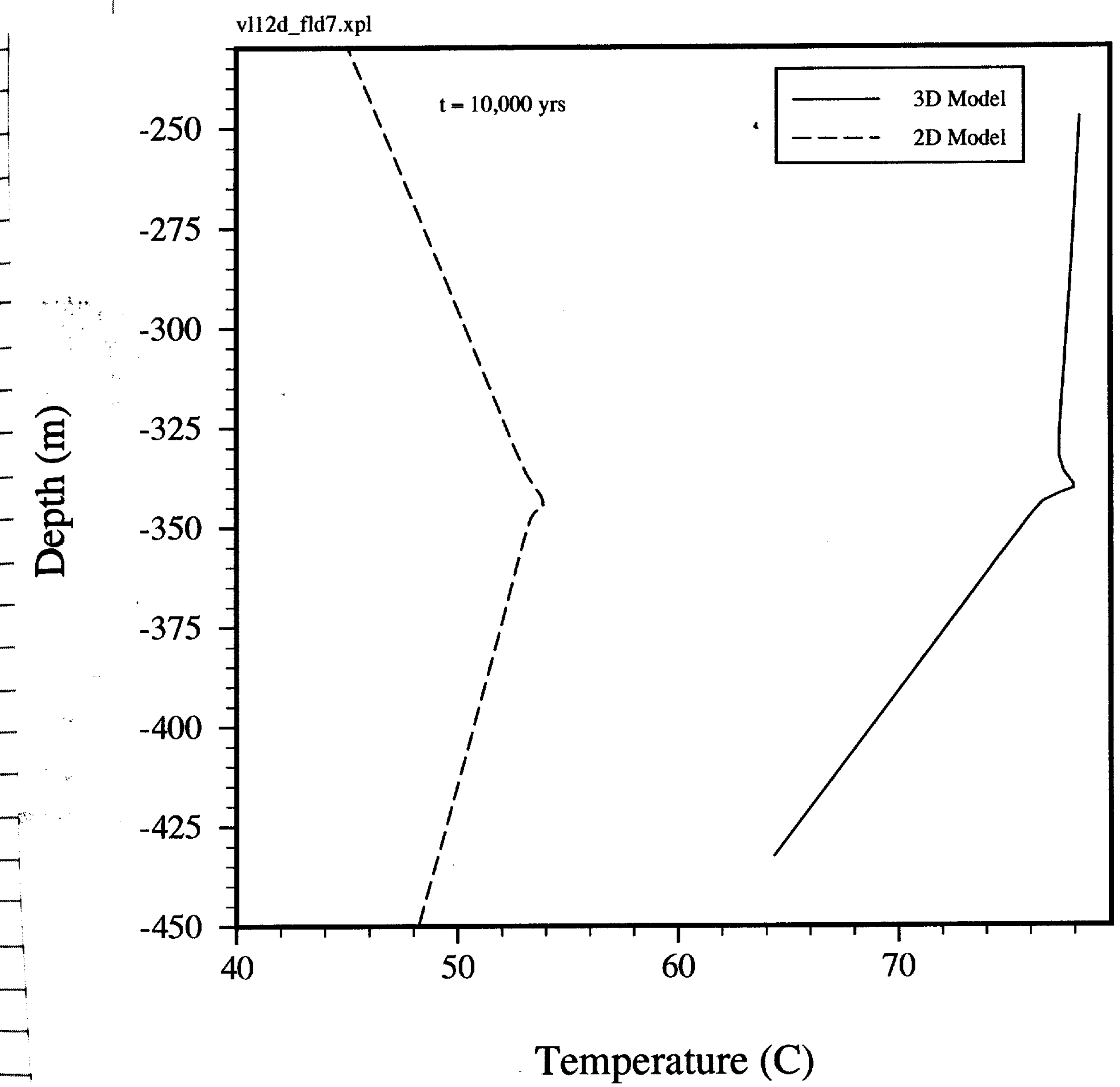
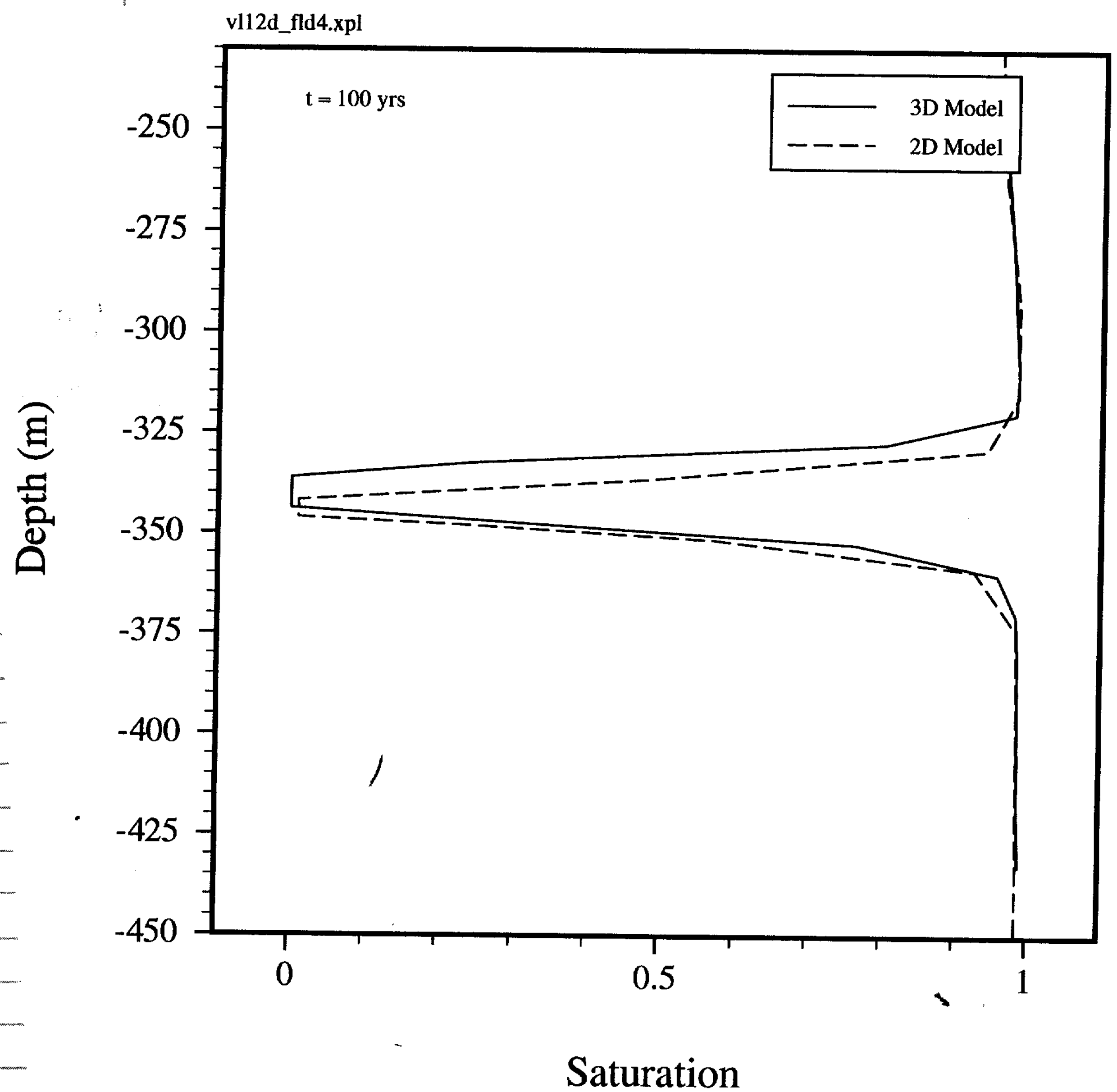
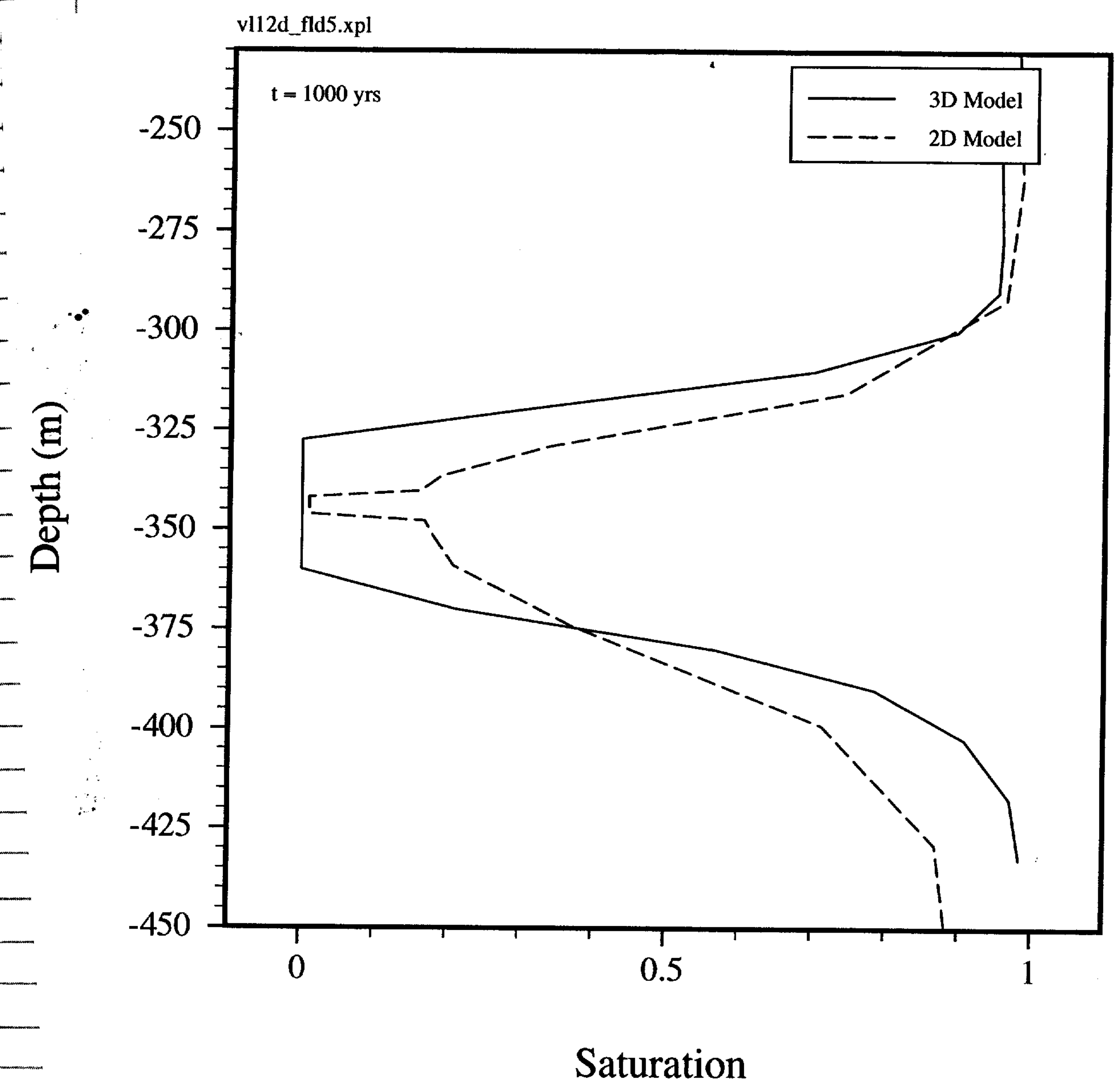



vl12d_fld5.xpl
t = 1000 yrs
3D Model
2D Model
Depth (m)
-250
-275
-300
-325
-350
-375
-400
-425
-450
80
90
100
110
120
130
Temperature (C)

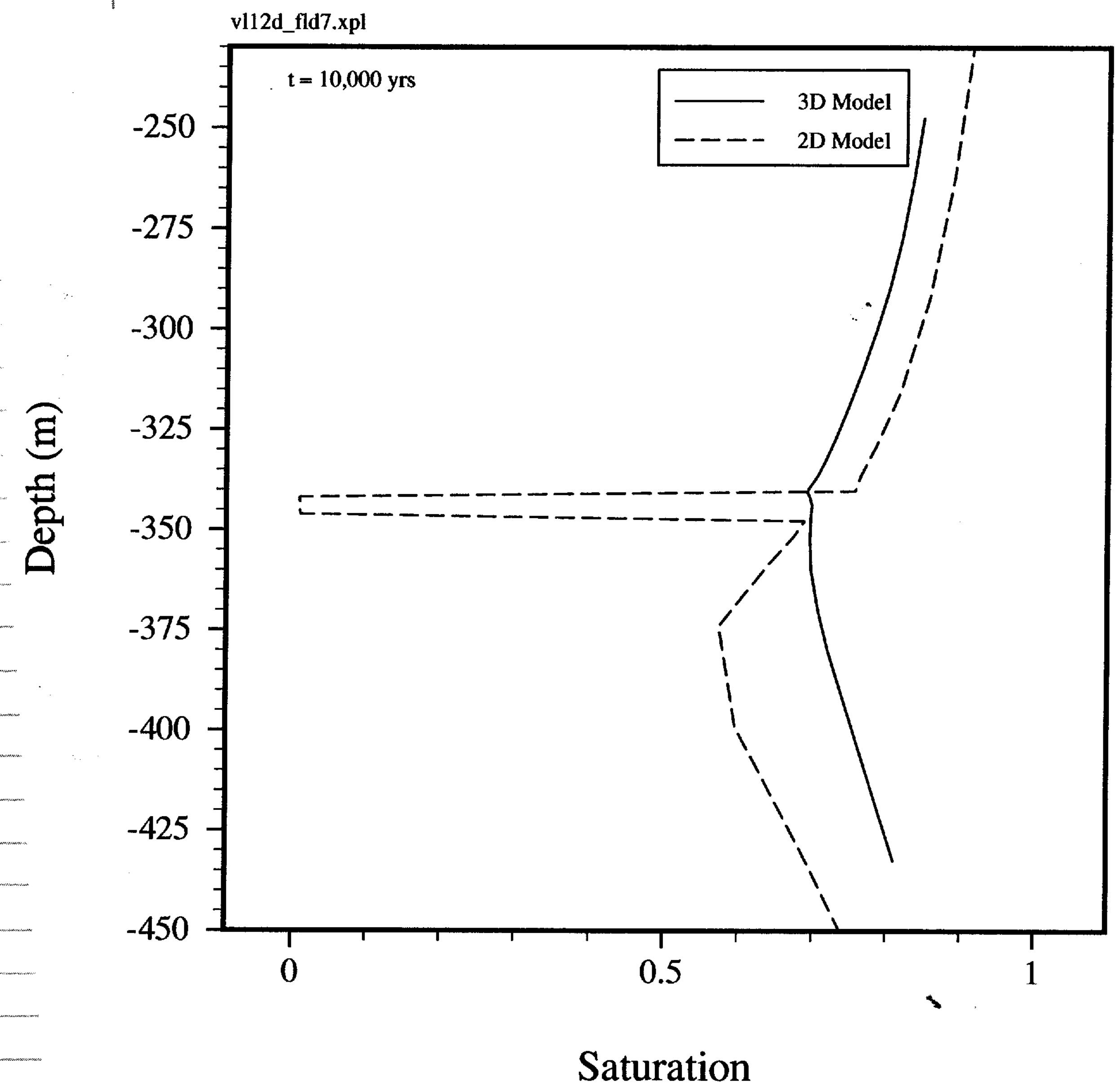

vl12d_fld7.xpl
t = 10,000 yrs
3D Model
2D Model
Depth (m)
-250
-275
-300
-325
-350
-375
-400
-425
-450
40
50
60
70
Temperature (C)



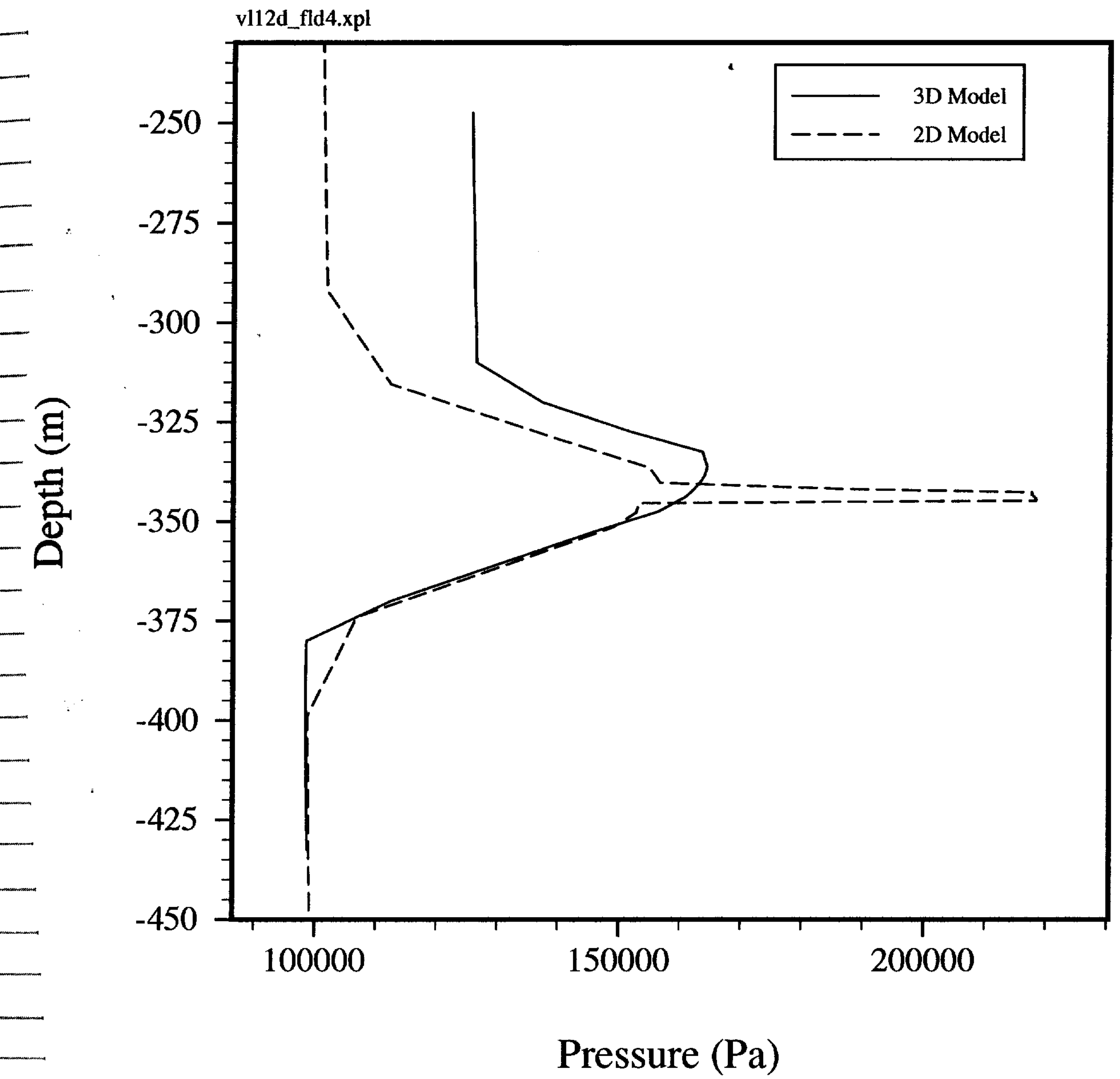
vl12d_fld4.xpl
t = 100 yrs
3D Model
2D Model
Depth (m)
-250
-275
-300
-325
-350
-375
-400
-425
-450
0
0.5
1
Saturation

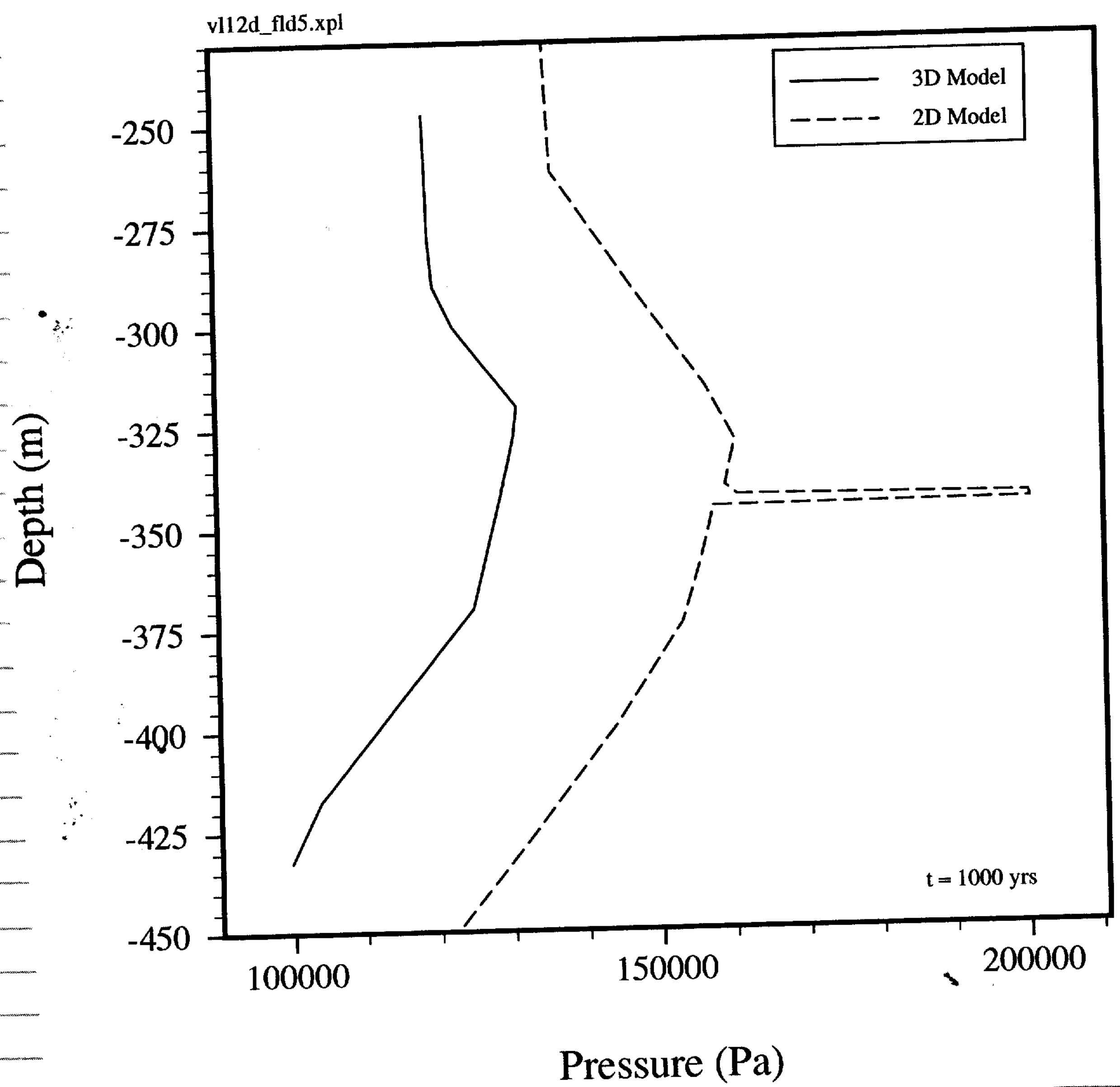


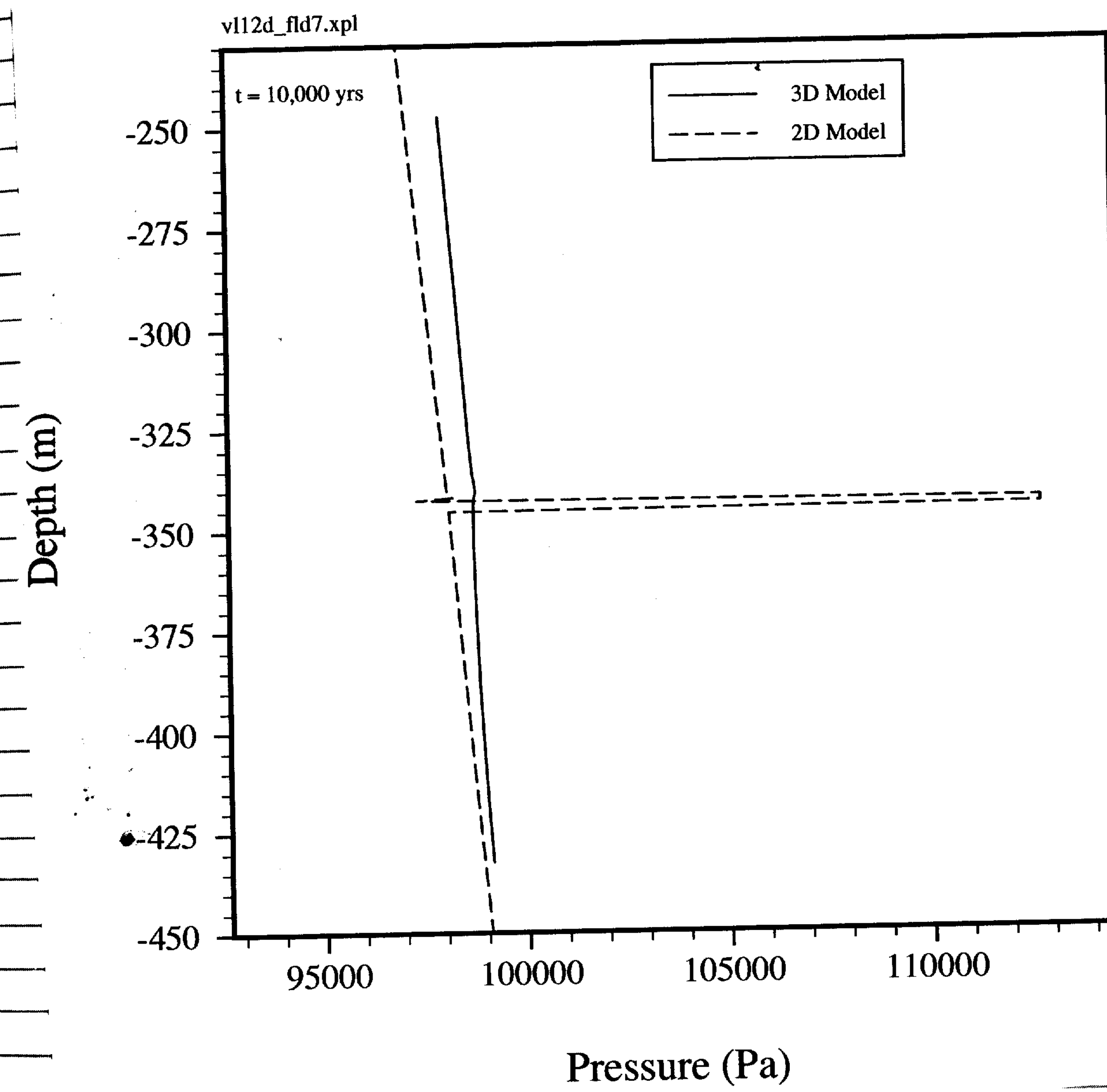
vl12d_fld5.xpl
t = 1000 yrs
3D Model
2D Model
Depth (m)
-250
-275
-300
-325
-350
-375
-400
-425
-450
0
0.5
1
Saturation


vl12d_fld7.xpl
t = 10,000 yrs
3D Model
2D Model
Depth (m)
-250
-275
-300
-325
-350
-375
-400
-425
-450
0
0.5
1
Saturation

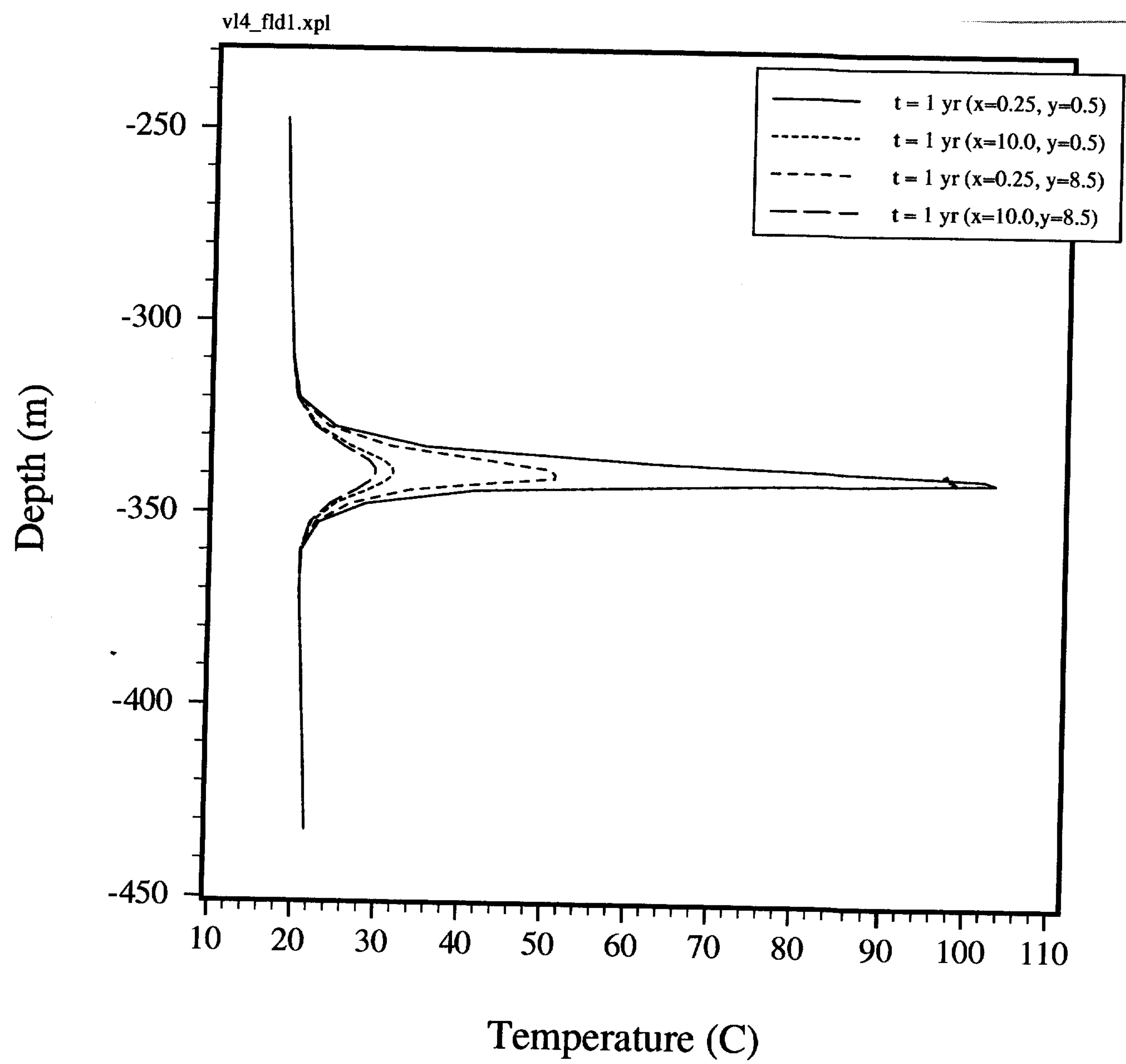
100 years

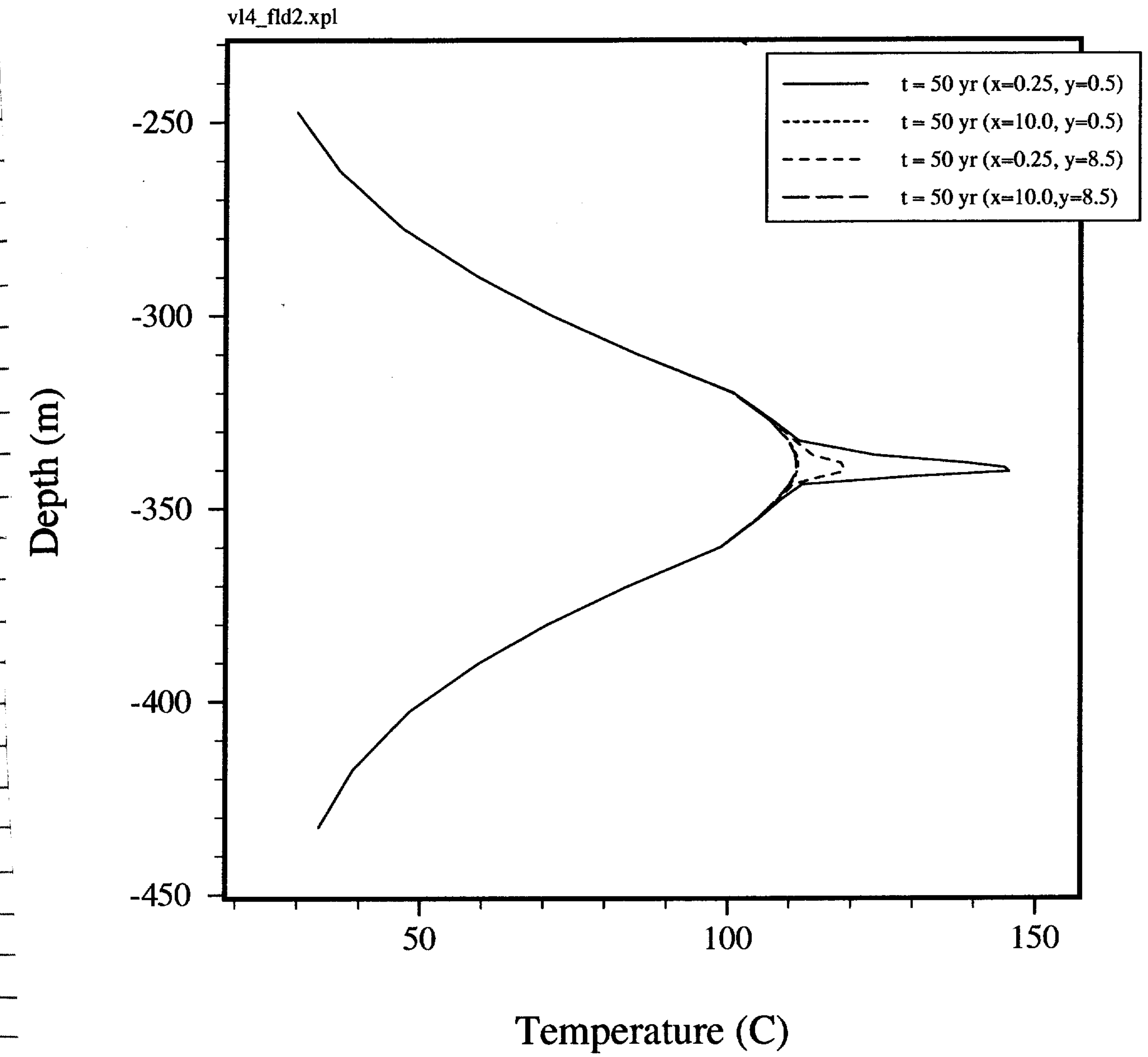

vl12d_fld4.xpl
3D Model
2D Model
Depth (m)
-250
-275
-300
-325
-350
-375
-400
-425
-450
100000
150000
200000
Pressure (Pa)

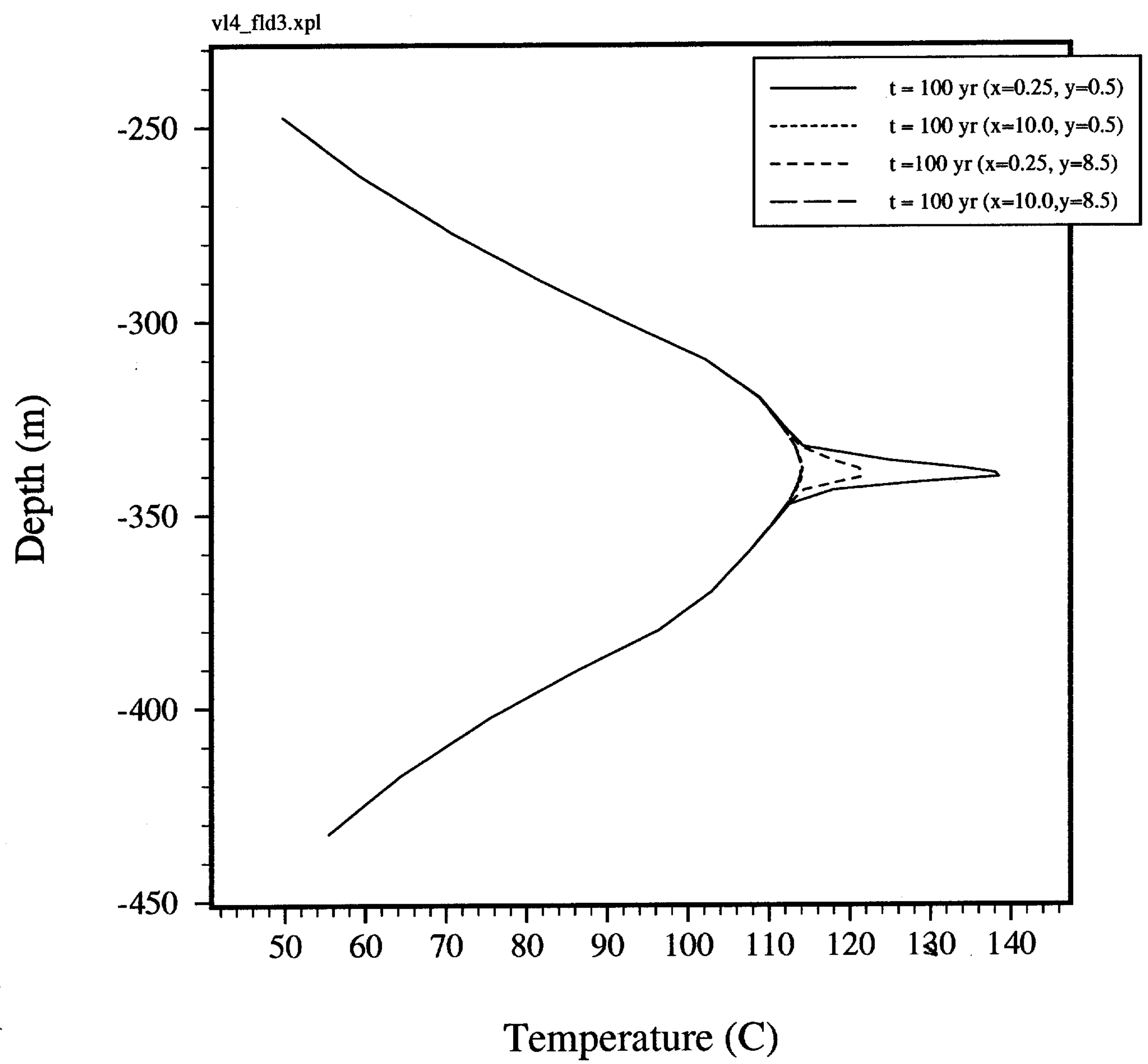

vl12d_fld5.xpl
3D Model
2D Model
t = 1000 yrs
Depth (m)
-250
-275
-300
-325
-350
-375
-400
-425
-450
100000
150000
200000
Pressure (Pa)

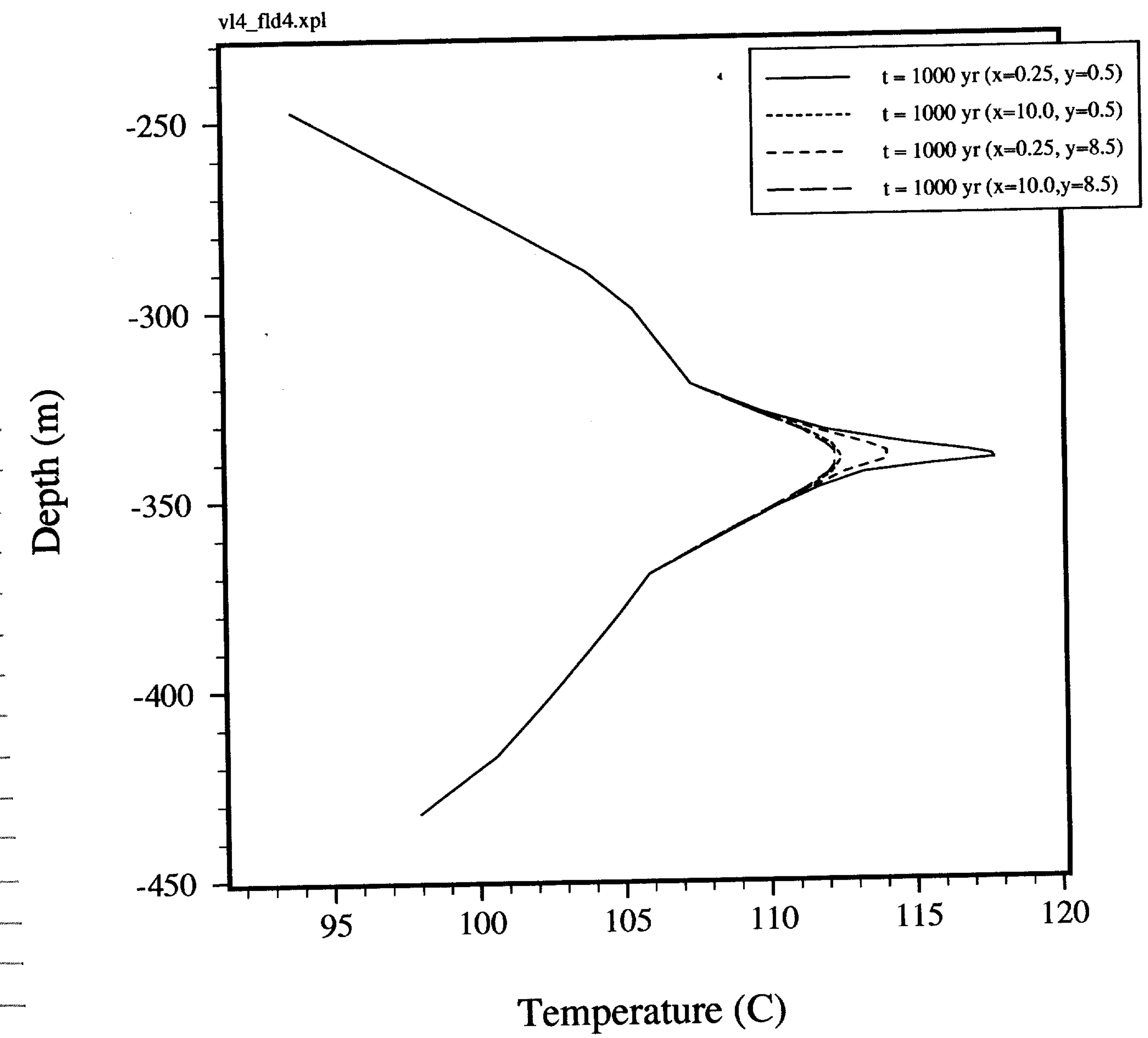

vl12d_fld7.xpl
t = 10,000 yrs
3D Model
2D Model
Depth (m)
-250
-275
-300
-325
-350
-375
-400
-425
-450
95000
100000
105000
110000
Pressure (Pa)

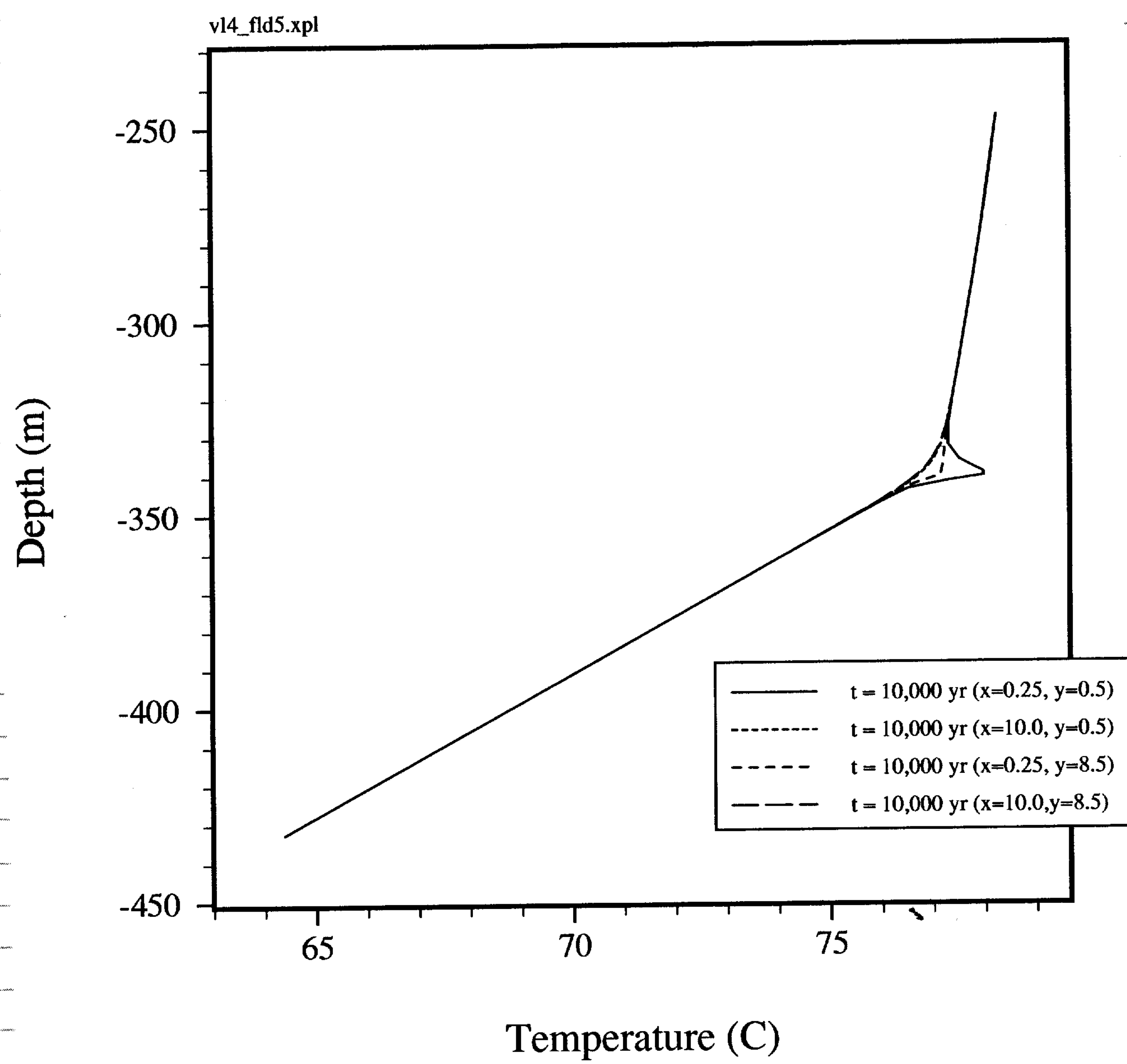
The following set of plots show a revised and improved 3D model run [data file — C3-th5bc.dat] in which the hydrologic properties of the air are modeled in addition to TSw2. Air porosity was set to 99.90% and the permeability several orders of magnitude less than TSw2 [i.e. 1.e-20 m²]. Results are plotted at times t=1, 50, 100, 1000, & 10,000 yrs] along vertical lines at all 4 corners of the 3D submodel.

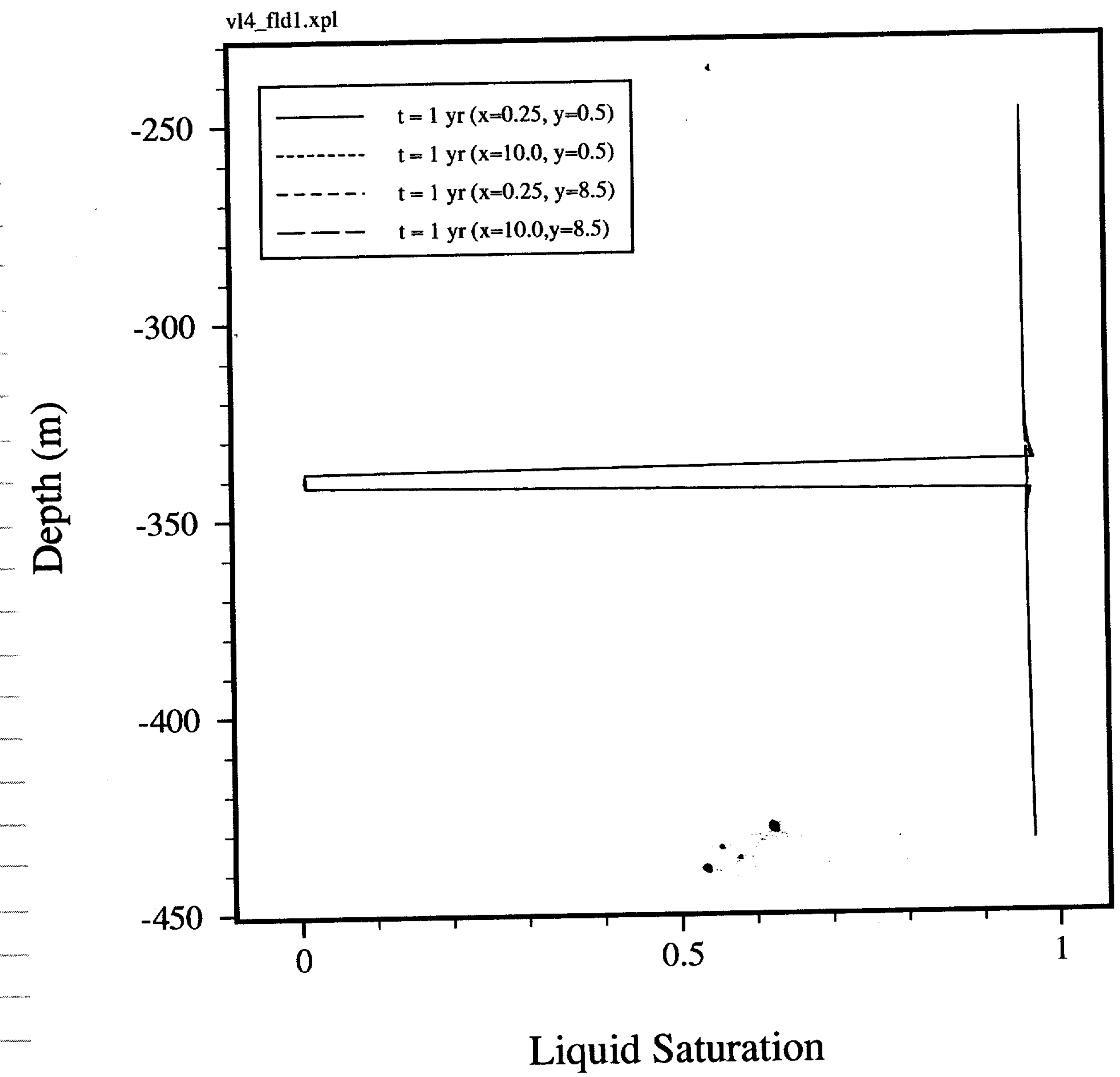


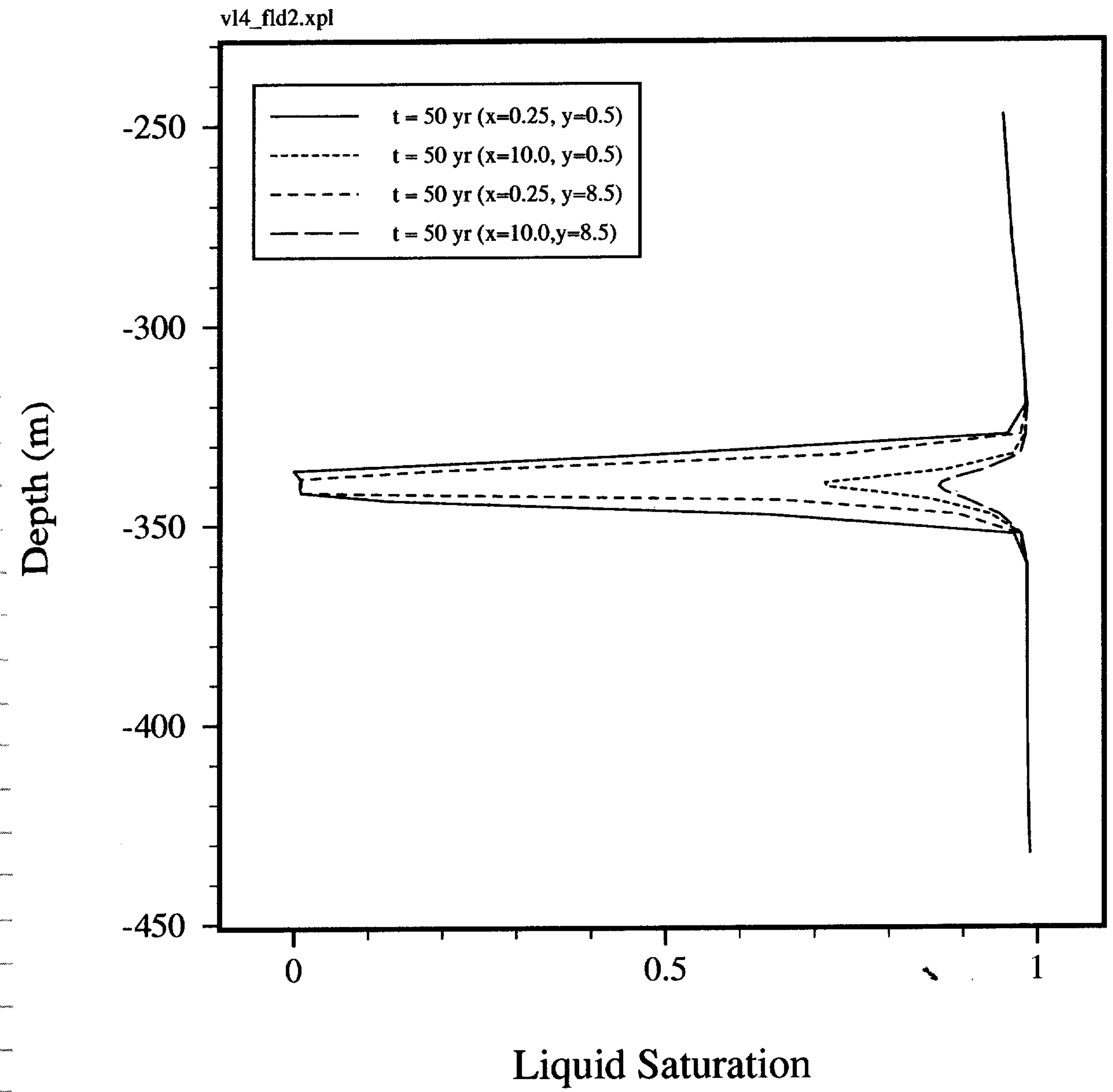


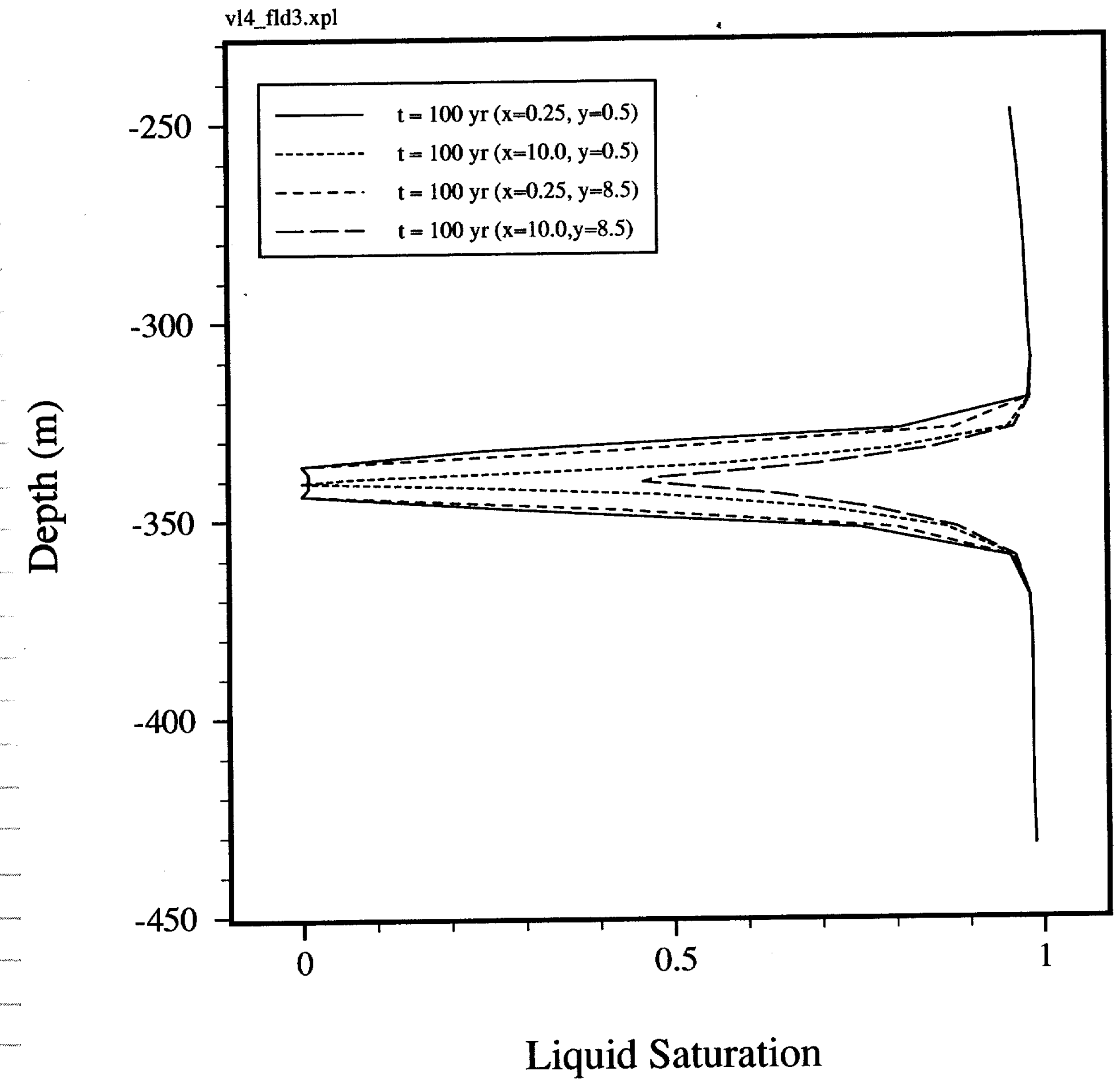

vl4_fld3.xpl
t = 100 yr (x=0.25, y=0.5)
t = 100 yr (x=10.0, y=0.5)
t =100 yr (x=0.25, y=8.5)
t = 100 yr (x=10.0,y=8.5)
Depth (m)
-250
-300
-350
-400
-450
50 60 70 80 90 100 110 120 130 140
Temperature (C)


vl4_fld4.xpl
t = 1000 yr (x=0.25, y=0.5)
t = 1000 yr (x=10.0, y=0.5)
t = 1000 yr (x=0.25, y=8.5)
t = 1000 yr (x=10.0,y=8.5)
Depth (m)
-250
-300
-350
-400
-450
95 100 105 110 115 120
Temperature (C)

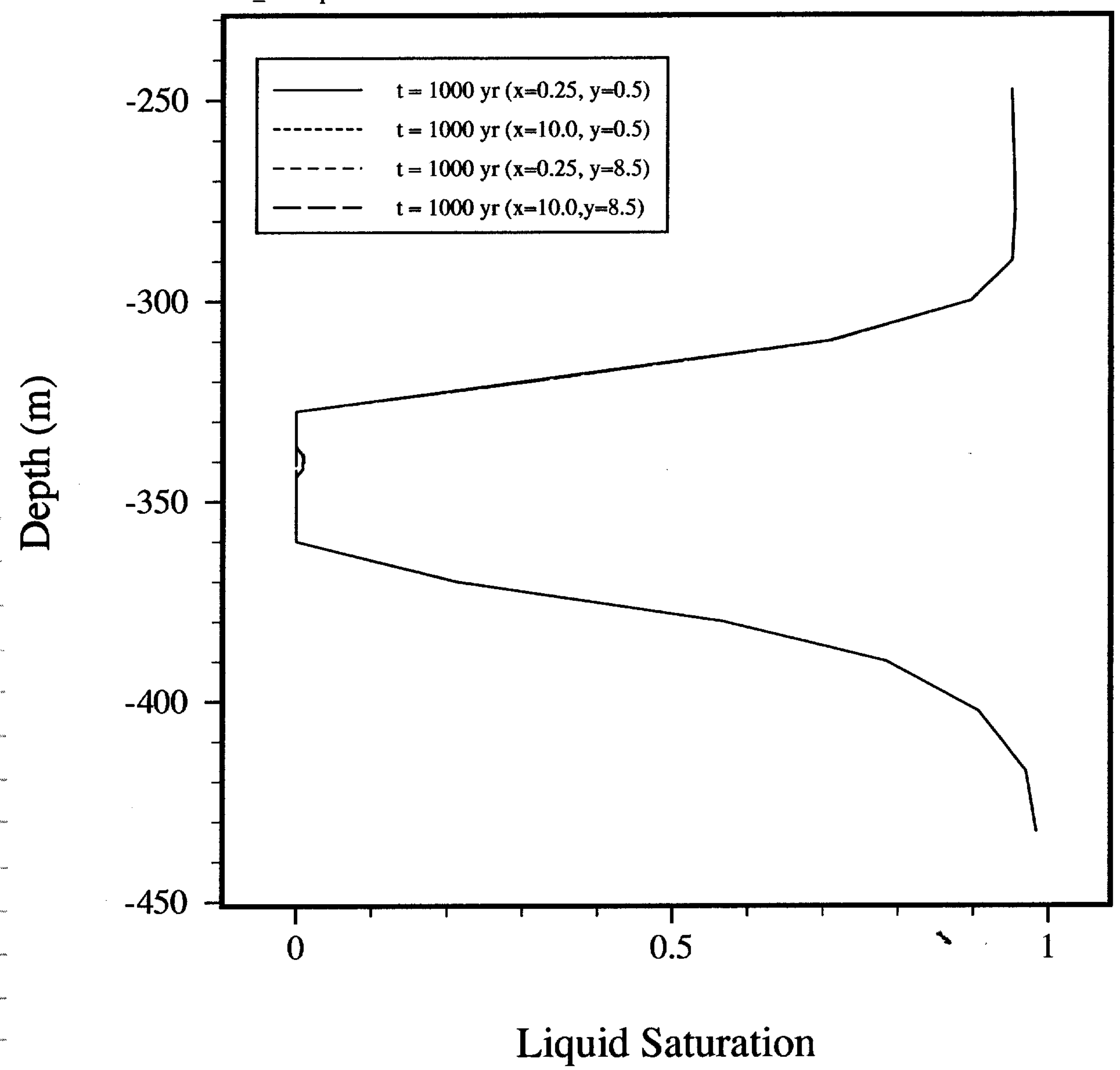

vl4_fld5.xpl
Depth (m)
-250
-300
-350
-400
-450
65
70
75
Temperature (C)
t = 10,000 yr (x=0.25, y=0.5)
t = 10,000 yr (x=10.0, y=0.5)
t = 10,000 yr (x=0.25, y=8.5)
t = 10,000 yr (x=10.0,y=8.5)


vl4_fld1.xpl
Depth (m)
-250
-300
-350
-400
-450
0
0.5
1
Liquid Saturation
t = 1 yr (x=0.25, y=0.5)
t = 1 yr (x=10.0, y=0.5)
t = 1 yr (x=0.25, y=8.5)
t = 1 yr (x=10.0,y=8.5)

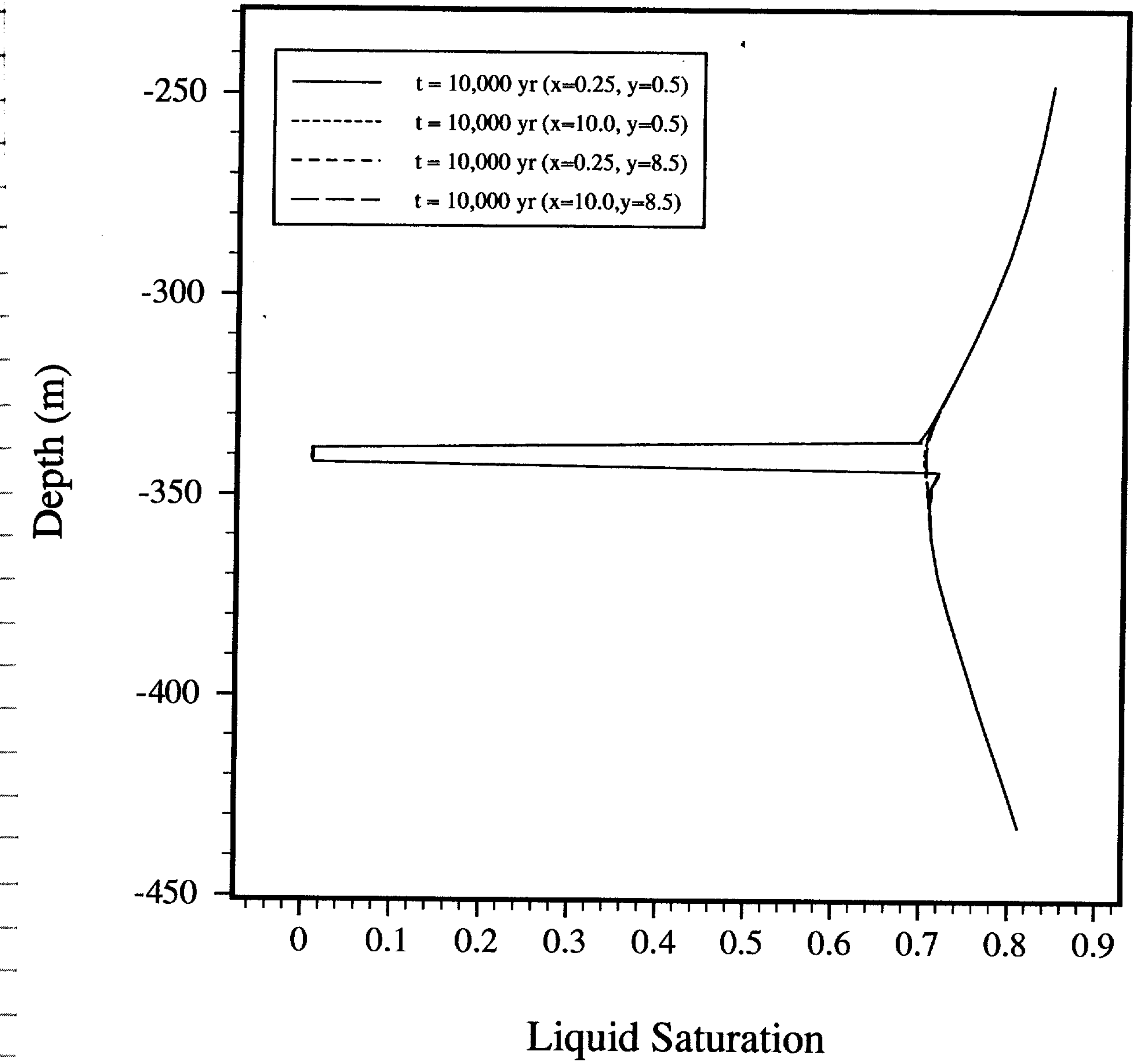

vl4_fld2.xpl
t = 50 yr (x=0.25, y=0.5)
t = 50 yr (x=10.0, y=0.5)
t = 50 yr (x=0.25, y=8.5)
t = 50 yr (x=10.0,y=8.5)
Depth (m)
-250
-300
-350
-400
-450
0
0.5
1
Liquid Saturation


vl4_fld3.xpl
t = 100 yr (x=0.25, y=0.5)
t = 100 yr (x=10.0, y=0.5)
t = 100 yr (x=0.25, y=8.5)
t = 100 yr (x=10.0,y=8.5)
Depth (m)
-250
-300
-350
-400
-450
0
0.5
1
Liquid Saturation

vl4_fld4.xpl



vl4_fld5.xpl



I have reviewed This Scientific notebook and find it in compliance with QAP-001. There is sufficient information regarding procedures used for conducting tests, acquiring and analyzing data so that another qualified individual could repeat the activity.

[signature]

5/30/2000

Manager - MGPE