Volume VIII – TEF Edge Effect

8/9/02 RF

Initial Entry

In order to help Chandrika Manepally describe the edge effect in thermohydrologic modeling of the repository drifts, I had the conduction model extracted out of TPA so that we could compare it directly to Chandrika's MathCad mountain scale conduction model. This was the MathCad conduction model she inherited from Debra Hughson and has been trying to verify and correct all year. Her initial comparisons showed that the TPA code was running 20 C cooler than her MathCad sheet at early times, but that the comparison curves had crossed over by 10,000 years.

George Adams extracted the code segment from TPA 4.2 that calculates the temperature history for each subarea. We then modified it to calculate the temperature profile along a drift at a specified time. George's validation check was against the TPA code output and all of our modifications for the condxyzt driver are recorded in his scientific notebook as follows:

George Adams: Scientific Notebook # 532e

Initial entries: page 3; In-process Entries (for building the driver and verification testing) on pages 4 and 5.The scientific notebook is 532E-Vol2.

Chandrika Manepally: Scientific Notebook #478e

My working directories are:

Bubo (WinNT box) E:\TEF_kti\Chandrika RF 12/12/05
~~Bubo (WinNT box): E:\TEF-EdgeEffect*~~ Bubo (WinNT box): E:\AVData\TEF-EdgeEffect*
Spock (SUN) ~rfedors/EdgeEffect/

Primary computer running WindowsNT 4.00.1381 is called bubo (Acer, x86 Family 6 Model 4 Stepping 2; AT compatible with 512 MBytes RAM).

ArcView version 3.2a
ArcExplorer version 2.0.800
Adobe Acrobat & Distiller version 5.0
Adobe Illustrator 8.0
Adobe Photoshop version 5.0.2
Corpscon version 5.11.08 (U.S. Army Corps of Engineers)
ENVI version 3.6
Excel 97 SR-2
HYDRUS-2D version 2.05
Lahey/Fujitsu Fortran 95 version 5.0
MathCad 2000
Mathematica version 4.2.0.0
MrSID Geospatial Encoder version 1.4
NIST Standard Reference Database 10, version 2.2
Sigma Plot2000 version 6.00

Surfer version 6.04
Word 97 SR-2
Word Perfect version 8.00

UNIX (use uname –X on SUNs and uname -msR) as of March 2003
SGI: Io with a IP27 cpu board, 64-bit, running IRIX64 version 6.5 6.5.14m
ERDAS Imagine version 8.5
Earth Vision 5.1 (Dynamic Graphics)

SUN:
Spock is a SUN sparc Ultra 4 (4 cpu), 64-bit,
running SunOS version (Kernel ID) Generic_108528-17 release 5.8
fortran 77 version 5.0 (SUN Workshop Compiler FORTRAN 77 version 5.0)

Condrive Module

I determined during the work on the condxyzt driver that the drifts in the TPA code were different than the drifts in Chandrika's MathCad sheet. TPA still uses drifts angled at 105 degrees so that they can retain the subarea outlines (TPA still bases the drifts on the top boundary of subareas 1 and 2, which is consistent with old DOE drift designs; TPA didn't particularly care if their drifts lined up with the DOE's drifts, in part, because it doesn't matter given how the TPA treats the heat load). Chandrika used the EDA-II layout with actual coordinates obtained from DOE for the Site Recommendation vintage layout.

Another difference was in the handling of pre-closure ventilation. TPA code separately integrates time= 0 to 50 yr (closure time) and time= 50 to 10,000 yrs (or whatever the time is during post-closure when temperatures are needed). The MathCad conduction model was not integrating the 2nd integral from 50 to 10,000, it instead still integrated from time=0. Since this was not easy to fix, we will go with the extracted conduction model from TPA.

To evaluate if DOE properly incorporated edge effects, by analyzing all the way to the end of the drift (none of their LDTH chimneys are near an edge) or by using the correct lithology (none of their chimneys are in the lower nonlith), we will use the same drifts as Buscheck used in the MSTH model (Rev00 ICN02).

8/16/02

I took Chandrika's drift coordinates
Bubo: E:\TEF_kti\Chandrika\MSTHM_dft1.xls
(EDA-II design) and converted the state plane coordinates to UTM NAD27 (m), then created an input file for the condxyzt driver. The coordinate conversion was done using Corpscon v. 5.11.08.

See file in bubo: E:\TEF_kti\Chandika\MSTHM_dft1.crv, which was exported from worksheet "UTM" in MSTHM_dft1.xls. This file was formatted to read into the condrive.e (extracted conduction model from TPA) as the drifts.dat input file. The drifts.dat file is incorporated here in the table below (see page 3 of volume VIII) for reference.

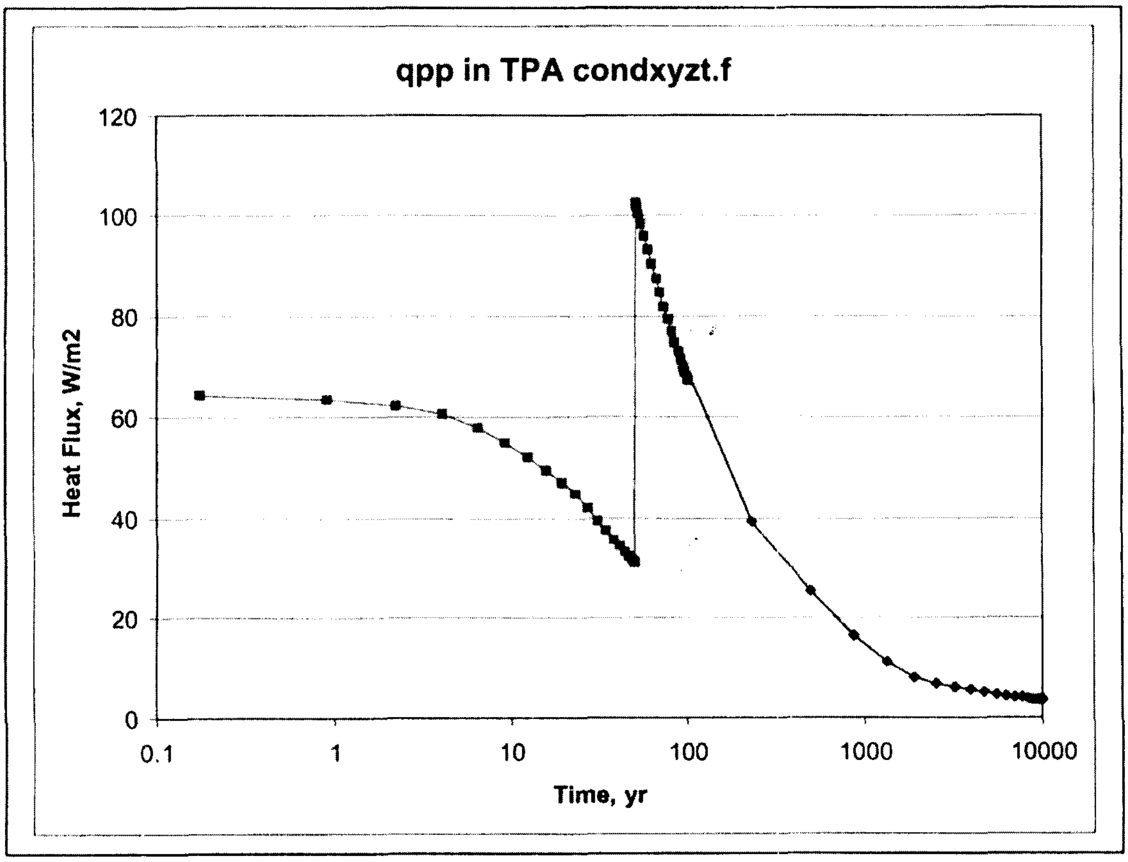
```
TITLE:
**
**
Emplacement Block
           1
**  Drift Endpoints
**   x1              y1              x2              y2          numWP
 5.48664741E+05 4.08090214E+06 5.47846144E+05 4.08116496E+06  1
 5.48661617E+05 4.08086062E+06 5.47817558E+05 4.08113162E+06  2
 5.48655679E+05 4.08077748E+06 5.47760377E+05 4.08106493E+06  3
 5.48651583E+05 4.08069374E+06 5.47727876E+05 4.08099032E+06  4
 5.48647486E+05 4.08061001E+06 5.47716904E+05 4.08090879E+06  5
 5.48643390E+05 4.08052628E+06 5.47712037E+05 4.08082531E+06  6
 5.48639303E+05 4.08044255E+06 5.47707159E+05 4.08074182E+06  7
 5.48635207E+05 4.08035880E+06 5.47702292E+05 4.08065834E+06  8
 5.48631110E+05 4.08027507E+06 5.47697415E+05 4.08057485E+06  9
 5.48627014E+05 4.08019134E+06 5.47692548E+05 4.08049137E+06  10
 5.48622917E+05 4.08010761E+06 5.47687671E+05 4.08040788E+06  11
 5.48618821E+05 4.08002387E+06 5.47683284E+05 4.08032424E+06  12
 5.48614724E+05 4.07994014E+06 5.47679188E+05 4.08024051E+06  13
 5.48610627E+05 4.07985640E+06 5.47675091E+05 4.08015678E+06  14
 5.48606541E+05 4.07977267E+06 5.47670994E+05 4.08007304E+06  15
 5.48602444E+05 4.07968893E+06 5.47666898E+05 4.07998930E+06  16
 5.48598348E+05 4.07960520E+06 5.47662811E+05 4.07990557E+06  17
 5.48594251E+05 4.07952147E+06 5.47658715E+05 4.07982184E+06  18
 5.48590155E+05 4.07943774E+06 5.47654618E+05 4.07973810E+06  19
 5.48586058E+05 4.07935399E+06 5.47645267E+05 4.07965606E+06  20
 5.48581961E+05 4.07927026E+06 5.47618611E+05 4.07957957E+06  21
 5.48577865E+05 4.07918653E+06 5.47588463E+05 4.07950419E+06  22
 5.48573778E+05 4.07910280E+06 5.47558314E+05 4.07942883E+06  23
 5.48569682E+05 4.07901906E+06 5.47528175E+05 4.07935345E+06  24
 5.48565585E+05 4.07893533E+06 5.47504172E+05 4.07927611E+06  25
 5.48561488E+05 4.07885159E+06 5.47495201E+05 4.07919394E+06  26
 5.48557392E+05 4.07876786E+06 5.47486831E+05 4.07911158E+06  27
 5.48553295E+05 4.07868412E+06 5.47478461E+05 4.07902921E+06  28
 5.48549199E+05 4.07860039E+06 5.47470100E+05 4.07894686E+06  29
 5.48545102E+05 4.07851666E+06 5.47461730E+05 4.07886449E+06  30
 5.48541015E+05 4.07843292E+06 5.47453370E+05 4.07878212E+06  31
 5.48536919E+05 4.07834918E+06 5.47445000E+05 4.07869977E+06  32
 5.48532822E+05 4.07826545E+06 5.47436639E+05 4.07861740E+06  33
 5.48528725E+05 4.07818172E+06 5.47428269E+05 4.07853504E+06  34
 5.48524629E+05 4.07809799E+06 5.47419899E+05 4.07845268E+06  35
 5.48520532E+05 4.07801425E+06 5.47411539E+05 4.07837031E+06  36
 5.48516435E+05 4.07793051E+06 5.47403168E+05 4.07828795E+06  37
 5.48512339E+05 4.07784678E+06 5.47394808E+05 4.07820559E+06  38
 5.48508252E+05 4.07776305E+06 5.47386438E+05 4.07812323E+06  39
 5.48504155E+05 4.07767932E+06 5.47378067E+05 4.07804086E+06  40
 5.48500059E+05 4.07759558E+06 5.47369707E+05 4.07795849E+06  41
 5.48495962E+05 4.07751185E+06 5.47372636E+05 4.07787251E+06  42
 5.48491865E+05 4.07742811E+06 5.47387166E+05 4.07778279E+06  43
 5.48487769E+05 4.07734438E+06 5.47401705E+05 4.07769308E+06  44
 5.48483672E+05 4.07726064E+06 5.47416234E+05 4.07760336E+06  45
 5.48479575E+05 4.07717691E+06 5.47430763E+05 4.07751365E+06  46
 5.48475488E+05 4.07709318E+06 5.47445292E+05 4.07742393E+06  47
 5.48471392E+05 4.07700945E+06 5.47459821E+05 4.07733422E+06  48
 5.48467295E+05 4.07692570E+06 5.47474350E+05 4.07724450E+06  49
 5.48463198E+05 4.07684197E+06 5.47488880E+05 4.07715480E+06  50
 5.48459102E+05 4.07675824E+06 5.47503409E+05 4.07706508E+06  51
 5.48457058E+05 4.07671637E+06 5.47510673E+05 4.07702022E+06  52
```

Simulations using condrive.e (see Spock: ~rfedors/EdgeEffect/build/*) for source code and ~rfedors/EdgeEffect/run/* and ./data/* for data inputs) were performed on Spock (SUN). As noted previously, George Adams, scientific notebook 532E, did the verification testing for condrive.e.

The parameters used to do the comparison between condxyzt driver and the MathCad conduction model are (Buscheck's data):
h - ht. of overburden h = 324 m (this changes based on the location and this value is for I4c3)
k = thermal conduction of liquid in saturated rock (host rock - Tsw35) = 2.02 W/m K
Cp = rock specific heat (host rock - Tsw35) = 900 (J/Kg K)
r = rock density=2540 Kg/m^3
AML = areal MTU loading = 938.4 MTU/acre

The integral from Carslaw and Jaeger (1965, Conduction of Heat in Solids) takes "qpp" (TPA terminology) as heat flux input. A plot of this parameter from the condrive.e utility is included below (page 4 of Volume VIII). This plot is stored in the Excel 97 SR-2 spreadsheet E:/TEF_kti/Chandrika/heatFlux.xls

And uses 50 years of ventilation at 70% reduction of AML during ventilation and the thermal parameter values noted above:



Profiles for Drifts 4, 25, 49

Lithologic contacts along drifts were attempted from the faces file of GFM3.1. ISM3.1 and GRM3.1 are the official DOE releases of the Geologic Framework Model 3.1 and Integrated Site Model 3.1. The GFM3.1 faces file is stored at:
(io: /data/3dvis/ISM3.1/GFM3.1/GFM3_1_HiRes.unsliced.faces) by requesting cross-sections from the faces file using Earth Vision 5.1. However, constant Z horizon, well path, and traverse approaches all failed. So I just created 2000 x 2000 resolution images of the appropriate elevations (varies between 3428 and 3612 feet for the drifts). Images for each elevation were saved. The east and west ends of the drifts were specified in the "Manipulate" coordinates minimum and maximum. The coordinates of the drifts were again taken from the Buscheck drifts (MSTHM_dft1.xls file) of the MSTHM AMR Rev00. The output rgb files were cropped, saved as tif files, and world files (*.tfw) files were created. The cropping was done in Photoshop 5.0; the tif format saved used IBM PC ordering and no LZW compression on the tif files. The world file information was based on pixel resolution [number of pixels in each direction (image size) versus actual distances] and state plane coordinates outlining all drifts.

The tif files were read into ArcView 3.2a (since the ERDAS license has been busy). The state plane nad27 outline of the repository and ESF were also displayed in Arc View to verify that I had created the world files correctly.

The project file for ArcView
bubo E:\AVData\TEF-EdgeEffect\edge.apr
and the image files
bubo E:\AVData\TEF-EdgeEffect\Gfm3.1* with elevation as part of the file names

		Drift 4	Drift 25	Drift 49	Drift 52
West End	Easting, ft	559139.4	558385.7	558264.5	558381.2
	Northing, ft	773699.2	768076.2	761409.4	760672.9
East End	Easting, ft	562167.4	561865.0	561519.5	561483.5
	Northing, ft	772715.4	766945.7	760351.8	759665.0
Width of Tptpmn, tsw34	ft	-	950	-	-
Width of Tptpll, tsw35	ft	3096	2705	2588	2376
Width of Tptpln, tsw36	ft	95	-	788	852
Width of Tptpln, tsw37	ft	-	-	56	38
Drift Length (actual)	ft	3183.8	3664.5	3422.4	3261.9

Widths in the table were estimated using the ruler tool in ArcView, and may not necessarily add up to the actual length of a drift (but should be close).

Note that tsw36 and tsw37 have the same thermal properties.

Infiltration Boundary Condition

Used the shallow infiltration results from TPA 4.1j version of ITYM printed out for 30 m pixels and the modern climate (17.38 C and 162.8 mm/yr precipitation). This file and the program used to reformat the data for ArcView were saved in:

E:\AVData\TEF-EdgeEffect\Maidtbl\maidtbl-tpa41j-30m.dat
.\dem.for and dem.exe

The fortran program was last modified in June 2002 while doing performance checking for TPA 5.0.

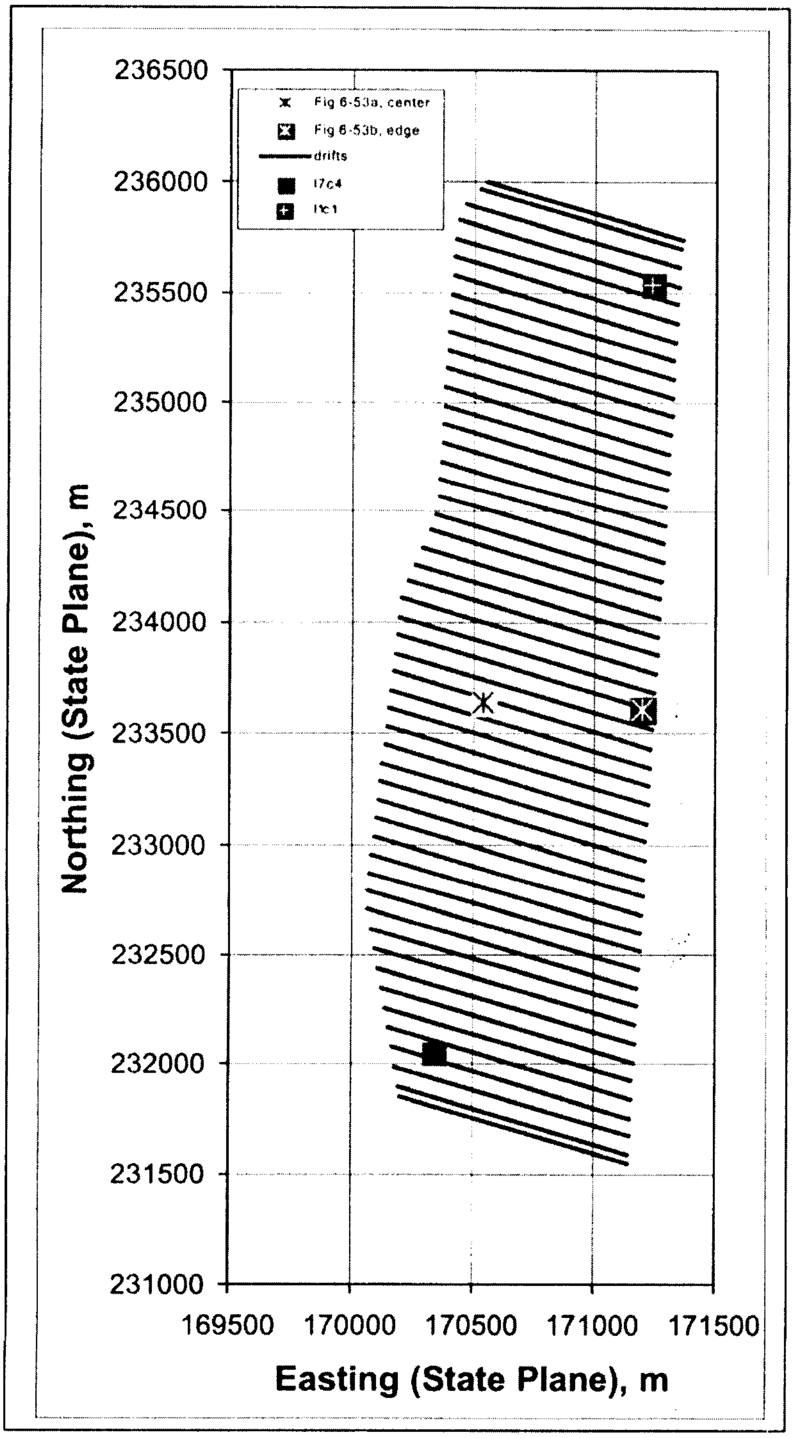
```
C     Last change:  RWF   30 Aug 2002    12:25 pm
        program dem
c Script reformats ITYM external data for input to ArcView in grid format
c
c RFedors  June 4, 2002
c
c23456789 123456789 123456789 123456789 123456789 123456789 123456789 12
      implicit  none
      integer ioread, iowrit, mxx, i, j, k, nrows, ncols
      parameter (mxx=200000)
      real*8 array(mxx,3),  xpos, ypos
      real*8 xllcorner, yllcorner, cellsize
      character*12 file1, file2, fvar, junk
      character*60 header
      character*1 comment

c set input and output unit numbers
      ioread = 7
      iowrit = 8

c read in DEM of infiltration; note that the coordinates of the
c southwest corner of the domain are given in the header, but the
c ordering of data is row-major starting from the northwest corner.

      write(*,1010)
 1010  format(' enter input filename ')
      read(*,'(a12)') file1
      write(*,1013)
 1013  format(' enter output filename ')
      read(*,'(a12)') file2
      write(*,1016)
 1016  format(' enter dependent variable ')
      read(*,'(a12)') fvar

      open(unit = ioread, file = file1, status = 'unknown')

c Note that Stofhoff used 2 or 4 comment lines and flip-flops the
c order of listing NROWS and NCOLS
      k = 0
      do i = 1, 4
         read(ioread,'(a1,a60)') comment, header
         if(comment.ne."N")    k = k+1
      enddo
      rewind(ioread)

      do i = 1, k
          read(ioread,'(a60)') header
      enddo
      read(ioread,'(a5,i10)')  junk, nrows
      if(junk.eq."NROWS") then
         read(ioread,'(a5,i10)') junk, ncols
       else
```

```
         ncols = nrows
         read(ioread,'(a5,i10)') junk, nrows
      endif
      read(ioread,'(a9,f16.6)') junk, xllcorner
      read(ioread,'(a9,f16.6)') junk, yllcorner
      read(ioread,'(a9,f16.6)') junk, cellsize
      read(ioread,'(a60)') header
      read(ioread,'(a60)') header
      read(ioread,'(a60)') header
      print*, ncols, nrows, cellsize, xllcorner, yllcorner

      ypos = yllcorner + cellsize * dfloat(nrows-1)
      xpos ■ xllcorner
      k = 1
      do i = 1, nrows
        do j = 1, ncols
          read(ioread,*) array(k,3)
          array(k,1) = xpos
          array(k,2) = ypos
          xpos = xpos + cellsize
          k = k + 1
        enddo
        ypos = ypos - cellsize
        xpos = xllcorner
      enddo
      close(ioread)

c write out reformatted data including easting and northing locations
      open(unit=iowrit, file=file2, status='unknown', form='formatted')
c      open(unit=iowrit, file='maidtbl.txt', form='formatted')
      write(iowrit,1050) fvar
      do k = 1, nrows*ncols
         write(iowrit,1080)  array(k,1), array(k,2), array(k,3)
      enddo

 1050  format(' easting,', ' northing, ', a12)
 1080  format(e16.7,",",e16.7,",",e16.7)
      close(iowrit)
      stop
      end
```

Extracted net infiltration (percolation) rates are in the table below. Net infiltration value from the closest cell is recorded in the 4th column. Minimum and maximum values of surrounding cells are recorded in the 5th and 6th columns.

coordinate	easting, m UTM NAD27	northing, m UTM NAD27	percolation mm/yr	min mm/yr	max mm/yr	comment
l1c1	548537.3	4080704.5	6.5	6.0	8.7	
fig 6-53a (center)	547844.8	4078807.9	19.8	14.6	21.2	
Fig 6-53b (edge)	548504.8	4078775.2	9.8	9.4	21.2	adjacent to caprock
our edge (drift 25)	548515.1	4078951.6	9.5	9.2	21.6	adjacent to caprock
our center (drift 25)	548034.2	4079044.1	9.1	7.2	20.5	adjacent to caprock
l7c4	547653.4	4077217.0	19.5	18.3	20.3	caprock

Buscheck's center of repository and edge examples (Figure 6-53a,b of the MSTHM AMR, Rev00 ICN02), as determined from the figure below, are in drifts 27 (edge) and 29 (center). Thus, condrive.e was run for these drifts also. The plot on this page was developed in worksheet "drift plot" of the MSTHM_dft1.xls spreadsheet file.



Drift 52, West End

Extracted geology from ISM3.1 (GFM3.1) using EarthVision version 5.1. The annotation from file and well path file from the cross-section extraction using the following faces file are:

Bubo: E:\TEF-kti\Chandrika\drift52-west.path (well path input file)
Bubo: E:\TEF-kti\Chandrika\drift52-westend.ann (annotation output file)
Io: /data/3dvis/ISM3.1/GFM3.1/GFM31_lores.unsliced.faces

Unit Name	Top Elevation (feet)	Thickness (feet)
tcw11	none	
tcw12	4832.8	294.5
tcw13	4538.3	27.6
ptn21	4510.7	11.6
ptn22	4499.1	7.6
ptn23	none	
ptn24	4491.5	16.2
ptn25	4475.3	6.5
ptn26	4468.8	35.1
tsw31	4433.7	1.1
tsw32	4432.6	89.8
tsw33	4342.8	128.1
tsw34	4214.7	221.5
tsw35	3993.2	285.9
tsw36	3707.3	96.7
tsw37	3610.6	48.3
tsw38	3562.3	48.3
tsw39	3514.0	33.6
ch1	3480.4	42.1
ch2,3,4,5	3438.3	94.6
ch6	3343.7	47.2
pp4	3296.5	23.1
pp3	3273.4	132.1
pp2	3141.3	67.5
pp1	3073.8	218.4
bf3	2855.4	370.1
bf2	2485.3	211.6
tr3	2273.7	448.9
tr2	1824.8	400.6
bottom of Trambt	1424.2	

Assume no ptn23, since the Yucca Tuff is so thin here. Then divide the Yucca Tuff between ptn22 and ptn24. Top of Tpy is at 4494.1 ft elevation; top of Tbt3 is at 4489.0 ft

The grouping of stratigraphic horizons into hydrostratigraphy followed the info in the following table

GFM3.1 Lithology	PMR/AMR vintage Berkeley UZ Model Hydrostratigraphy	Hydrogeologic Unit (Flint, 1998)
Tpcr	tcw11	CCR,CUC
Tpcp	tcw12	CUL,CW
Tpcpv3, Tpcpv2	tcw13	CMW
Tpcpv1	ptn21	CNW
Tpbt4, Tpy	ptn22	BT4
Tpy (welded), present if >10m thick	ptn23	TPY
Tpy, Tpbt3	ptn24	BT3
Tpp(Pah)	ptn25	TPP
Tpbt2, Tptrv3, Tptrv2	ptn26	BT2
Tptrv1	tsw31	TC
Tptrn	tsw32	TR
Tptrl, Tptrf, Tptul	tsw33	TUL
Tptpmn	tsw34	TMN
Tptpll	tsw35	TLL
Tptpln (upper 2/3)	tsw36	TM2
Tptpln (lower 1/3)	tsw37	TM1
Tptpv3	tsw38	PV3
Tptpv2	tsw39	PV2
Tptpv1,Tpbt1	ch1	BT1a, BT1
Calico	ch2, ch3, ch4, ch5	CHV or CHZ
Calicobt (Thtbt)	ch6	BT
Prowuv (Tcpuv)	pp4	PP4
Prowuc (Tcpuc)	pp3	PP3
Prowmd (Tcpm), Prowlc (Tcplc)	pp2	PP2
Prowlv, Prowbt, Bullfroguv	pp1	PP1
Bullfroguc,Bullfrogmd,Bullfroglc	bf3	BF3
Bullfroglv, Bullfrogbt, Tramuv	bf2	BF2
Tramuc, Trammd, Tramlc	tr3	-
Tramlv, Trambt	tr2	-
Tund, Paleozoic		

Calculation of Net Infiltration for All Climates

Use scripts from sci ntbk #432e, Volume VI, pages 1-8. Specifically, extract.f to get net infiltration values from dem-style output of ITYM. The modern, monsoon, and glacial transition net infiltration maps were created back in July 2001 (sci ntbk #432, Volume VI).

I see that I wrote extract.f to read in "maidtbl.out." Hence, I have to copy whichever climate infiltration map to "maidtbl.out" to get values of different climates. Putting the new coordinates in the tefd.txt file, all climates were rerun (modern.m, glacial.lb, glacial.ub, and monsoon.ub were all used as maidtbl.dat)

Calculations were collated in the "chimney coord" worksheet of file:
bubo: E:\TEF-kti\Chandrika\ConductionModelCalc\MSTHM_dft1.xls

	Fig 6-53a, center	Fig 6-53b, edge	our edge, dft-25	I1c1	I4c1	I4c3	I7c4
	center	edge	drift 25				
	MAI mm/yr	MAI mm/yr	MAI mm/yr	MAI mm/yr	MAI mm/yr	MAI mm/yr	MAI mm/yr
modern lower-bound	6.2	2.9	3.0	2.0	6.9	2.8	6.1
modern mean	13.2	6.3	6.4	4.3	14.7	6.0	13.0
modern upper-bound	20.2	9.6	9.8	6.7	22.5	9.2	19.9
monsoon lower-bound	13.2	6.3	6.4	4.3	14.7	6.0	13.0
monsoon mean	37.6	18.9	19.0	14.5	39.9	18.2	37.5
monsoon upper-bound	62.1	31.6	31.6	24.7	65.0	30.3	61.9
glacial lower-bound	24.6	12.6	12.7	9.4	26.4	12.2	24.4
glacial mean	57.7	32.8	33.0	26.8	59.2	32.2	57.8
glacial upper-bound	90.8	53.1	53.2	44.1	92.1	52.2	91.2

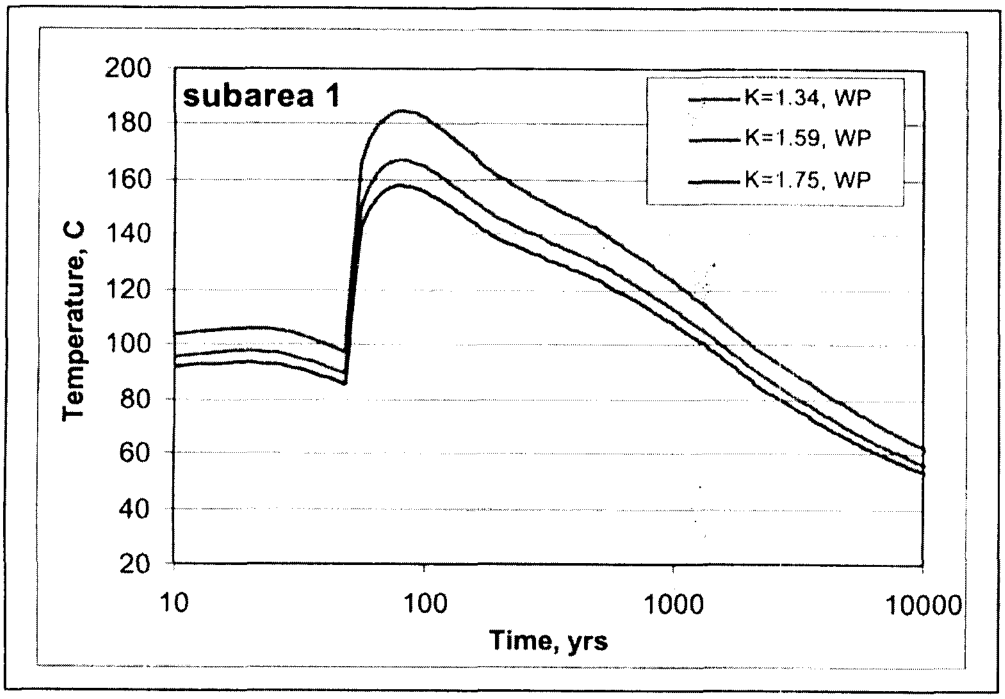
November 6, 2002

MRS Paper with Sitakanta and Chandrika

I ran the TPA 4.1j code and pulled temperatures and relative humidity at the waste package. The uncertainty distribution for thermal conductivity were used (i.e., lower bound, mean, and upper bound). These values were 1.34, 1.59, and 1.75 W/mK. Chandrika compared her thermohydrologic results with the TPA results to help us judge the reasonableness of the TPA range when the hydrologic effects on temperature are included. The plots (figure VIII-12a,b) contributed to the Material Society Paper by Mohanty, Fedors, Manepally, and Esh. Subarea 1 data was used because the center of subarea 1 is essentially a center location for the repository. The driftwall data for these 3 thermal conductivity values are from the same file (temprep heading in the spreadsheet, tempwp is waste package temperature in degrees C).

TPA 41.j files saved in spock: ~/EdgeEffects/Oct21_2002/run/TPA/*;
Excel file w/ TPA4.1j data bubo: E:\TEF-kti\Chandrika\ConductionModelCalc\condrive-MRS.xls

Figure VIII-12a. Waste package temperatures for different effective thermal conductivity values.



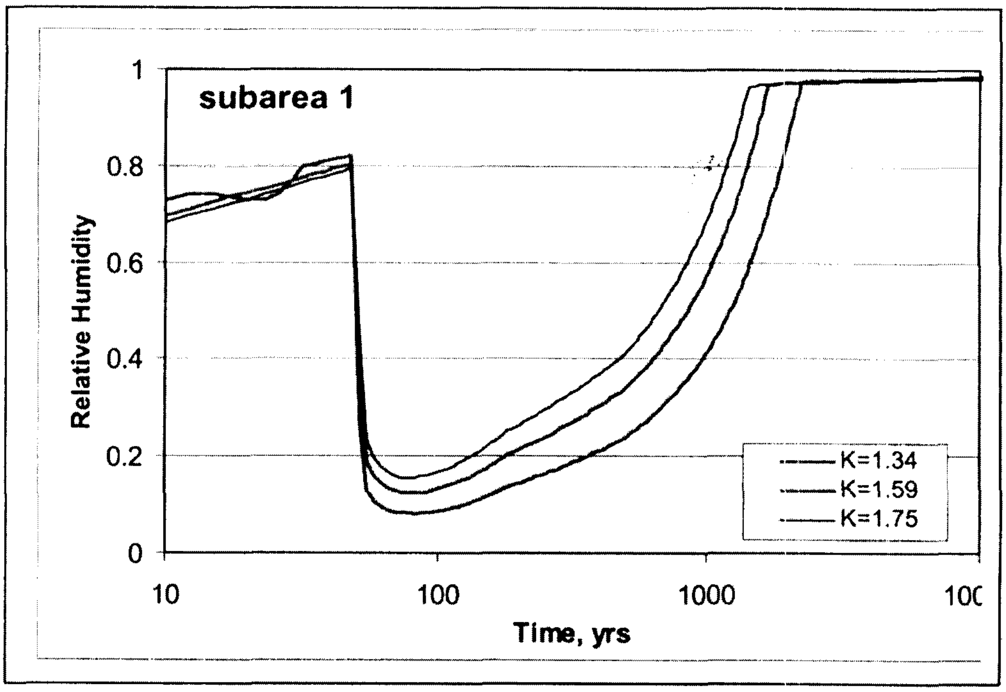


Figure VIII-12b. Waste package relative humidity for different effective thermal conductivity.

November 20, 2002

Condrive Temperature Calculations

A filter scans through the condrive.e output to extract estimates of the drift portion that see a significant temperature difference compared to the drift center. This fortran script is drift.f.

Created on using Lahey Fortran 95 on a laptop (Dell, CNWRA #2592) while on travel. Transferred to the bubo, where it still ran correctly.

bubo: E:\TEF-kti\Chandrika\Code\drift.f
bubo: D:\TEF-kti\Chandrika\ConductionModelCalc\condrive11Nov.xls
(see drift4-tsw35 worksheet for check that script works properly)

Drift.f is just a more efficient way of calculating these values repeatedly (for each drift) than manually chunking through each drift worksheet.

This script outputs:

1. temperature profiles along the drift and temperature change relative to the drift center
    - at peak temperature
    - when drift center drops below boiling point (100 C)
    - when drift center drops below 80 C
2. time versus drift length showing significant temperature difference

The output for drift 4 was imported into condriveNov11.xls spreadsheet as worksheet "drift4-tsw35Lengths" for initial plotting. Plotting in SigmaPlot will be the preferred figure generator.

Cross-checked code by comparing temperatures in output directly with spreadsheet values. Drift 4 was used for the checks (see worksheet drift4-tsw35 in spreadsheet file condriveNov11.xls). Temperature differences between drift center and edge were also calculated in spreadsheet and compared with drift.f output, which produced the same values. To check drift lengths, the plot of differences gives a visual estimate of the appropriate drift length and how it changes over time. The drift length plot appears to be consistent with the temperature difference plots. One point on the drift length plot was hand-calculated using data from the original spreadsheet (output from condrive) for drift 4. At 69.1 years, a 0.5 °C drop going away from the center occurs at –387.48 m (cell P175 in worksheet drift4-tsw35, record ID#164), the edge of the drift is at –485.37 m. Thus a difference of 97.89 m was manually calculated. This agrees with the drift.f calculation of 97.89 m.

The drift length calculation accounts for flat temperature profiles early in the heat pulse by requiring a 0.5 drop in temperature for the middle of the drift. And later in time, the flat profile near the edge of the drift also is uses the 0.5 C increase to define the portion of the drift affected. Figure VIII-14a illustrates the shapes of the profiles and the increase in the extent of the edge effect (creeps inward with increasing time). Figure VIII-14b compares the time profiles of the center and edge locations, illustrating the decrease in the magnitude of the difference with increasing time. Figure VIII-15 plots the temperature difference relative to the temperature at the center location of the drift, the plot shows the variation along the half-drift.

Figure VIII-14a. Plot illustrating the change in the shapes of the drift profiles over time.

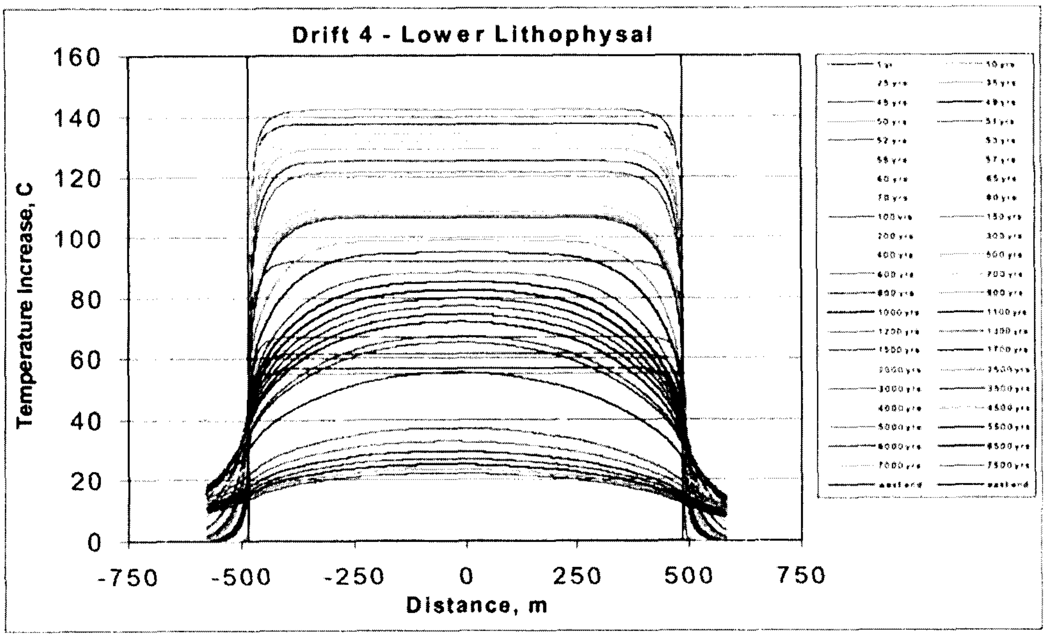


Figure VIII-14b. Temperature time profile for drift 4 center and edge, and Chandrika's chimney location

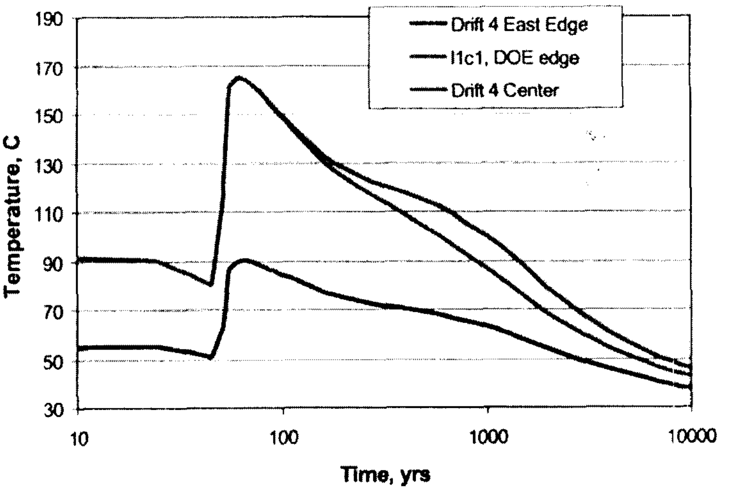
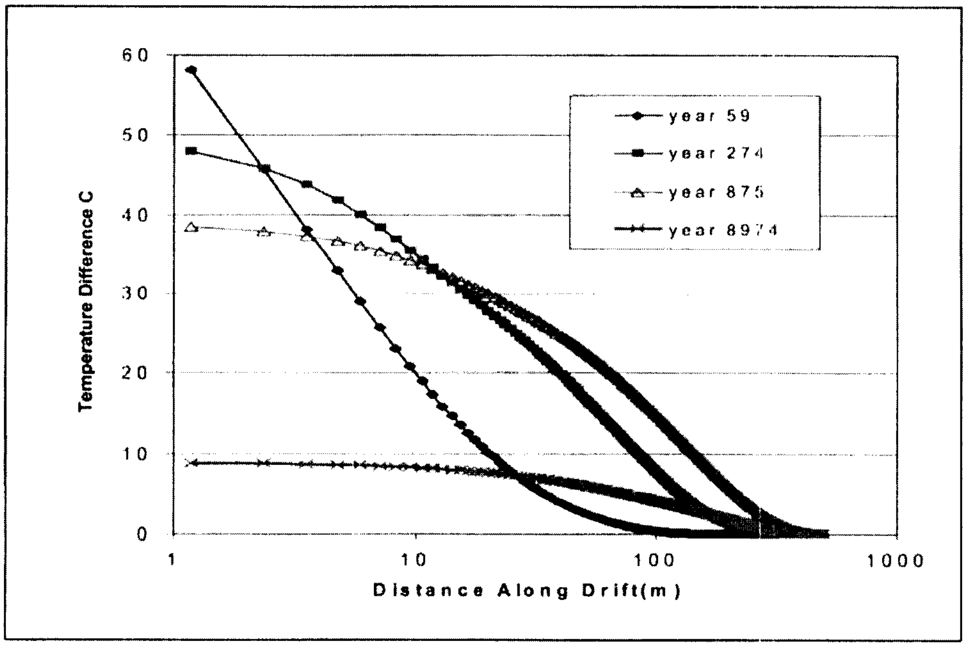


Figure VIII-15. Temperature difference relative to that of drift center



12/2/02 ℱ

Development of figures for IHLRWMC proceedings paper

bubo: E:\TEF-kti\Chandrika\ConductionModelCalc\condriveIHLRWC2002.xls
Conduction model run in:
    spock: ~rfedors/EdgeEffect/Oct21_2002/run/Condrive/*
Drift.exe script run in:
    bub0: E:\TEF-kti\Chandrika\Code*

Steps:

1. Run condrive.e on spock for a drift to get spatial and temporal variation in temperature
2. Import into spreadsheet for simple plotting check of results
3. Export to "drift.csv" in comma delimited format
    1st record is column headings: x, y, distance from center (m), time 1, time 2, time 3, ...
    all other records are temperatures at each locations
4. Run "drift.exe" (compiled from drift.f, see also volume VIII page13 description, and printout included on volume VIII page 18) on bubo (WinNT) to get portions of drifts with temperature gradients. Input file name is drift.csv and output file name is output.txt). Need to rename as appropriate.
    distance from center (m) for next 6 columns
    profile at peak temperature time
    difference with center for peak temperature time
    profile when center is at boiling temperature
    difference with center for boiling temperature time
    profile when center reaches 80 C

difference with center for 80 C time
time (yr) for next 2 columns
length of half drift with large temperature gradient (account for flat part of curve in center)
length of half drift with large temperature gradient (remove both flat portions of curve)

drift0.0.exe sets tolerance to 0.5 C and drift2.0.exe sets tolerance to 2.0 C

Drift 25
From Darrell Sims slice (non-horizontal, through the emplacement drifts) of GFM3.1, the ArcView measured (using the ruler tool) portion of drift 25 that was middle nonlithophysal was 898 feet. The total length of drift 25 was measured to be 3660 ft. From the coordinates in MSTHM_dft1.xls, drift 25 was 1114.8 m [3657.5 ft]. Hence, the ArcView measured value was pretty close to the actual given the resolution of using the ruler tool.

557.4m – (898ft * .3048m/ft) = 283.7m from center of drift 25, location of Tptpmn/Tptpll contact

Worksheet "drift25Combined-avgK" contains temperature data from condrive.e using tsw35 properties on the west and tsw34 properties on the east. Comma delimited file (.\Code\drift25-tsw345-avgK.csv) saved from this worksheet to be used as input to drift.f.

Spreadsheet condriveIHLRWC2002.xls, worksheet "dft4&25Lengths-K1.61&1.945-z2.5" contains the data for figures; figure VIII-16 has the temperature differences wrt center temperature for positions along the half drift. Figure VIII-17a shows the difference between using a threshold of 0.5 and 2.0 C in drift for the temperature difference in defining the portion of the drift experiencing a gradient. Figure VIII-17b contains the results for portions of the two drifts experiencing a gradient, note that half-drifts are included here.

Figure VIII-16

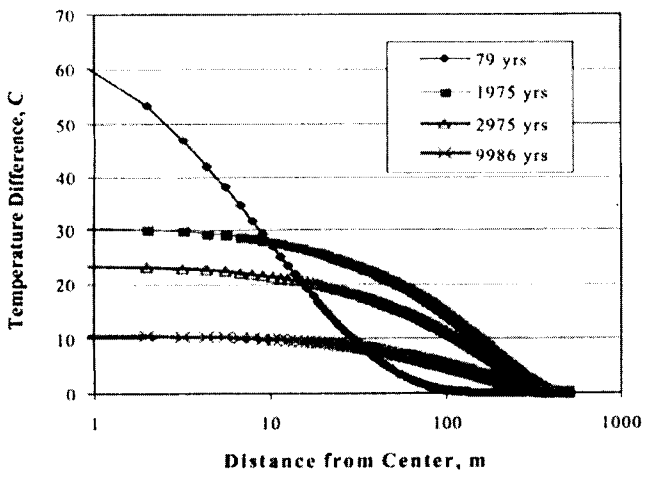


Figure VIII-17a.

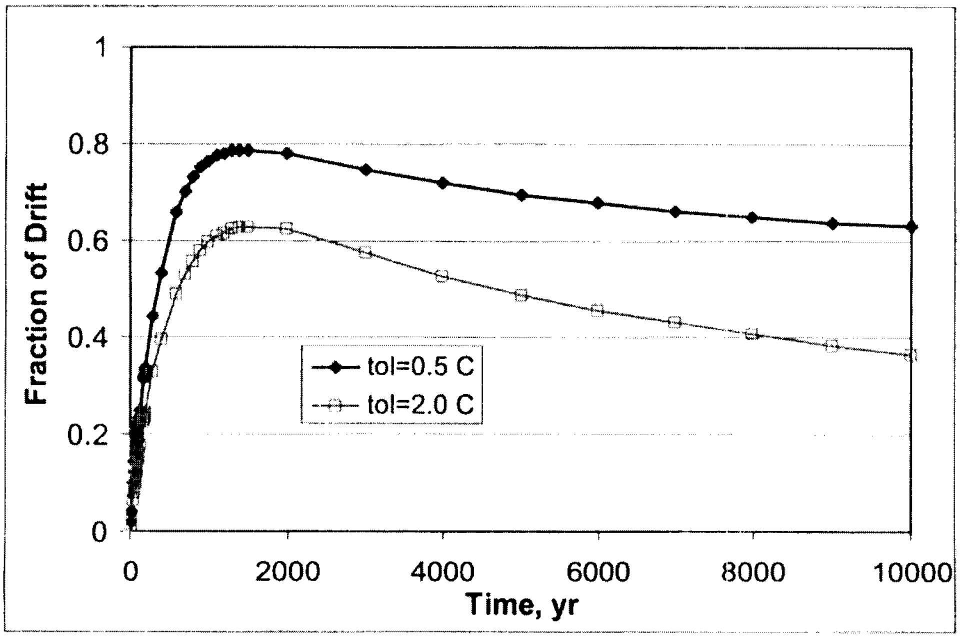
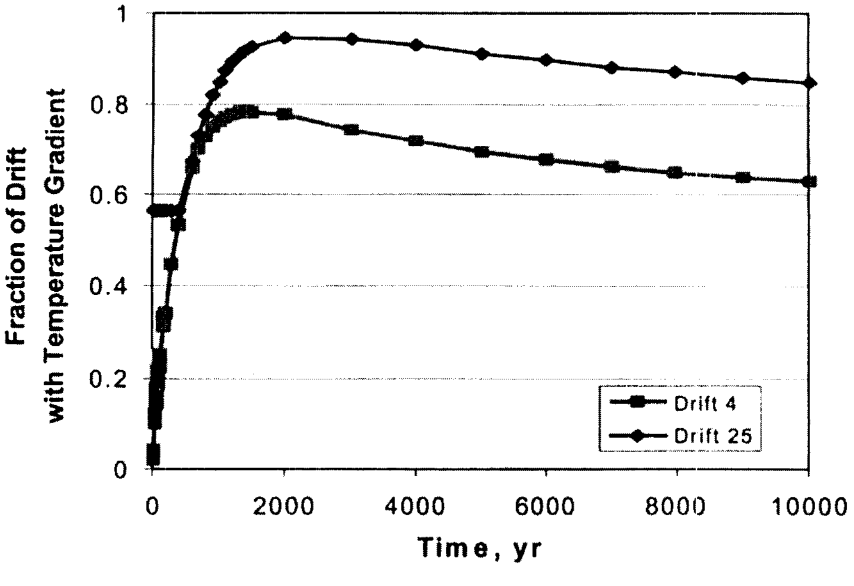


Figure VIII-17b. Note that the portion of the drift increases rapidly as the effect of the edge creeps inward, then decreases slowly as the temperature profile smooths out along the outer portion of the drift and into the adjacent rock outside the repository. Note that drift 25 has a change in rock type.



The drift.f fortran script is included below for reference:

```
program drift
c script for reading conduction model output and reformatting for plots
c   of drift length seeing edge effect over time
c RFedors  Nov 14, 2002
c  created on laptop using Lahey Fortran, comma-delimited input used because of
c  limitation in record length in Excel our favorite business spreadsheet program)
c  Input file has only headers (1 record) and temperatures at 1000 locations.
c  Column headings are: Easting(m), Northing(m), Distance(m), Times(j=4,47)
c23456789 123456789 123456789 123456789 123456789 123456789 123456789 12
      integer  ioread, iowrit, mx, ncl, i, j, ncols, nrows
      parameter (mx=2000, ncl=60)
      real*8  array(mx,ncl), array_old, plot(mx,12), ambient, dTmin
      real*8  columns(ncl)
      integer  iedge, icenter, kpeak, k100, k80, itmp(ncl), itemp(ncl)
      character*20  junk1, junk2, junk3

c set input and output unit numbers and number of columns in input file
      ioread = 7
      iowrit = 8
      ncols = 47
      nrows = 1000
      iedge = 84
      icenter = 500
c set threshold cutoff for calculating length of drift, in degrees celcius
      dTmin = 0.5
c      dTmin = 2.
c open and read in the comma delimited file (written from Excel)
      open(unit = ioread, file = 'drift.csv', form = 'formatted')
      read(ioread,*)  junk1, junk2, junk3, ( columns(j), j = 4, ncols )
      do i = 1, nrows
         read(ioread,*) ( array(i,j), j = 1, ncols )
      enddo
      close(ioread)

c find times at which center location i) peak; ii) below 100 C; iii) below 80 C
c if condrive version was early, then add ambient temperature; check if 1st T entry =
0
      ambient = 0.
      if(array(2,4).lt.0.1) ambient = 23.35

      array_old = 0.
      do j = 4, ncols
         if(array(500,j).gt.array_old)  kpeak = j
         array_old = array(500,j)
      enddo

      array_old = 100. - ambient
      do j = ncols, kpeak, -1
         if(array(500,j).lt.array_old)  k100 = j
      enddo

      array_old = 80. - ambient
      do j = ncols, kpeak, -1
         if(array(500,j).lt.array_old)  k80 = j
      enddo

c write temperature differences to plot array for peak, 100 C, and 80 C
      do i = iedge, icenter
         plot(i-iedge,1) = array(i,3)
         plot(i-iedge,2) = array(i,kpeak) + ambient
         plot(i-iedge,3) = array(500,kpeak) - array(i,kpeak)
         plot(i-iedge,4) = array(i,k100) + ambient
```

```
          plot(i-iedge,5) = array(500,k100) - array(i,k100)
          plot(i-iedge,6) = array(i,k80) + ambient
          plot(i-iedge,7) = array(500,k80) - array(i,k80)
          plot(i-iedge,8) = array(i,ncols) + ambient
          plot(i-iedge,9) = array(500,ncols) - array(i,ncols)
       enddo
c calculations of drift length over which gradient occurs, account for no edge effect
c in center of drift; depends on order going from east edge (i=84) to center (i=500);
c note that first 3 columns of headers() were not read in;
c note that length depends on tolerance value dTmin.
        do j = 4, ncols
          do i = iedge, icenter
             if((array(icenter,j)-array(i,j)).gt.dTmin) itemp(j) = i
          enddo
          plot(j-3,10) = columns(j)
          plot(j-3,11) = array(itemp(j),3) - array(iedge,3)
       enddo
c calculate length of significant temperature change, using above calc position,
c and then accounting for flat temperature profile near edge at late times
       do j = 4, ncols
          do i = iedge, icenter
             if((array(i,j)-array(iedge,j)).lt.dTmin) itmp(j) = i
          enddo
          plot(j-3,12) = array(itemp(j),3) - array(itmp(j),3)
       enddo

c writing out the data for plotting in SigmaPlot or Excel
       open(unit = iowrit, file = 'output.txt', form = 'formatted')
c       write(iowrit,*) 'distance',',','Peak T',',','100 C',',' '80 C'
c       write(iowrit,*)
c      &'distance,Peak T,DiffPeak,100 C,Diff100,80 C,Diff80,Time,Len1,Len2'
       write(iowrit,*) 'times ', columns(kpeak), columns(k100),
     &                             columns(k80), columns(ncols)
       do i = 1, ncols-3
          write(iowrit,*)  ( plot(i,j), j = 1, 12 )
       enddo
       do i = ncols-2, icenter-iedge
          write(iowrit,*)  ( plot(i,j), j = 1, 9 )
       enddo
c 100   format(2(f11.2,','),f10.5)
       stop
       end
```

2/24/03

Lithologic Contacts for Drifts, EDA-II Design

Coordinates of stratigraphic contacts sent to George; contacts estimated in ArcView. Lengths in table calculated in MSTH_dft1.xls in "UTM" worksheet. Drifts 25 and 49 are included as representative drifts that have a lithologic change.

	Drift 25 easting and northing (m)		Drift 49 easting and northing (m)	
west	5.47504172E+05	4.07927611E+06	5.47474350E+05	4.07724450E+06
contact	5.48305100E+05	4.07901940E+06	5.47712900E+05	4.07716830E+06
east	5.48565585E+05	4.07893533E+06	5.48467295E+05	4.07692570E+06
total length, m	1114.8		1042.9	
tsw34 length, m	273.7		-	
tsw35 length, m	841.1		792.4	
tsw36 length, m	-		250.4	

Thermal properties taken from MSTHM AMR REV00 ICN01, Table 4-4.

unit	dry thermal conductivity, W/(mK)	average thermal conductivity, W/(mK)	wet thermal conductivity, W/(mK)	bulk density, kg/m^3	specific heat, J/(kg K)
tsw34	1.56	1.945	2.33	2530	948
tsw35	1.2	1.61	2.02	2540	900
tsw36	1.42	1.63	1.84	2560	865
tsw37	1.42	1.63	1.84	2560	865

2/28/03

Instead of doing just drifts 25 and 49, I modified the edge.apr file and named it
bubo: E:\AVData\TEF-EdgeEffect\edge_gadams.apr
In ArcView 3.2a, George created drifts and then shape files that mark all the contact points (where the lithological contact crosses each drift). Then I exported these to ascii files for input to the condrive module. George's work on this, and all the files, should be found in his TEF scientific notebook. I used ERDAS Imagine version 8.5 on the SGI (Io) machine to export the shape files. Note that the exporter in ArcView loses prominent significant figures (rounds off to nearest 10 meters!). Since GFM3.1 is in State Plane, NAD27(ft), conversions to the exported ascii files were needed to get the coordinates into UTM NAD27 (m). Corpscon 5.11.08 was used in batch file format.

==

Entries made into Scientific Notebook #432e for the period August 26, 2002, to March 6, 2002, have been made by Randall Fedors (April 25, 2003).

No original text or figures entered into this Scientific Notebook has been removed

04/25/2003

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RL 4/10/2008

Volume VIII – TEF Edge Effect

5/15/03

TPA 5.0 – DRIFT DEGRADATION & EDGE EFFECT & COLD TRAP

Collaborators
George Adams: Scientific Notebook # 532e
Chandrika Manepally: Scientific Notebook #478e
Steve Green (Division 18): Scientific Notebook #536e

My working directories are:

Bubo (WinNT box) E:\TEF_kti\Chandrika
Bubo (WinNT box): E:\AVData\TEF-EdgeEffect*
Spock (SUN) ~rfedors/TPA50d/

No changes to computers (bubo WinNT box, or Spock the SUN machine) nor software since last scientific notebook submittal

Effect of cold-trap process on number of waste package failures

This section is part of the sensitivity analyses being done with TPA 5.0d to illustrate the effect of the edge effect, cold trap process, and drift degradation. Many of the changes and approaches used to show the cold trap effect are also used for the other two phenomena.

TPA 5.0d work done on spock (SUN machine, SunOS)
~/TPA50d/*

Need to set the following environment variables to run tpa.e (and variants) from any directory:

```
setenv TPA_DATA $HOME/TPA50d
setenv TPA_TEST $HOME/TPA50d
```

Some General Changes Used for Testing

Start with the basecase tpa.inp and create the tpameans.out file by aborting the basecase TPA 5.0 simulation. This tpameans.out file, created by TPA 5.0, is used as the basecase mean value input file (replaces tpa.inp), thus a deterministic run (1 realization) can be done. The tpameans.out file calculates the mean values for each parameter in the tpa.inp file that has a distribution assigned to it.

1. To run just one subarea (e.g., subarea 2), change the tpa.inp

```
StartAtSubarea
1
StopAtSubarea
1
```

2. Need to use external file for RH and temperature (tefkti.inp) instead of relying on conduction model to estimate temperatures and then resultant temperatures to control RH near the waste package. To use tefkti.inp, change the parameter "TabularTemperatureRHFlag" flag from 0 to 1 in tpa.inp. Then also change "nsetUsedToPickTempRHDataSet" to whichever of the 4 sets in tefkti.inp to use.

3. Need to use external file (drythick.dat) to adjust dry out thickness for cold trap causing an earlier rewetting of the wallrock. Note that drythick.dat has 18 entries with the last one setting the dryout thickness to zero at 1000 years. However, the first entry in the file is "17", which is suppose to be the number of records that follow. Thuse, the 18th record is ignored and the dryout thickness never goes back to zero. I will change the first entry to "18" so that the dryout thickness does go back to zero.

Change tefkti.inp by inserting chimney model results.
bubo: E:\TEFkti\SensitivityReport2003\tpa-ColdTrap.xls

The worksheet "tefkti_Chimney" was exported as a comma-delimited file, then saved as a UNIX ascii file using TextPad (ascii editor program) named tefkti_Chimney.inp after deleting header lines and extra commas appearing part way down the file and at the bottom. The worksheet "tefkti_Chimney" was created (linked entries) from the "Compare" worksheet, which itself was derived from Chandrika's Teftpa1.xls file (METRA results); I got the temperatures and relative humidities from Chandrika's Teftpa1.xls by following the source data of the figures she included as separate worksheets. Note that the limit of 2000 lines in TPA 5.0 for tefkti.inp forced me to delete some records; I chose to delete alternating times at the beginning of Sets 1 and 2. After saving as a comma delimited file from Excel 97 SR-2, the file was named tefkti_Chimney.inp and saved in the ~rfedors/TPA50d/data/ directory for TPA simulations on Spock.

tefkti_Chimney.inp
Set 1: Chimney model results for center of Drift 25 direct from Chandrika
Set 2: Chimney model results for center of Drift 25, except relative humidity set to a high value (needs to be above critical relative humidity, which is sampled from .254 to .65; mean value case is 0.42).
Set 3: Chimney model results for West end of Drift 25 (no lithologic change from center location. Relative humidity stays near saturated condition always, but temperature only goes above boiling for a short time.
Set 4: Chimney model results for East end of Drift 25, lithologic change from TSw35 (lower lith unit) to TSw34 (middle nonlith unit). The latter has a larger value for saturated thermal conductivity and thus the temperature never approaches the boiling point.

Besides changing the relative humidity, I changed value of chloride concentration from the basecase mean value (constant, "Indrift_Cl_PostTemperaturePeak[mol/L]", 4.48E-2) to 0.5 mol/L. Also changed the "Indrift_Cl_PreTemperaturePeak[mol/L]" value, which was 4.47E-2, to the same 0.5 mol/L value. Under basecase, mean conditions, no localized corrosion was occurring. Localized corrosion needs ecorr>ecrit; these are included in the TPA 5.0 output file "corrode.out" or run failt.e to see similar output of corrosion modes.

I don't believe that the Epoch 1 situation (pre-thermal peak) ever occurs unless there is no dryout period when temperatures go above boiling. The pathway described by the chemistry model implemented in TPA 5.0 (not in version 4.1) seems to be in error.

None of the other chemistry or corrosion parameters were changed.

The table used by PA and ENFE folks is included below:

Strategy to select ion concentrations (chloride, fluoride, pH, carbonate) and DeltaECrit

Temperature (C)	**Relative Humidity (%)**	**Time (year)**	**Chemistry Data Source**	**Sampled/Constant parameter name from *tpa.inp***
T < 97	all values	all values	**multifbe.dat** if before dry-out period and **multifaf.dat** if after dry-out period	N/A
97 < T	**RH** < CriticalRelativeHumidityAqueousCorrosion	all values	*tpa.inp* constant values for dry period (dummy values)	Cl_conc_Dry = 0 Fl_conc_Dry = 0 pH_Dry = 7 CO3_Dry = 0 DeltaECrit_Dry=0
	CriticalRelativeHumidityAqueousCorrosion < **RH**	**t** < TimeOfPeakTemperature	*tpa.inp* sampled parameters for epoch 1.	Cl_epoch_1 Fl_epoch_1 pH_epoch_1 CO3_epoch_1 DeltaECrit_epoch_1
		TimeOfPeakTemperature < **t**	*tpa.inp* sampled parameters for epoch 2.	Cl_epoch_2 Fl_epoch_2 pH_epoch_2 CO3_epoch_2 DeltaECrit_epoch_2

Parameters currently available in tpa.inp
BoilingPointOfWater[C] : Constant = 97 C
CriticalRelativeHumidityAqueousCorrosion : Uniform[0.242, 0.56]

Need to introduce to tpa.inp
Cl_epoch_1 : loguniform[2.0E-4,10.0]
Fl_epoch_1 : loguniform[1.15E-4,0.52]
pH_epoch_1 : uniform[5.78, 11.0]
CO3_epoch_1 : uniform[0.0,0.8324]
DeltaECrit_epoch_1 : constant=0.0

Cl_epoch_2 : loguniform[2.0E-4,10.0]
Fl_epoch_2 : loguniform[1.15E-4,0.52]
pH_epoch_2 : uniform[5.78, 11.0]
CO3_epoch_2 : uniform[0.0,0.8324]
DeltaECrit_epoch_2 : constant=0

Local variables
The following are just local variables and should not have any influence on the results. They are just dummy constants, and there is no need to specify them in tpa.inp
Cl_conc_Dry = 0
Fl_conc_Dry = 0
pH_Dry = 7
CO3_Dry = 0

DeltaECrit_Dry=0

The following variable changes from subarea to subarea and from realization to realization:
TimeOfPeakTemperature

This variable must be computed for every realization and subarea

==

5/30/03

George rebuilt the TPA 5.0d code to include the logic tree switch of 80 C instead of using the boiling point, this switch enables the switch of the multifbe.dat and multifaf.dat chemistries to the Epoch 1 and 2 chemistries. This change was made in NFENV.f by George as a test to illustrate an affect on performance; the temperature point at which chemistry values change was modified to 80 C from the current tpa.inp parameter value of "BoilingPointOfWater[C]" (currently set to 97.0 C). Note that the boiling point temperature was not modified. I will rename the executable to:

Spock: ~/TPA50d/tpa80.e

Tracing this change to George's notebook, the modified tpa5.0d code is located in:
~gadams/tpabuild_study/tpa50dmod5-29-03.
A description of the code change is located in:
~gadams/tpabuild_study/modifiedfiles50d5-29-03.

I made the following TPA 5.0 and modified-TPA5.0 (uses 80 C, instead of boiling point) simulations:

BaseCaseK2.02
BaseCaseK2.02-80
ChimneyCenter-80-Cl
ChimneyCenter-Cl
ChemneyCenter-Cl-Set2
BaseCaseK1.56
BaseCaseK1.64
BaseCaseK1.7

where the "BaseCase" refers to using the mean values for tpa.inp, except for what is noted by the rest of the directory name; "K2.-02" means the thermal conductivity was changed to 2.02 W/mK; "80" refers to the use of George's modified-TPA5.0 code; "Cl" refers to my changing the mean value for chloride to 0.5 mg/l (well within the sampled range, and suggested by Osvaldo Pensado); "ChimneyCenter" means that I used the external tefkti.inp file for temperature and relative humidity instead of the conduction model in TPA; "set2" refers to using the 2nd set of T and RH in the external file tefkti.inp;

Also from Darrell Dunn and his early 2003 data (why isn't this in the TPA5.0 release?), I used repassivation values per the emails messages:

```
===============================================================================
- These parameters:

OuterOverpackErpIntercept[mVSHE]     2006.0
  temperature coef                    -15.2
OuterOverpackSlope[mVSHE/C]      -590.7
```

```
  temperature coef                4.3
```

were from some preliminary results for Alloy 22. After more extensive testing we found that the alloy was more susceptible to localized corrosion. The revised values for the mill annealed alloy are correct and the original values (above) should be discarded.

I suspected that the code still used the older values. That is the reason I provided the correct values.

Please let me know if you have any other questions.

-----Original Message-----
From: Randy Fedors [mailto:rfedors@cnwra.swri.edu]
Sent: Monday, June 02, 2003 9:10 AM
To: 'Darrell Dunn'
Subject: RE: tpa question

Darrell,

It appears to me that TPA 5.0 is using your values for "as good as it gets" for the weld, and going in the opposite direction for the regular overpack.

Here are the values currently in the basecast tpa.inp file (mean values for distribution, if relevant):

```
ErpInterceptWeld[mVSHE]     1541.2
  temperature coef         -13.1
ErpSlopeWeld[mVSHE/C]     -362.7
  temperature coef          2.3
OuterOverpackErpIntercept[mVSHE]     2006.0
  temperature coef                   -15.2
OuterOverpackSlope[mVSHE/C]     -590.7
  temperature coef                4.3
```

Is there something I am missing here?

--Randy

----Original Message-----
From: Darrell Dunn [mailto:ddunn@cnwra.swri.edu]
Sent: Friday, May 30, 2003 3:53 PM
To: Randall Fedors
Subject: FW: tpa question

Well, this was not as complete as I thought. I transmitted a paper to the NRC that was referred to in the original message. You can read the original questions below if you are interested. Here are some repassivation potential parameters for mill annealed Alloy 22. The mill annealed alloy is in the as-received condition and is, in simple terms, "as good as it gets"

Asub1 = Outer overpack Erp intercept
Asub2 = Temperature coefficient for outer overpack Erp intercept (Increase temp and Erp decreases)

Bsub1 = Outer overpack Erp slope (Increase Chloride concentration and Erp goes down)
Bsub2 = Temperature coefficient for outer overpack Erp slope (slightly positive)

Asub1 = 1,541
Asub2 = -13.1

Bsub1 = -362.7

Bsub2 = 2.3
Critical chloride concentration = 0.5 molar

I provided these because I am not sure what the code presently has for there parameters

Now for the welded material or "what you really get"

Asub1 = 1,041
Asub2 = -10.0

Bsub1 = -584.2
Bsub2 = 3.7
Critical chloride concentration = 0.01 molar

Also,

-----Original Message-----
From: Darrell Dunn [mailto:ddunn@cnwra.swri.edu]
Sent: Friday, February 14, 2003 5:51 PM
To: 'AEP@NRC.gov'
Cc: Gustavo Cragnolino; Vijay Jain
Subject: RE: tpa question

There are several things that need to be clarified here.

First, the parameters used in the TPA code are based on some initial tests from several years ago. Since then, we have completed many additional tests. I have attached the latest paper that will be presented at Corrosion 2003 in March. In the paper the repassivation parameters are provided in Table 2. The parameters in Table 2 are same as those used in the TPA code although the values are different. Below is a description

Corrosion 2003 paper #697 = TPA parameter definition

Asub1 = Outer overpack Erp intercept
Asub2 = Temperature coefficient for outer overpack Erp intercept

Bsub1 = Outer overpack Erp slope
Bsub2 = Temperature coefficient for outer overpack Erp slope

Also, the parameters in the Corrosion 2003 paper are in mV vs SCE. For the TPA code, one needs mV vs SHE. The conversion is:

mV vs SHE = mV vs SCE + 241.

For the mill annealed alloy: Asub1 = 1,541 mV vs SHE (1,300 mV vs SCE)

For the thermally aged specimens that behave very similarly to the welded material: Asub1 = 1,041 mV vs SHE (800 mV vs SCE).

Notice that these values are different from the older values used in the TPA code.

The addition of nitrate does not alter repassivation potential of Alloy 22 when the nitrate to chloride concentration ratio is 0.1 or less. When the nitrate to chloride concentration ratio is 0.2 or greater, localized corrosion is inhibited. As an additional note, I would like to point out that higher nitrate to chloride concentration ratios are needed to inhibit localized corrosion on less resistant passive alloys such as Stainless Steels. Also, nitrate is not an inhibitor for all metals and alloys.

I am not sure about the validity of altering the repassivation potential parameters to simulate the effect of nitrate. If altering the parameters is the only way you have to do this then you could set the slope (Bsub1 and Bsub2) to low values. Because the slope is negative (i.e. the repassivation potential decreases with increasing chloride concentration) choosing a slope of 0 will artificially increase the repassivation potentials values. If Bsub1 and Bsub2 are set to 0, the repassivation potential for mill annealed Alloy 22 at 95 C will be

1,541 + (-13.1*95) = 296 mV vs SHE.

This really is not that high and does not reflect what we actually observe. For example with a nitrate to chloride concentration ratio of 0.2 or greater, no localized corrosion is observed even at potentials above 500 mV vs SHE. It may be possible to get corrosion potentials above 300 mV vs SHE but to get corrosion potentials above 500 mV vs SHE requires a system that has either a low pH or is very oxidizing. In addition to altering the B values, you could alter the Asub2 value (-13.1). The problem is that if you set Asub2 to zero then the repassivation potential is constant (Erp=Asub1). For predicting localized corrosion in systems with high nitrate to chloride concentration ratios this approach may be acceptable because localized corrosion will not be predicted in the TPA code realizations. However, the low passive dissolution rate cannot be maintained above about 600 mV vs SHE. At high potentials, transpassive dissolution will occur even if the nitrate to chloride ratio is high. This is not addressed in the TPA code.

In order to correctly account for the inhibitive effects of nitrate, a change in the TPA code is necessary.

I hope this information is helpful. Please let me know if you have additional questions.

Darrell S. Dunn

From these results, I compared different effective thermal conductivity values to use that, mostly to see what value would best match waste package temperatures estimated by Chandrika and her thermohydrologic model. Previously, we had been focusing on comparing drift wall temperatures between the thermohydrological and TPA conduction models (MRS paper in December 2002, IHLRWC paper March 2003). A value of effective thermal conductivity of 1.64 W/mK in TPA5.0 best matched waste package temperatures estimated by the thermohydrological model. Note that drift wall temperatures were best matched in TPA by using a saturated thermal conductivity value of 2.02. These comparisons were done for a center repository location.

As for the waste package failure, and all the other simulations noted above, please NOTE:

All testing stopped. Effect of cold trap cannot be incorporated into TPA at this time:

1. Geochemists blew up when they heard that we changed the hydrologic conditions under which evaporation would occur and thus residue would form leading to high chloride concentrations. I still maintain that evaporation will occur on the waste packages and drip shield as the thermal pulse is dissipating, way beyond the temperature of 80 C. The geochemists insist that evaporation stops when the waste packages reach boiling point (i.e., they believe that no evaporation occurs below 97 C). Evaporation occurring between 80 C

and the boiling point, using the current NFENV approach, would lead to chloride chemistries equivalent to the ambient percolating water chemistry (~6.e-3 mg/l) – the effect of deliquescence and localized corrosion cannot be incorporated for this temperature range. The geochemists promised to reassess (later) the hydrological model inherent in their chemistry model for TPA.

2. Weird results from the corrosion module indicated that waste packages were failing before the welds failed. Also, using Darrell Dunn's values of the passitivations for the Alloy 22 and for the weld, I could flip-flop the values and not see a difference. Something does not appear to be working with the corrosion model.

Thus, we will limit the metric for all components (cold trap, edge effect, and drift degradation) to changes in environmental conditions that are important for affecting chemistries and corrosion rates.

The metric will be waste package temperature and relative humidity; and NO cold trap.

6/13/03

Calculation of Relative Humidity at Waste Package

bubo E:\TEF-kti\ColdTrap\Conduction\RH1.xls
bubo E:\TEF-kti\ColdTrap\Conduction\Psat.xls
bubo E:\TEF-kti\ColdTrap\KelvinEqn*.nb

Two factors come into play (1) relative humidity reduction in the porous media at high temperatures, and (2) relative humidity reduction from the RH at the drift wall to the RH near the waste package purely due to a temperature increase. MULTIFLO accounts for the former, but not the latter. Hence, Chandrika needs to modify the MULTIFLO output.

To make the modification, however, a simplification is used such the air mass is assumed to be well mixed between the drift wall and the waste package. Thus, the Clausius-Clapeyron equation does not have to be used because of this well-mixed air assumption. Thus, knowing the drift wall relative humidity (from MULTIFLO output), one can calculate waste package relative humidity assuming that the vapor pressure is the same between the two points (well-mixed assumption):

$$RH_{WP} = RH_{DW} \frac{P_{sat}(T_{DW})}{P_{sat}(T_{WP})} \qquad \text{Equation VIII-28}$$

Note that the TPA5.0 also assumes that the drift wall RH is equal to 1, thus

$$RH_{WP} = \frac{P_{sat}(T_{DW})}{P_{sat}(T_{WP})} \quad \text{or if above boiling temperature} \quad RH_{WP} = \frac{P_{sat}(T_{BoilingPoint})}{P_{sat}(T_{WP})}$$

The difficulty lies in calculating the saturated vapor pressure. Since the TPA5.0 output of relative humidity does some funky zig-zagging near boiling point, I checked the TPA5.0 approximation of the saturated vapor pressure as a function of temperature

The saturation pressure of water vapor was approximated by the Keenan, Keyes, Hill, and Moore formula (Keenan, J. H., Keyes, F. G., Hill, P. G., Moore, J. G., Steam Tables: Thermodynamic Properties of Water, Including Vapor, Liquid, and Solid Phases, John Wiley and Sons, Inc, 1969. As cited in Chapter 5 of ASHRAE Handbook and Product Directory, 1977

Fundamentals, Third Printing, American Society of Heating Refrigeration and Air Conditioning Engineers, Inc., New York, p. 52.),

$$\ln\left(\frac{P_{v,sat}}{217.99}\right) = \frac{0.01}{T}(374.136 - t)\left[-741.9242 + \sum_{i=1}^{7} F_i(0.65 - 0.01\,t)^i\right]$$

where

$F_1 = -29.72100$ $F_2 = -11.55286$ $F_3 = -0.8685635$

$F_4 = +0.1094098$ $F_5 = +0.439993$ $F_6 = +0.2520658$

$F_7 = +0.05218684$

Equation VIII-29

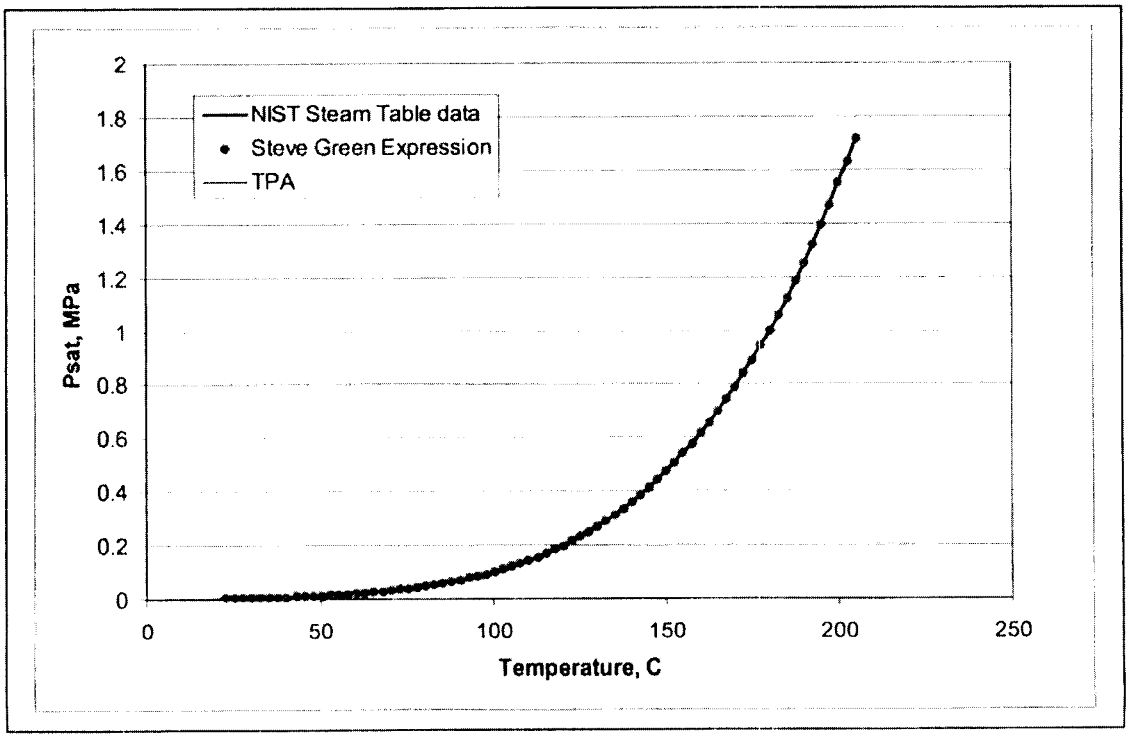
where T is temperature expressed in K, t is temperature expressed in °C, $P_{v,sat}$ is saturated vapor pressure expressed in atmospheres.

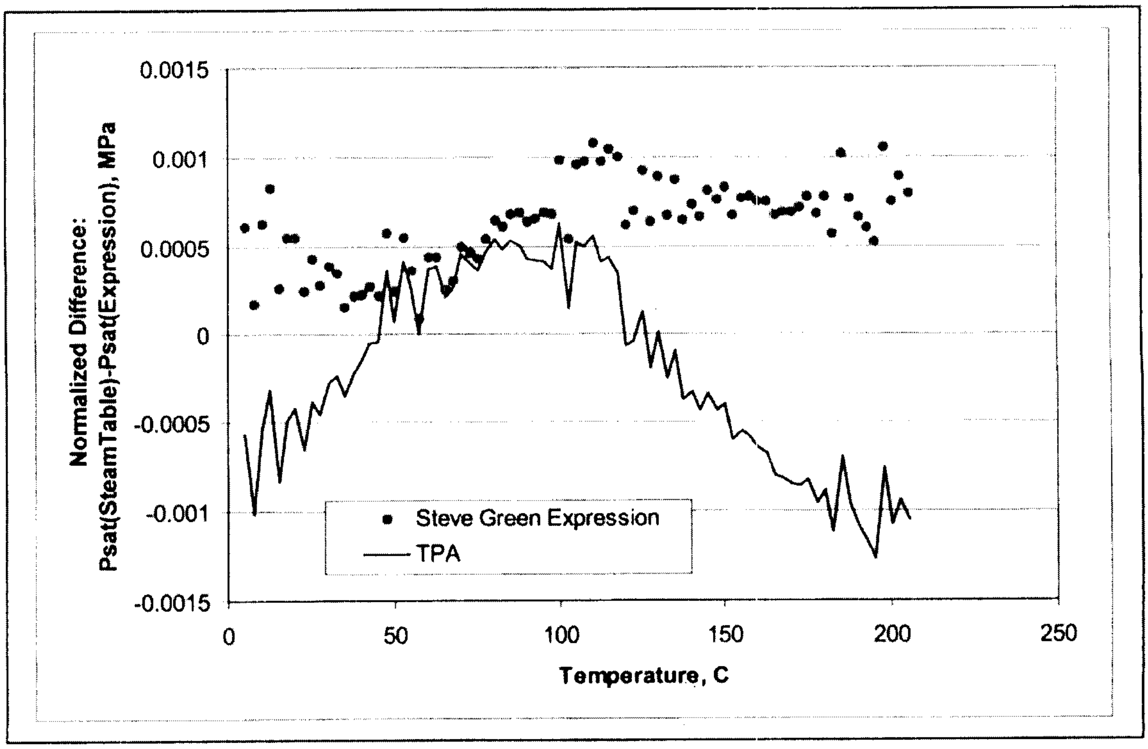
To modify the MULTIFLO output, just use the expressions in Equations VIII-28 and VIII-29. The first is the relationship of saturated vapor pressures and drift wall RH to the waste package RH. The second is a good approximation of the saturated vapor pressure as a function of temperature. This eliminates our previous avoidance of presenting in-drift relative humidity plots in reports.

To answer how well the TPA5.0 approximates relative humidity (ignoring the TPA approximation that the vapor pressure at start, dictates the amount of moisture in the drift throughout the entire period of the simulation), I compared the TPA5.0 approximation to NIST Steam Table data and to results from Equation VIII-29. The following figure shows that there is a good match between 20 and 200 C between all three results. Therefore, the TPA approach seems pretty good, but then I still don't know why the zig-zags occur early in the post-closure period, for cases when the temperatures barely peak out above boiling.

The following figures are from the "RH,KelvinEqn" worksheet in Psat.xls. The first figure (VIII, page 30) shows a pretty good match.

A closer inspection, and thus development of the 2nd plot, of the differences can be see in the normalized difference plot (normalized to the NIST Steam Table value for that temperature. Note that there is a slight positive bias for Equation VIII-29 results, and that the TPA5.0 approach wanders more (as a function of temperature) and may get even worse at higher temperatures. This was not considered important, since relative humidity at the higher temperatures can not lead to the presence of liquid phase water (deliquescence).


NIST Steam Table data
Steve Green Expression
TPA
Psat, MPa
0
0.2
0.4
0.6
0.8
1
1.2
1.4
1.6
1.8
2
0
50
100
150
200
250
Temperature, C


Normalized Difference:
Psat(SteamTable)-Psat(Expression), MPa
0.0015
0.001
0.0005
0
-0.0005
-0.001
-0.0015
0
50
100
150
200
250
Temperature, C
Steve Green Expression
TPA

The Kelvin equation (one form of it is in the MULTIFLO documentation) estimates the relative humidity drop across the curved surface of water in partially saturated porous media. Just to check the sensitivity of RH at the drift wall to temperature, I took the derivative using Mathematica, and checked the results using the NIST Steam Table; use NIST steam table program (database 10, version 2.2) to get enthalpies (gas and liquid), "Calculate Saturation Table", then vary temperature).

The code snipped from TPA 5.0d for calculating RH at waste package:

```
tboil = 97 C
temprep(it) = temperature of the repository at a time step
tempwp(it) = temperature of the waste package at a time step
relhumwp(it) =  pvap( dminl( temprep(it), tboil ) ) /
     &                pvap( tempwp(it) )

c=======================================================================
      function pvap( t )
c=======================================================================
c vapor pressure of water as a function of temperature
c
c t = input, double precision, temperature in units of [C]
c pvap = output, double precision, vapor pressure of water in
c               units of [Pa] which also is [N/m^2]
c
c  equation from R.C. Reid, J.M. Prausnitz, B.E. Poling,
c  "The Properties of Gases
c and Liquids, Fourth Edition, McGraw-Hill, Appendix A
c
      implicit double precision (a-h,o-z)
      data vpa, vpb, vpc, vpd / -7.76451, 1.45838, -2.77580, -1.23303 /

       x  = 1.0 - (t+273.0)/647.3
       pvap = 221.2D+5 *dexp( (vpa * x +vpb * x**(1.5)  + vpc * x**3 +
     1      vpd * x**6 )/ (1 - x))

       return
       end
```

end of TPA5.0 code for Psat

Derivative of Kelvin Equation

One form of the Kelvin equation is

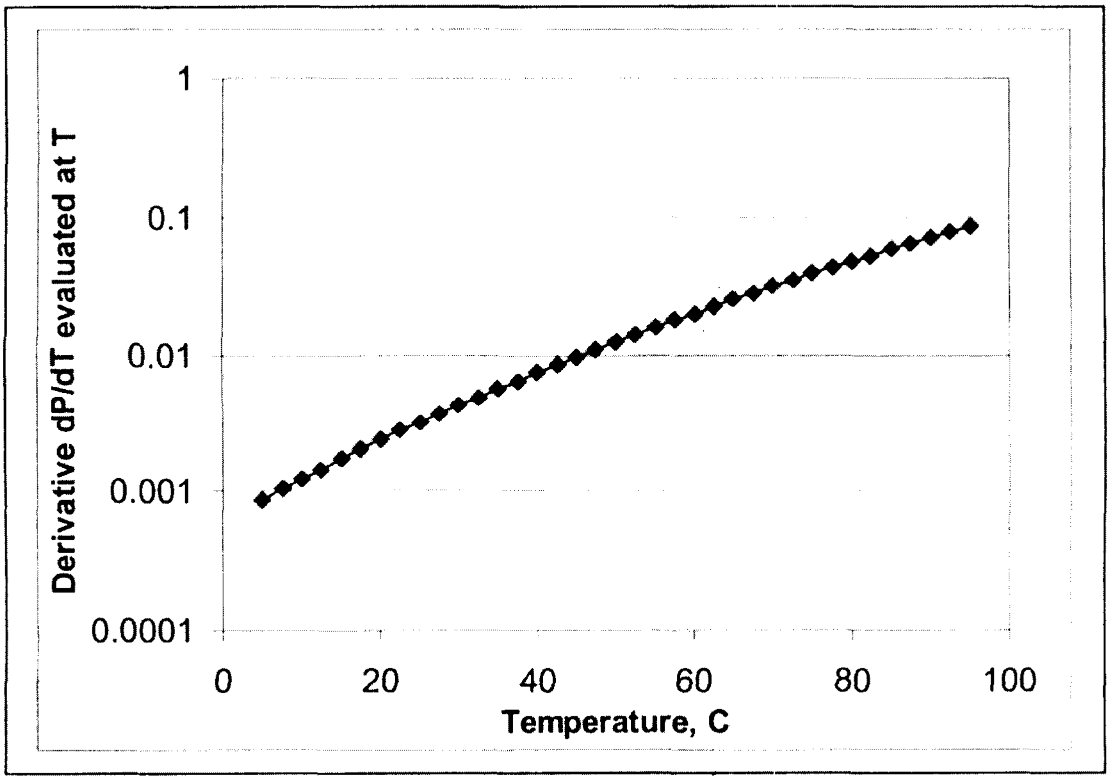
$$RH = \frac{P_v}{P_{sat}} = \exp\left\{\frac{M(-P_c)}{\rho RT}\right\}$$

where P_v and P_{sat} are vapor pressure and saturated vapor pressure (at that temperature), P_c is capillary pressure, M is molecular weight of water, R is ideal gas constant, T is temperature in Kelvin, and ρ is density of water.

See Psat.xls spreadsheet and dPdT.nb and dPsi_dT.nb Mathematica sheets for calculations.

bubo E:\TEF_kti\KelvinEqn\dPdT.nb
checks to make sure that derivative of pressure wrt T is same as derivative of Psi (capillary head) wrt T; this is an implementation check on my Mathematica inputs

.\dPsi_dT.nb derivative of capillary head wrt to temperature
The first part of dPsi_dT.nb is a check to make sure that the equation for saturated vapor pressure (Equation VIII-29) is implemented correctly - the results agree with the NIST Steam Table standard table 10, version 2.2



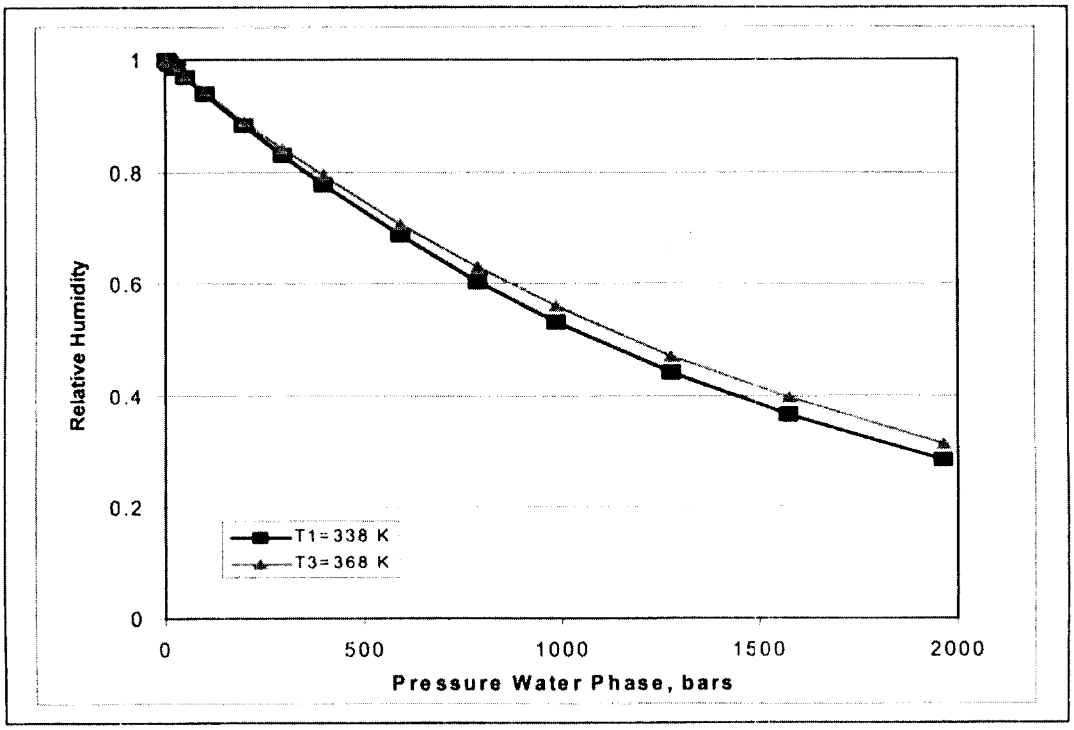
This figure gives one a feel for the rate of change of the saturated vapor pressure curve as boiling point is approached. This plot is from the worksheet "MathematicaOutput" in Psat.xls.

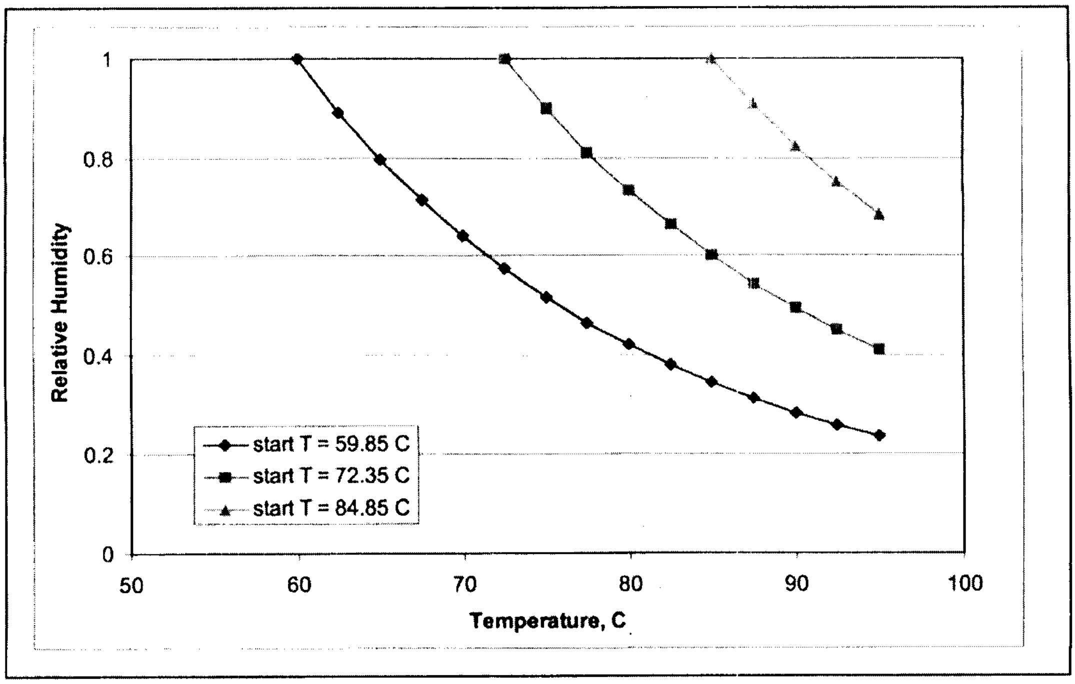
One can also get a feel for the effect of temperature and capillary pressure head directly on the relative humidity in the porous media (and hence at the drift wall) by plotting relationships based on the Kelvin equation.

1st plot: For the relative humidity as a function of capillary pressure head, note that ambient pressure heads are in the range of 0.1 to 1 bars.

2nd plot: For the wallrock temperature in the legend, assume the relative humidity is 1. Then the higher temperatures will reduce the relative humidity by the amount shown on the plot.

Note that the Kelvin equation should not be used to evaluate temperature difference between the waste package and drift wall (it's only for RH drop across a curved interface). The Clausius-Clapeyron equation really should be used instead.


Relative Humidity
1
0.8
0.6
0.4
0.2
0
0
500
1000
1500
2000
Pressure Water Phase, bars
T1=338 K
T3=368 K


Relative Humidity
1
0.8
0.6
0.4
0.2
0
50
60
70
80
90
100
Temperature, C
start T = 59.85 C
start T = 72.35 C
start T = 84.85 C

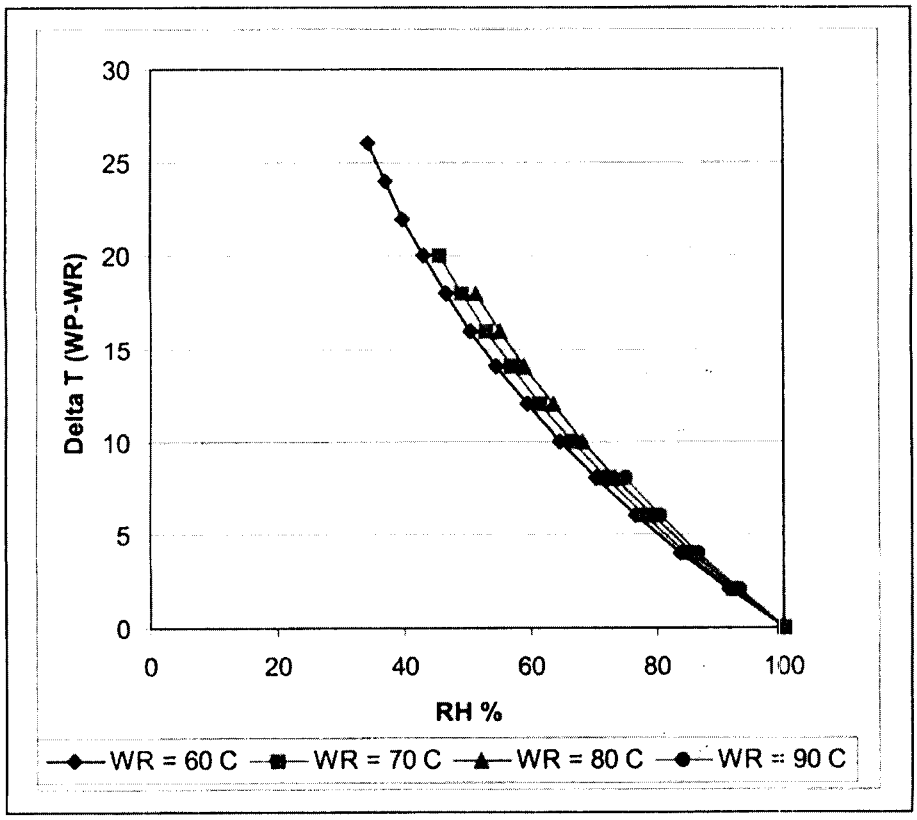
Clausius-Clapeyron Equation

The Clausius-Clapeyron (see page 162 of Klotz, I, and R.M. Rosenberg, Chemical Thermodynamics, Third Edition, W.A. Benjamin, Inc, Menlo Park, CA. 1972) estimates the RH when there is a temperature drop in the air mass.

Use NIST steam table program (database 10, version 2.2) to get enthalpies (gas and liquid), "Calculate Saturation Table", then vary temperature. Just to get a feel for the magnitude in the drop of relative humidity between the drift wall and the waste package, relative humidity as a function of temperature difference was calculated using the Clausius-Clapeyron equation. These calculations are shown in the following figures.

$$\ln[RH] = \frac{\Delta H}{R\left(\frac{1}{T_2} - \frac{1}{T_1}\right)} \quad \text{where } \Delta H = H_g - H_l$$

where R is the gas constant, and H_g and H_l are the enthalpies for gas and liquid at the appropriate temperatures. For my calculations, I just used the enthalpies at the lower temperature as an approximation. In the figure below, WR is the wall rock, WP is the waste package. Note that the wall rock is assumed to be at RH=1, which is not a bad approximation for lower temperatures when there is at least some water in the matrix, but gets marginal as boiling point is approached. For a temperature difference of 10 C (drift wall to waste package), the RH drop is about 35% (from 1.0 to 0.65); 10 C difference is typical for YM.

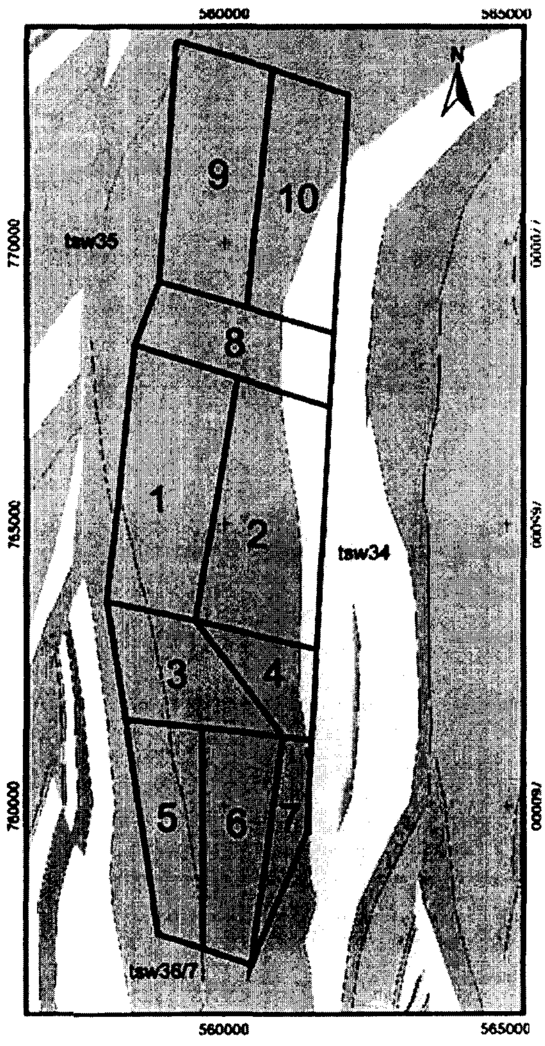


6/17/03

Geologic Map of Repository Horizon

Darrell Sims sliced a non-horizontal geologic map of the repository horizon using the coordinates of EDA-II design (elevation and state plane projection, NAD27) from the DOE Earth Vision model GFM3.1 of Yucca Mountain. I converted the TPA subarea coordinates from UTM NAD27 (m) to State Plane NAD27 (ft) so as to plot on top of the geologic map in ArcView 3.2a. The conversion was done using ERDAS Imagine 8.5. Areas of each rock type in the repository block were estimated using the ArcView area calculation on the shape file I created by outlining each rock type with polygons (areas.shp): tsw34=5028901 ft2 (9.8%); tsw34=40209324 ft2 (78.6%); tsw36/7=5924600 ft2 (11.6%).

E:\AVData\TEF-EdgeEffect\sensitivity2003.apr ArcView project file
E:\AVData\TEF-EdgeEffect\gfm_slice\Repos_slice.tif and .tfw header file
E:\AVData\Tpa\subareasSP* arcinfo files
E:\AVData\TEF-EdgeEffects\areas.shp (and associated files)
shape files for areas of each rock type within repository outline



10/03/03

Entries made into Scientific Notebook #432E Volume VIII for the period April 3, 2002 to September 30, 2003 have been made by Randall Fedors (October 3, 2003).

No original text or figures entered into this Scientific Notebook has been removed

10/03//2003

RL
4/10/2008

5/5/03 RF

Volume VIII – TEF Edge Effect

Evaluate the Effect of Drift Degradation on Temperature and Relative Humidity

Objectives:

Over the past year, we have been performing iterative assessments of the TPA code at the behest of Sitakanta. We are now at the stage of exploring how to evaluate the effect of drift degradation on the temperature history. Our objective is to develop an in-drift heat transfer algorithm that links the temperature estimate to the drift degradation rate derived from MechFail. After testing and demonstration of importance, this in-drift heat transfer algorithm would be provided to TSPAI KTI for their consideration for eventual incorporation into the TPA code. Note that relative humidity is a function of the drift wall and waste package temperatures.

Collaborators:

George Adams: Scientific Notebook # 532e
Steve Green (Division 18): Scientific Notebook # 536e
Chandrika Manepally, Scientific Notebook # 478e

Work is contained in the directory

Bubo: E:\TEF-kti\Sensitivity-June2003*

Evaluate Current TPA In-Drift Heat Transfer Algorithm

Steve Green was tasked to go through the TPA documentation and code to determine the reasonableness of the in-drift heat transfer algorithm currently in the TPA code. His analysis is provided in Sci Ntbk #536e.

His analysis indicated that there were errors in the algorithm that needed to be corrected before we linked created the link with the drift degradation module (MechFail). One error was in the denominator of the radiation term, which appeared to lead to small errors in temperature. A more significant error was in how the drip shield was included in the algorithm. Radiation and convection were allowed to operate in the postclosure as if there were no drip shield. The drip shield, however, should force the algorithm to include two separate legs in series. One leg is from the waste package to the drip shield, and other leg is from the drip shield to the drift wall. The third error was in the estimate of temperature when natural backfill was emplaced. As currently coded, emplaced backfill did not lead to increased temperatures of the waste package compared to the no-backfill scenario. Obviously, this is incorrect.

Steve also checked the reasonableness of the linearized approach for convection and radiation. Both of these should be nonlinear problems (update the coefficients when new temperatures are estimated). Steve ran a spectrum of cases to show the linear approach led to sufficiently accurate results for the Yucca Mountain configuration. This may require further analyses with more relevant parameters latter.

5/27/03

Temperature Estimates Linked to Drift Degradation

Revised Abstraction to Link Temperature to Drift Degradation

This section is a documentation of the algorithm that George Adams has been implementing. The three modes of heat transfer of conduction, convection, and thermal radiation are considered for the three scenarios:

(1) Preclosure when no drip shield or backfill is included
(2) Postclosure with waste package, invert, and drip shield
(3) Postclosure with waste package, invert, drip shield, and backfill with or without air space above the backfill. The backfill thickness will vary with time.

For the thermal network analysis, the assumption is made that axial temperature variations or heat flux are negligible. In addition, the translation of the two-dimensional geometric configuration in a cross section of the drift to a radially oriented configuration centered on the drift centerline is also assumed acceptable. Also note that the temperature estimates for the center of each subarea, in the base case TPA, is intended to be representative of the entire subarea. These are the same assumptions needed for the current TPA in-drift heat transfer algorithm.

Expressions for heat load (Q_p) as a function of effective thermal conductances (G) and the temperature difference between the waste package (T_p) and the drift wall (T_w) are developed from thermal networks used to describe each scenario. Waste-package surface temperature is calculated after the effective thermal conductance terms have been evaluated and the drift-wall temperature has been specified. The effective thermal conductance is defined as the inverse of the resistance using the electrical network analog. This thermal network approach follows that presented in Mohanty, et al. (2002, TPA User Guide). Errors are noted in the radiation component and the thermal network paths for scenarios 2 and 3 in Mohanty, et al. (2002) that lead to significant errors in waste-package surface temperatures when the drift degradation effect is analyzed.

The multimode thermal network for the preclosure scenario (scenario 1) has radiation and convection laterally and upward through the air and conduction through the floor all acting in parallel, thus leading to the following equation for the heat load

$$Q_p = \left[\frac{1}{R_k} + \frac{1}{R_{cpw}} + \frac{1}{R_{rpw}}\right](T_p - T_w) = \left[G_k + G_{cpw} + G_{rpw}\right](T_p - T_w) \tag{1}$$

where the resistance and effective conductance terms are defined to represent

R_k — conduction through the floor
R_{cpw} — convection between waste package and drift wall
R_{rpw} — radiation between waste package and drift wall
G_k — conduction through the floor
G_{cpd} — convection between waste package and drift wall
G_{rpd} — radiation between waste package and drift wall

Because conduction through the floor, convection, and radiation operate in parallel, they can simply be added.

For postclosure scenarios, where a drip shield is in place, thermal processes act in series above the waste package. The drip shield blocks direct convection and radiation between the waste package and drift wall. The high thermal conductivity of the drip shield and small thickness lead to a much smaller thermal resistance than for other components of heat transfer. Thus, the drip shield can be neglected from the thermal network for heat transfer, but its effect on radiation and convection must still be included. The multimode thermal networks lead to the following equations for the no-backfill scenario (scenario 2)

$$Q_p = \left\{ G_k + \left[\frac{1}{G_{cpd} + G_{rpd}} + \frac{1}{G_{cdw} + G_{rdw}} \right]^{-1} \right\} \left(T_p - T_w \right) \tag{2}$$

where the effective conductance terms are defined to represent

G_{cpd}	—	convection between waste package and drip shield
G_{rpd}	—	radiation between waste package and drip shield
G_{cdw}	—	convection between drip shield and drift wall
G_{rdw}	—	radiation between drip shield and drift wall

and for the backfill scenario (scenario 3)

$$Q_p = \left\{ G_k + \left[\frac{1}{G_{cpd} + G_{rpd}} + \frac{1}{G_b} + \frac{1}{G_{cbw} + G_{rbw}} \right]^{-1} \right\} \left(T_p - T_w \right) \tag{3}$$

where the effective conductance terms are defined to represent

G_b	—	conduction through the backfill
G_{cbw}	—	convection between backfill and drift wall
G_{rbw}	—	radiation between backfill and drift wall

Inner drip-shield temperature T_d and outer backfill temperature T_b can be calculated after the waste-package surface temperatures have been estimated using the following expressions

$$Q_p - G_k \left(T_p - T_w \right) = \left(G_{cpd} + G_{rpd} \right) \left(T_p - T_d \right) \tag{4}$$

and

$$Q_p - G_k \left(T_p - T_w \right) = \left(G_{cbw} + G_{rbw} \right) \left(T_b - T_w \right) \tag{5}$$

Effective thermal conductance terms for each scenario are presented below, organized by thermal process. Development of the equations for the conductance terms follows the approach used by Mohanty, et al. (2002, TPA User Guide).

For conduction through the invert,

$$G_k = \frac{2\pi(1-f_c)(L_p + 2\delta)k_f}{\ln\left(\frac{D_w}{D_p}\right)} \quad (6)$$

where

π — 3.14...
L_p — length of waste package
2δ — gap between waste packages
f_c — fraction of waste-package cylindrical surface available for convection and radiation
k_f — thermal conductivity of floor (invert) material
D_w — inner diameter of drift wall
D_p — outer diameter of waste package

For conduction through the backfill,

$$G_b = \frac{2\pi f_c(L_p + 2\delta)k_b}{\ln\left(\frac{D_b}{D_d}\right)} \quad (7)$$

where

k_b — thermal conductivity of backfill material
D_b — outer diameter of backfill
D_d — diameter of drip shield, thickness assumed negligible

For convection, it is assumed that the effective thermal conductivity, k_{nc}, value does not change with temperature and temperature difference over which convection is occurring. Thus, the same value of k_{nc} is used for convection (i) from the waste package to the drift wall, (ii) from the waste package to the drip shield, and (iii) from the drip shield or backfill to the drift wall.

For convection,

$$G_{cio} = \frac{2\pi f_c(L_p + 2\delta)k_{nc}}{\ln\left(\frac{D_o}{D_i}\right)} \quad (8)$$

The subscripts for G_{cio} refer to convection, inner diameter, and outer diameter where the

diameters refer to waste package (*p*), drip shield (*d*), and drift wall (*w*) in Eqs. (1) through (3).

Substitutions for G_{cio}, D_i, and D_o for specific legs of the thermal networks for each scenario [Eqs. (1) through (3)] are defined in Table zzxx, below.

For radiation,

$$G_{rio} = \frac{\sigma \pi f_c \left(L_p + 2\delta\right)}{\dfrac{1}{D_i \varepsilon_i} + \dfrac{1}{D_o} \dfrac{1 - \varepsilon_o}{\varepsilon_o}} 4T_w^3 \qquad (9)$$

where

σ — Stefan-Boltzman constant
ε_i — emissivity of inner surface material (i.e., waste package, drip shield)
ε_o — emissivity of outer surface material (i.e., drip shield, drift wall)

The subscripts for G_{rio} refer to radiation, inner surface, and outer surface where the surfaces are the waste package (*p*), drip shield (*d*), and drift wall (*w*). Similar to the convection substitutions, G_{cio}, D_i, D_o, ε_i, and ε_o for specific legs of the thermal networks for each scenario [Eqs. (1) through (3)] are defined in Table zzxx. The use of the drift-wall temperature cubed in Eq. (7) is a linearization of the nonlinear radiation equation following the approach of Mohanty, et al. (2002). For waste package to drift wall radiative heat transfer, the linearization assumes that, for example, $4T_w^3 \approx \left(T_w^2 + T_p^2\right)\left(T_w + T_p\right)$ for scenario 1.

Table zzxx. Substitutions of Inner and Outer Diameters to Use for Eq. (8) (Convection) and Diameters and Emissivities to Use for Eq. (9) (Radiation) Depending on the Specific Leg of the Thermal Network

Scenario	**Description**	**Effective Conductance G_{cio} or G_{rio}**	*Inner Diameter Di*	*Outer Diameter Do*	*Inner Emissivity ε_i*	*Outer Emissivity ε_o*
1 Preclosure	*Waste package to drift wall*	G_{cpw} or G_{rpw}	D_p	D_w	ε_p	ε_w
2 and 3	Waste package to drip shield	G_{cpd} or G_{rpw}	D_p	D_d	ε_p	ε_d
2 Backfill	Drip shield to drift wall	G_{cdw} or G_{rpw}	D_d	D_w	ε_d	ε_w
3 Backfill	Backfill to drift wall	G_{cbw} or G_{rpw}	D_b	D_w	ε_b	ε_w

Calculations

It was presumed that natural backfill occurring as a result of drift degradation would have a significant impact on waste package surface temperature. In order to see this effect, version

5.0d of the TPA code was modified to incorporate three heat transfer equations associated with the following three test cases:

- Case 1 occurs during the ventilation period and accounts for the heat transfer from the waste package to the drift wall in parallel with the heat transfer through the invert.
- Case 2 occurs after the ventilation period when a drip shield is in place. It accounts for heat transfer from the waste package, through the drip shield, and out to the drift wall in parallel with heat transfer through the invert.
- Case 3 also occurs after the ventilation period but in this case, both the drip shield is in place and backfill is emplaced within the drift. It accounts for heat transfer from the waste package, through the drip shield and backfill, and out to the drift wall in parallel with heat transfer through the invert.

In addition, version 5.0d of the TPA code was modified to place drift height and area of fallen rock in a result file. These terms were used to calculate an equivalent radius for the drift and outer radius of the backfill versus time. The equivalent radius for the drift and backfill can then retrieved by the modified TPA code and used in the heat transfer equations for Case 3 above.

George documented the exploratory changes to the TPA code, provided hand calculations to verify the changes were acting properly, and provided the calculations in spreadsheets of the final results (waste package and drift wall temperatures). I just had to modify or create the figures as needed, and write the chapter of the intermediate milestone.

Equivalent Thickness of Rubble

The rubble pile was hand calculated by George using an area based approach to convert the degraded drift ceiling heights to an equivalent rubble pile thickness and ceiling height. The rate of degradation (time dependent) and bulking factor were incorporated into the spreadsheet calculation

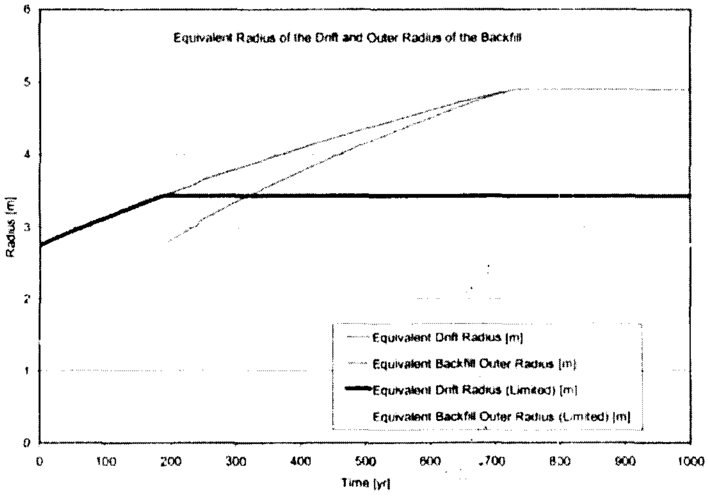
.\Sensitivity-June2003\Drift Degradation_In Drift_Original.xls (provided by George)
.\Sensitivity-June2003\Drift Degradation_In Drift.xls (my modifications of figures)

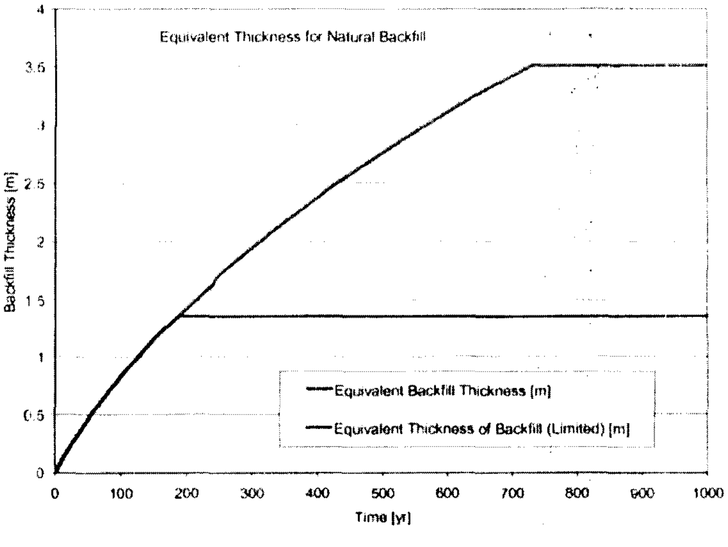
The parameter values needed to convert MechFail results to equivalent radii of drift and rubble are

Drip Shield Height [m]:	2.521
Invert Height [m]:	0.721
Drift Radius [m]:	2.75
Drip Shield Height (offset from drift center):	0.492
Fraction Not Covered by Pedestal/Floor:	0.75
Drip Shield Thickness [m]	0.015
Equivalent Outer Radius of the Drip Shield [m]:	1.39
Drift Void Area [m^2]	16.14754759
Fraction of Rock Type 1	0.75
Fraction of Rock Type 2	0.25
Average Bulking Factor Rock Type 1	1.325
Average Bulking Factor Rock Type 2	1.425
Weighted Average Bulking Factor	1.35

Time, static load height, and drift height are provided by MechFail for mean case TPA parameters; i.e., seismo.rlt file from a TPA 5.0d simulation.

The worksheet "Equivalent Height (mean)" contains the calculations and methods used to convert a mean case drift degradation result from MechFail (*seismo.rlt*) inTPA 5.0d *to the* equivalent radii and thicknesses needed for the in-drift module (see next two figures) (worksheets "Figure 2" and "Figure 3" in Degradation_In Drift.xls file).



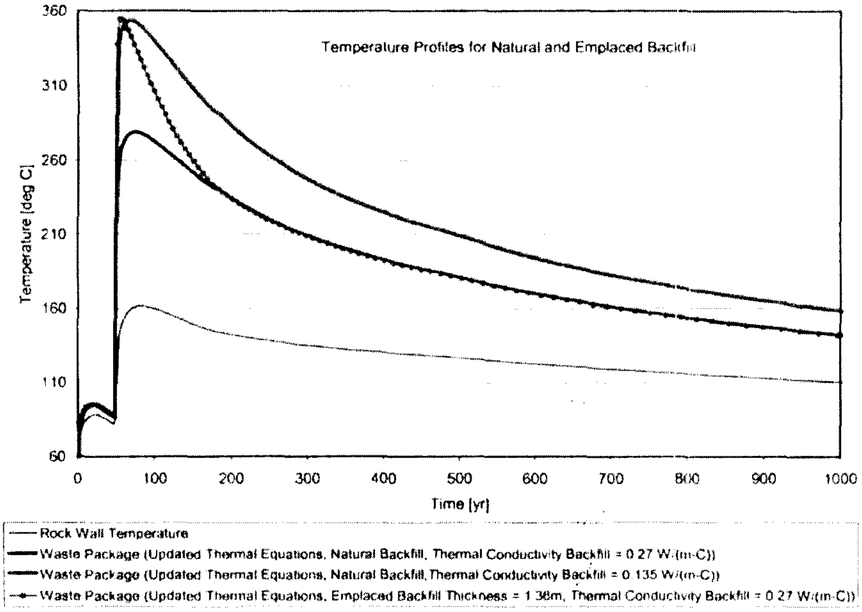


Note that a practical limit was imposed on the equivalent thickness of the rubble pile. The equivalent radii and thickness figures above show that the degradation of the drift and accumulation of natural backfill was limited such that the equivalent radius of the backfill did not exceed the original radius of the drift. Thus, natural backfill was limited to 1.36m, the same value used for the emplaced backfill in this study.

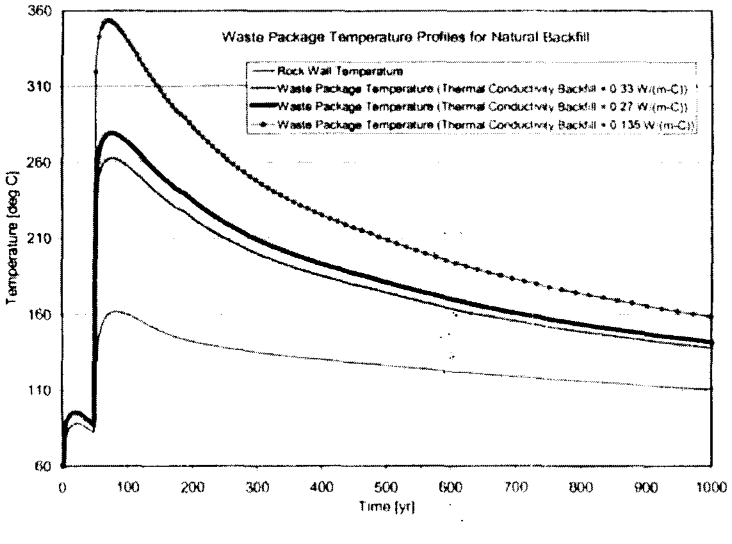
Calculations for In-Drift Heat Transfer

In order to see the effect of emplaced backfill on waste package surface temperature, version 5.0d of the TPA code was modified to incorporate the new heat transfer equations that utilize the rubble equivalent thickness. Note that it is assumed that the rubble builds up on the drip shield, and does not collapse the drip shield. The modified version of TPA 5.0d reads in the generated rubble thickness file and uses the revised in-drift heat transfer algorithm. Worksheet "Figure 1" in Degradation_In Drift.xls plots the temperatures for the first 1000 yrs for emplaced backfill and natural backfill (with two different rubble effective thermal conductivities). Again, George Adams provided the simulation results; and besides documenting the changes in his SciNtbk #532e, he completed a hand calculation to verify the algorithm was acting as expected, which I also retained for reference:

.\Sensitivity-June2003\Backfill-HadnCalc*

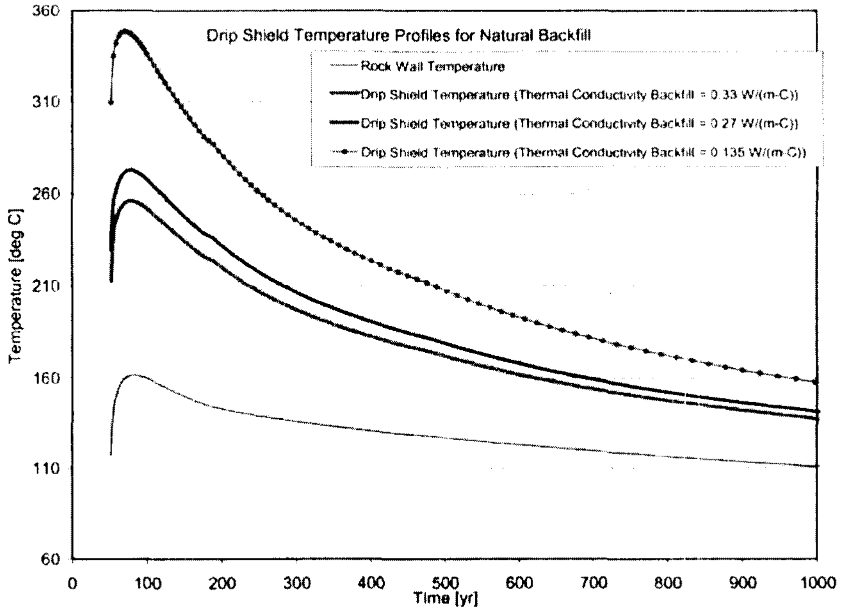


To better illustrate the uncertainty in thermal conductivity for natural backfill affects the temperature profiles (worksheet "Figure 4" in spreadsheet). At a value of 0.33 W/(m-K),



referenced in the Multiscale Themohydrological Model AMR (ANL-EBS-MD-000049 REV 00 ICN 01), the temperature peaks around 262 C. For a value of 0.27 W/(m-K), currently used in the TPA code for emplaced backfill, the waste package temperature peaks around 279 C. And for 0.135 W/(m-K), half the thermal conductivity used in tpa, the temperature peaks around 353 C. Thus, a factor of two reduction in the thermal conductivity for natural backfill results in a 26.5% increase in waste package temperature at the peak. Clearly, waste package temperature is highly sensitive to rubble pile thermal conductivity. Furthermore, rubble pile effective thermal conductivity is highly uncertain both because the topology/packing of the rubble is highly uncertain and because the heat transfer through rubble piles with high pore space (large fragments and poor packing). While thermal conductance in unconsolidated material is much smaller than the in the welded tuffs, convective and radiative heat transfer likely occur in rubble piles with large pore spaces. Rip-rap is an example that comes to mind. Currently, no information was readily found on thermal properties of rubble piles. Thus, this will be an important area for further literature search, modeling, or measurement.

With the new (high) temperatures being estimated when rubble builds up on the drip shield, Doug Gute has become concerned that the mechanical integrity of the drip shield should be reassessed. As expected, the drip shield temperatures (worksheet "Figure 4b" in spreadsheet Degradation_In Drift.xls) are close to the temperature values of the waste package; radiation and convection across the air gap are efficient at heat transfer at these temperatures.



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Adding Third Leg to Thermal Network

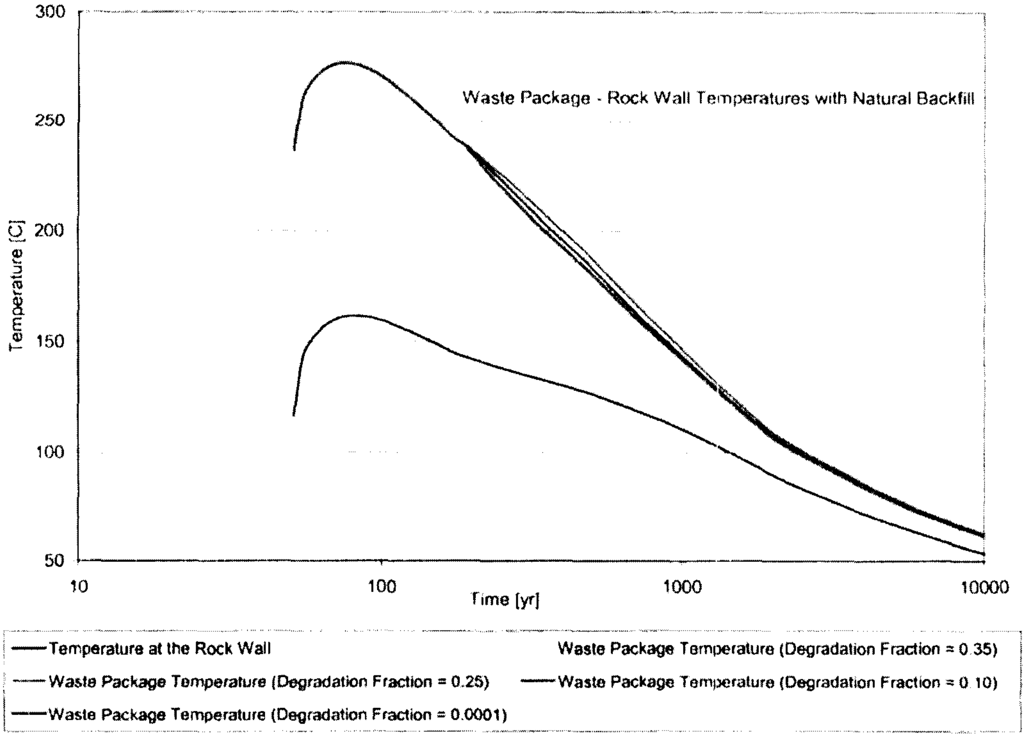
As part of the technical review of the intermediate milestone, Doug Gute questioned the radial symmetry assumption for the drift degradation and rubble pile formation. To address his question, we quickly added a third leg to the thermal network, and a new parameter that specified the portion of the arc taken up by the vertical leg (Leg 3 is vertical leg).

Leg 1: through the invert, same as before.

Leg 2: laterally from the waste package to drip shield through rubble on the side of the drip shield and to the drift wall. Note the springline of the drift wall does not degrade, and thus provides the maximum thickness constraint on the rubble in this leg.

Leg 3: vertically from waste package to drip shield through rubble pile and to ceiling of degraded drift. Note the ceiling of the drift degrades and changes position. Also note that the rubble pile can continue to increase thickness beyond the original position of the drift ceiling.

George made the changes to the routine, provided the hand calculations to verify the routine was acting as expected, and provided a spreadsheet with the results. The hand calculations are retained in self-explanatory files (George also probably has these as part of SciNtbk #532):
.\Sensitivity-June2003\Fraction-VerticalConductance*
The results are contained in the Excel 97 SR-2 spreadsheet
.\Sensitivity-June2003\vertical-testresults6-17-03.xls



From the figure (three legs of the heat transfer algorithm), it is noted that early on, no difference in temperature occurs. It is not until the rubble thickness has reached the side wall that a difference is noted. Then a 5-10 C difference is noted in waste package temperature.

Different fractions for the vertical leg arc were tried. Low values should collapse back to the two-leg algorithm results.

End Insert 6/17/03

6/2/03 RF

TPA-Based Results to Compare Against Metra Results (No-Degradation Scenario)

The analyses for one chapter of the intermediate milestone were to be provided by Chandrika Manepally

George Adams provided Chandrika TPA-based results to compare with her Metra results. See their respective scientific notebooks for details; George's (#532) and Chandrika's (#478). I provided guidance and made sure that George knew to use the corrected version of the in-drift heat transfer algorithm (George's TempSurf module modifications? See email below, and see his SciNtbk #532e). TPA had to be run for set locations (edge or center), which is a flexibility that the TPA approach has, and thus TPA approach automatically takes care of the heat load for edge and center locations. Note that Chandrika has to modify the heat load input for Metra to account for an edge location. George Adams used TPA4.1j code, made the modifications indicated to address the errors found by Steve Green (see previous entry on errors in TPA in-drift heat transfer algorithm), performed hand-calculations to verify that the routine was acting as expected, and documented all this in his sci ntbk #532e.

For the different cases, the thermal conductivity of the host rock in tpa.inp (TPA control input file) was set to a constant value and TPA was run to produce temperature profiles for Chandrika to compare with her thermohydrology results developed using Metra. To represent edge locations, a saturated thermal conductivity value was used (Kth=2.02 W/m-K) for the Tptpll (Topopah Springs lower lithophysal). To represent a center location, the TPA average thermal conductivity for the host rock was used (Kth=1.56 W/m-K). George ran the cases we requested and provided the output imported into Excel spreadsheets (Excel 97 SR-2).

From: George R Adams [george.adams@swri.org]
Sent: Tuesday, May 06, 2003 1:45 PM
To: Chandrika Manepally; Randy Fedors
Subject: TEMPERATURE AT THE WASTE PACKAGE SURFACE AND RELATIVE HUMIDITY

Randy, Chandrika,

Please find attached an Excel Spreadsheet showing some plots of waste package surface temperature and relative humidity information.

The first plot is waste package surface temperature and rock wall temperature. The upper curve is the output generated from the TempSurf module. I took the information from tpa4.1j and made corrections to the equations. The bottom plot is a base case tpa4.1j for one subarea and one realization run at 10,000 years. The spreadsheets show the hand calculations I did for the TempSurf code to verify its output.

The second plot, Tabular Temp-RH Comparison, is a run of the basecase tpa4.1j code using the tefkti.inp file of tabular temperature versus relative humidity information. Even though the file contains four sets of data, the four sets are all the same.

The third plot, Comparison Base-Tabular, is a comparison of the tpa4.1j base case temperature and relative humidity and the tabulated temperature and relative humidity.

George

11/5/03 RF

TPA 5.0 – DRIFT DEGRADATION TEMPERATURE ESTIMATES

Collaborators
George Adams: Scientific Notebook # 532e
Chandrika Manepally: Scientific Notebook #478e
Steve Green (Division 18): Scientific Notebook #536e

Objective:

We created the poster for Fall 2003 AGU Meeting on drift degradation using the spreadsheets that George has been maintaining for calculations using the thermal network algorithm for in-drift temperatures. The poster extended the analyses (using the same tools) presented in the intermediate milestone "THERMAL CONDUCTIVITY, EDGE COOLING, AND DRIFT DEGRADATION—ABSTRACTED MODEL SENSITIVITY ANALYSES FOR YUCCA MOUNTAIN" (R. Fedors, G. Adams, C. Manepally, S. Green, June 2003). George and I had modified the algorithms in the TPA 5.0 using Steve Green's recommendation for the basic equations. This modification was done on an exploratory basis to evaluate the approach prior to inserting the approach into the next version of TPA code.

One significant correction incorporated into the results for the AGU poster, compared to the Fedors et al. (2003) report, was that the time frame for MechFail module in TPA was made consistent with the pre-closure/post-closure distinction. Previously, RDTME folks thought TPA time started at the time of closure (they believed the 50 years of operation were not simulated by TPA). Hence, their MechFail calculations essentially had degradation starting during the operation period. The MechFail correction is outside the realm of our work, so is not discussed further here.

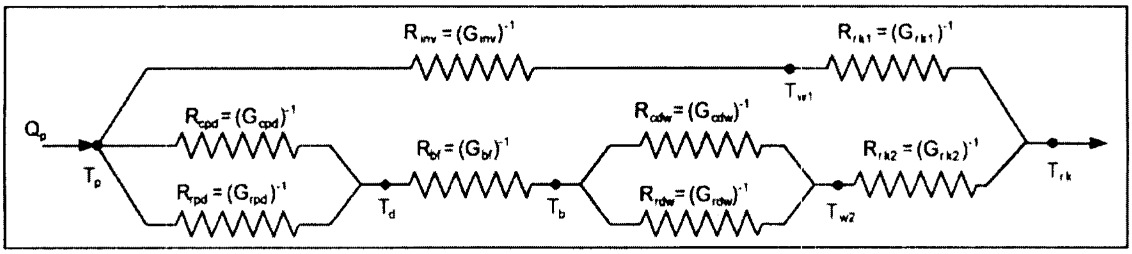
Three other aspects were explored in greater detail for the Fall 2003 AGU poster: (i) the effect of moving the outer boundary condition into the host rock, (ii) the 3-leg wedge thermal network to assess the effect of asymmetry, and (ii) the effect of the linearization of the nonlinear processes of radiation and convection.

Approaches

The figures in the Fall 2003 AGU poster were derived using the same tools as used for the Fedors et al. (2003) CNWRA report. The Fall 2003 AGU poster supports the submitted abstract: "Effects of Drift Degradation on Environmental Conditions in Drifts" by Chandrika Manepally, Randall W. Fedors, George Adams, Steve Green, Doug Gute. Doug Gute contributed the figures on drip shield alloys as a function of temperature.

Revised analyses in the poster that are not found in the Fedors et al. (2003) report are focused on calculations that used the outer boundary condition shifted from the TPA location at the drift wall (Z=2.5m, which is almost the drift radius) to 5 m from the drift wall. While the approach was discussed and presented in Fedors et al. (2003), the analyses were expanded to better illustrate the effect of the boundary condition. The position of the boundary condition was shifted from the drift wall to a position further into the host rock. This was done to lessen the effect of the conduction-only, mountain-scale analytical model estimate that was used as the drift wall temperature. Note that the 3-D conduction-only equation for mountain-scale heat transfer in TPA (i) does not account for radiation, convection occurring in the drift, (ii) it ignores the presence of airspace, and (iii) it treats the drift space as welded tuff. Asymmetry and linearization assumptions were also tested.

The basic thermal network and associated equation for the algorithm are:



$$Q_{wp} = \left\{ \left[\frac{1}{G_{inv}} + \frac{1}{G_{rk1}} \right]^{-1} + \left[\frac{1}{G_{cpd} + G_{rpd}} + \frac{1}{G_{bf}} + \frac{1}{G_{cdw} + G_{rdw}} + \frac{1}{G_{rk2}} \right]^{1} \right\} \left(T_{wp} - T_{rk} \right)$$

where Q_{wp} is the heat supplied by the waste package and G refers to the conductance terms, which are the inverse of the resistance, R. The subscript *inv* refers to the invert, *rk1* and *rk2* to conduction in the rock below the invert and above the drift, *cpd* and *rpd* to convection and radiation between the waste package and the drip shield, *bf* to conduction through the backfill if present, *cdw* and *rdw* to convection and radiation between the drip shield or backfill and the drift wall. T_{wp} and T_{rk} refer to temperatures at the waste package and in the rock. T_{rk} is the boundary condition for the in-drift algorithm and is obtained from the mountain-scale conduction-only model at the position further into the host rock (not z=2.75 m).

The Fall 2003 AGU poster also included more analyses using the 3-leg thermal network, which is also referred to a the wedge (the vertical thickness of the rubble pile can be much greater than the lateral thickness, thus the wedge terminology). The ceiling of the drift would degrade, thus an ever thickening pile of rubble would occur as the ceiling degraded. The sidewall of the drift would limit the thickness of the rubble pile laterally to the distance between the drip shield the original drift wall. Modifying the algorithm was straightforward and the revised routine was documented by George Adams (SciNtbk #532). The thermal network figure above, and the corresponding equation, were developed in response to a technical reviewer comment for Fedors, et al. (2003), but was not analyzed in great detail in that report.

These analyses are considered exploratory analyses to illustrate the effect of different aspects of the configuration and conceptual model. Analyses for (i) shifting the boundary condition further into the host rock, (ii) use of the 3-leg network or wedge (accounting for asymmetry), and (iii) the iterative approach are both described in George's scientific notebook (SciNtbk #532e). The equations for each of the G terms are described in the June 2003 intermediate milestone mentioned on page 37 of this notebook (Fedors, et al. 2003). George's scientific notebook #532 provides the documentation and software validation performed on the exploratory routines.

To create a linkage between the figures and information in the poster and the scientific calculations, I am listing the figures and spreadsheets that I used and the George Adams archives cited in George's scientific notebook, #532.

George Adams' archives:

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SPOCKHOMEtpabuild_teftef10-27-03.zip: Thermal Effects Report.xls, tef_backfill_thermal_conductivity_study.xls

SPOCKHOMEtpabuild_teftef10-2-03.zip: iterationreport.xls, handcalculations_iteration.txt, hand_calculations.txt

SPOCKHOMEtpabuild_tef.zip: testresults_wedge.xls, hand_calculationswedge.txt, thermal_0m.dat, thermal_1m.dat, thermal_2m.dat, thermal_3m.dat, thermal_4m.dat, thermal_5m.dat (thermal files for degradation located in directory: tpabuild_tef\documents\degradation)

===

Figures in the poster with spreadsheet and worksheet names, corresponding spreadsheets in George's archive are also listed.

Figure #	Location on Bubo in E:\TEF-kti* (except as noted)	Worksheet	George's spreadsheet name
3	.\Sensitivity2003\Revisions2003\ ThermalEffectsReport-27Oct.xls	"Figure 3-5a (2)"	"Thermal Effects Report.xls"
4	.\Sensitivity2003\Revisions2003\ ThermalEffectsReport-27Oct.xls	"Figure 3-6b 5m-AGU"	"Thermal Effects Report.xls"
5	.\Sensitivity2003\Revisions2003\testresults.xls	"Temperature(5m)"	"testresults_wedge. xls"
6	.\Sensitivity2003\Revisions2003\ iterationcalculation.xls	"temp_keff_nbf(0m)-AGU"	"iterationreport.xls"
7	.\Sensitivity2003\Revisions2003\testresults.xls	"temp_keff_bf(0m)-AGU"	"iterationreport.xls"
8	.\Sensitivity2003\Revisions2003\ tef_backfill_thermal_conductivity_study.xls	"Figure 3-7 5m-AGU"	"Thermal Effects Report.xls"
9	.\Sensitivity2003\Revisions2003\ testresults_wedge.xls	"wedge profile (2)"	"testresults_wedge. xls"
10	Data in both .\Sensitivity2003\Revisions2003\ ThermalEffectsReport-27Oct.xls **and** .\Sensitivity2003\Revisions2003\testresults.xls plotted in testresults.xls	"No Backfill 0m" and "No Backfill 5m" form 1st file added to 2nd file listed. Plotted in "Compare Twp"	"testresults_wedge. xls" **and** "Thermal Effects Report.xls"
11	from Doug Gute		

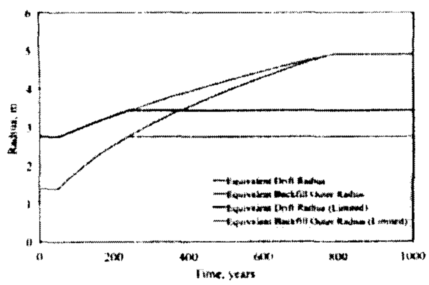

Figure 3.

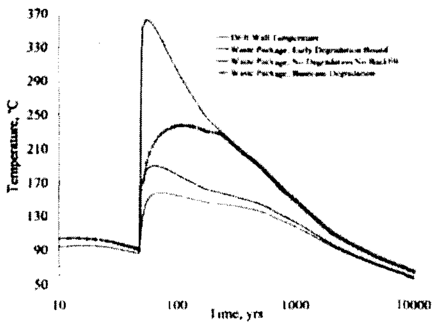

Figure 4.

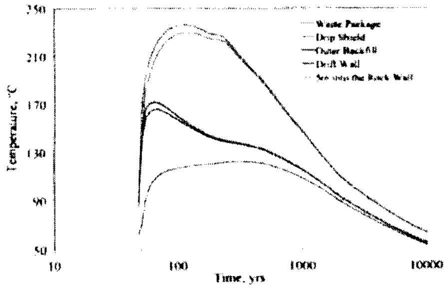

Figure 5

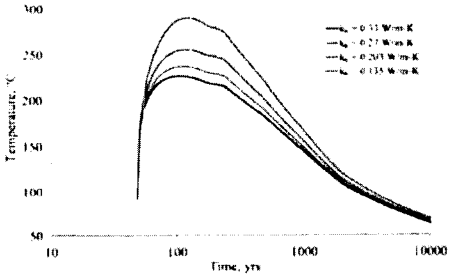

Figure 8

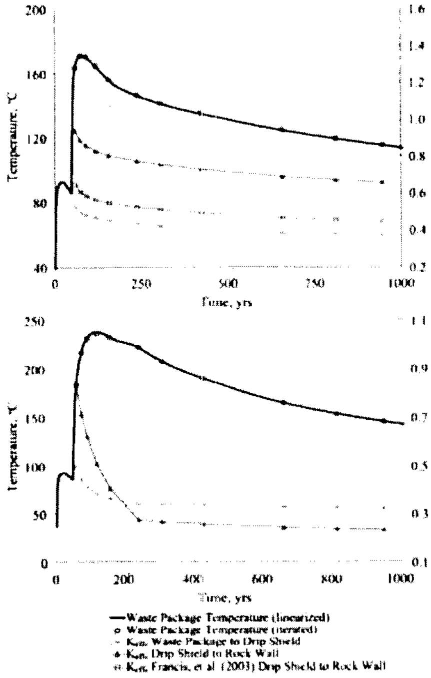

Figure 6 and Figure 7

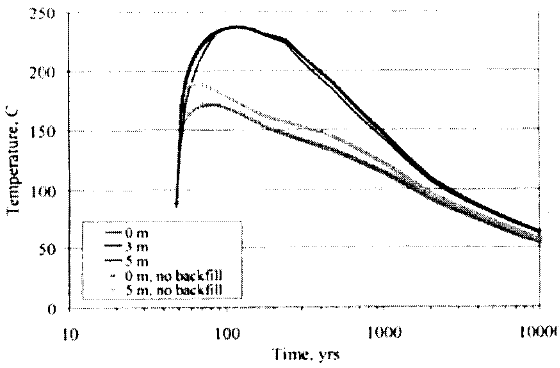

Figure 10

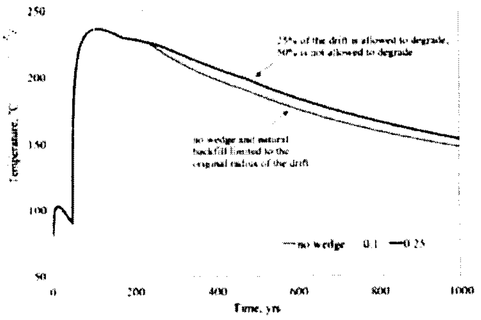

Figure 9

11/13/03

SME 2004 Proceedings Paper

Collaborators
George Adams: Scientific Notebook # 532e
Chandrika Manepally: Scientific Notebook #478e
Steve Green (Division 18): Scientific Notebook #536e

Objectives

I wrote the proceedings paper for the SME 2004 Annual Conference in Denver Colorado (Feb 22-24, 2004) titled: Evaluation of Large-Scale Temperature Gradients to Support Assessment of Convection and Cold-Trap Processes in Heated Drifts (Fedors et al.). The focus of the SME proceedings paper was to assess temperature gradients along a drift. The proceedings paper also included some of the results put in the Fall 2003 AGU poster

Analyses

George continued to maintain the algorithms and create the spreadsheets for using the heat transfer network algorithm for in-drift temperatures. The data and figures in the proceedings paper were derived from the analyses maintained in George's spreadsheets. Hence, all that is reported here is the linkage between George's archives and the data and figures in the paper. I created new plots or modified George's plots for the figures in the proceedings paper. Modifications to the heat transfer algorithm that I asked George to make since the AGU poster (see sci ntbk 432, pages 48-50) include the use of thermohydrologic modeling results as the boundary conditions at 5m for the in-drift heat transfer algorithm. Previously we had used the mountain-scale conduction-only model results for the boundary condition. The routine used to calculate gradients along the drift is described on pages 13-19 of this volume (SciNtbk #432, Volume VIII), and was modified by George (see SciNtbk #532).

George Adams Archive (see his SciNtbk#532):

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SPOCKHOMEtpabuild_teftef10-22-03.zip: EdgeEffectDegradation.xls
SPOCKHOMEtpabuild_teftef11-13-03.zip: early_east.xls
SPOCKHOMEcondxyzttemperaturegradientplots10-16-03.zip: condriveavgdrift25east.xls, condriveavgdrift25west.xls
SPOCKHOMEtpabuild_teftef10-2-03.zip: iterationreport.xls, handcalculations_iteration.txt, hand_calculations.txt

==

Figure #	Location on Bubo in E:\TEF=kti*	Worksheet and pdf file	George's Spreadsheet name
1	E:\AVData\TEF-EdgeEffect\sensitivity2003.apr	see sci ntbk #432, volume VIII, page 36	-
2	.\ColdTrap\Conduction\George2\ condriveavgdrift25east.xls	"TemperatureDifference" & "LocalGradient-Smoothed" .pdf	same name
3	.\ColdTrap\Conduction\George2\ condriveavgdrift25east.xls and condriveavgdrift25west.xls	"SignificantGradientPlot" in each spreadsheet; used 5-pt smoothing of noisy data	same name
4	.\Sensitivity2003\Revisions2003\ Chapter2_Figures.xls	"FigureE-WPRH TPAMetra" and "FigureD_WP Temp TPA Met(2)"	Chandrika's
5	.\Sensitivity2003\Revisions2003\	"temp_keff_nbf(0m)-SME"	same info as in

	iterationcalculations.xls	"temp_keff_nbf(0m)-SME" center-nobkfl-degrad.pdf	iterationreport.xls
6	.\Sensitivity2003\Revisions2003\ east-early-temperatureprofile1.xls	"east-center-SME" degrad-east-ctr.pdf	Combined "early-east.xls" and "temperatureprofile1.xls"
7	.\Sensitivity2003\Revisions2003\ east-early-temperatureprofile1.xls	"thermal_5m_drift25temps-SME" bound-degrad.pdf	Combined "early-east.xls" and "temperatureprofile1.xls"

Thermal conductivity values used for the host rock in the conduction-only model in the

1.945 W/m-K average of wet and dry thermal conductivity of the middle nonlithophysal unit, MSTHM AMR Rev00

1.61 W/m-K average of wet and dry thermal conductivity of the lower lithophysal unit, MSTHM AMR Rev 00

1.56 W/m-K mean case for the TPA 4.1j and 5.0

The thermohdyrological results were provided by Chandrika Manepally (SciNtbk #478). The thermohydrological results were used two ways (i) to compare with the conduction-only and in-drift heat transfer algorithm results, and (ii) as input to the in-drift heat transfer algorithm as a replacement for the conduction-only model.

A comparison was included in the SME paper between conduction-only results and the in-drift algorithm (includes degradation and hydrology):

	center & edge T °C	ΔT at Peak	center & edge T °C	ΔT At 1000 yrs	center & edge T °C	ΔT When Center Reaches 80 °C	Source spreadsheet
Conduction-Only Model	160	71 °C	113	46 °C	77	26 °C at 3960 yrs	condriveavgdrift25east.xls worksheet "condrive drift 25"
	89		66.5		51		
Base Case Drift Degradation, In-Drift Algorithm and Thermohydrologic Model	223	86 °C at 128 yrs	135	39 °C	79.3	20 °C at 6260 yrs	east-early-temperatureprofile1.xls plot in worksheet "east-center_SME"
	137		96		59.2		

An approximate temperature gradient over the simulated zone of condensation was calculated from figure 3-22 to 3-24 in Fedors, et al. (2003, "Laboratory and Numerical Modeling of the Cold-Trap Process," CNWRA Report)

The gradient was calculated for two distances from the 3 profiles in Figures 3-22, 3-23, and 3-24. Then the result was scaled according to Frank Dodge's scaling rules [see Sci Ntbk #432, Volume VII, or see Fedors, et al. (2003, Cold-Trap report)]. Approximate temperatures are read from graphs using the measured temperature data. The condensation zone comes from Figure 3-19 of the cold trap report.

For the axial distance from 0.279 m (heater) to profile at 0.165 m
$\Delta T/\Delta x$ = (45-32 °C)/ (0.279-0.165 m) = 114 °C/m

Scaling follows $\Delta T_{drift}=\lambda^{b}*\Delta T_{lab\ model}$ where b=1.75 and λ=0.01 (1% scale lab model)
which leads to $\Delta T_{drift}=(0.01)^{1.75}$ * 114 °C/m = 0.036 °C/m

For the axial distance from 0.279 m (heater) to profile at 0.0.063 m
$\Delta T/\Delta x$ = (45-29 °C)/(0.279-0.063 m) = 74.07 °C/m
Scaling follows $\Delta T_{drift}=\lambda^{b}*\Delta T_{lab\ model}$ where b=1.75 and λ=0.01 (1% scale lab model)
which leads to $\Delta T_{drift}=(0.01)^{1.75}$ * 74.07 °C/m = 0.023 °C/m

Since it is not clear which gradient to use, just use a range or take an intermediate value. Note that the condensation rate drops off asymptotically before the mid-point of the experiment drift is reached (mid-point = 0 m).

RF April 11, 2004

Metra Modeling of Radiation and Drift Degradation

Objective:

Help Chandrika Manepally and Alex Sun with Metra modeling of radiation and of drift degradation. The radiation inclusion is to assess in-drift heat transfer when air gaps are still present. The drift degradation part is to compare Metra results with the in-drift heat transfer algorithm/abstraction slated for TPA code. As part of my contribution, I checked the restart option in MULTIFLO so that Alex could use the restart with different property assignments to mimic transient rubble pile formation, and I checked TOLR and LIMIt settings for speeding up the simulations.

Lead: Chandrika Manepally

Collaborators: Alex Sun and Randy Fedors

Restart and Fine-Tuning Simulation Clock Times

Checking the restart option in MULTIFLO and TOLR and LIMIt settings for speeding up the simulations for Alex Sun and Chandrika.

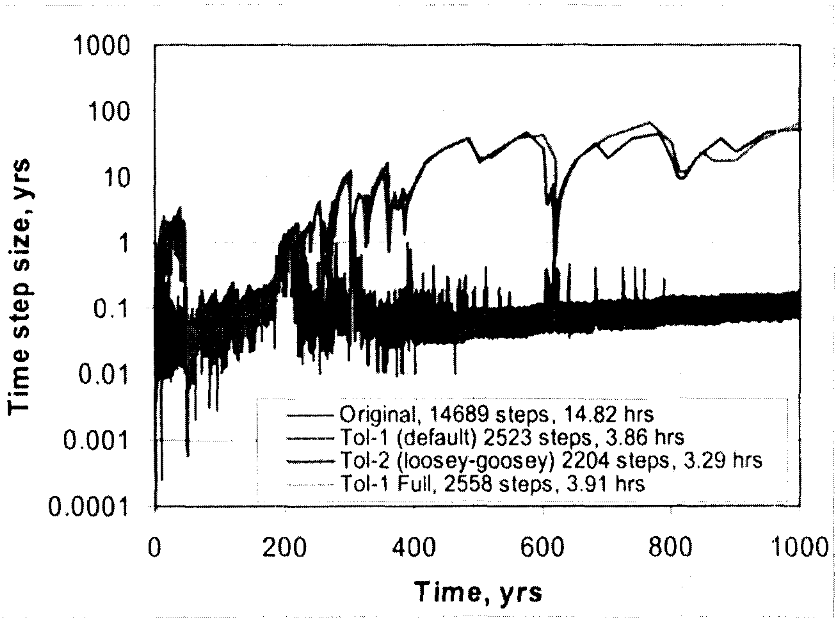
Used Alex's drift-scale unstructured grid (in case the restart worked for structured grids and not for unstructured grids).

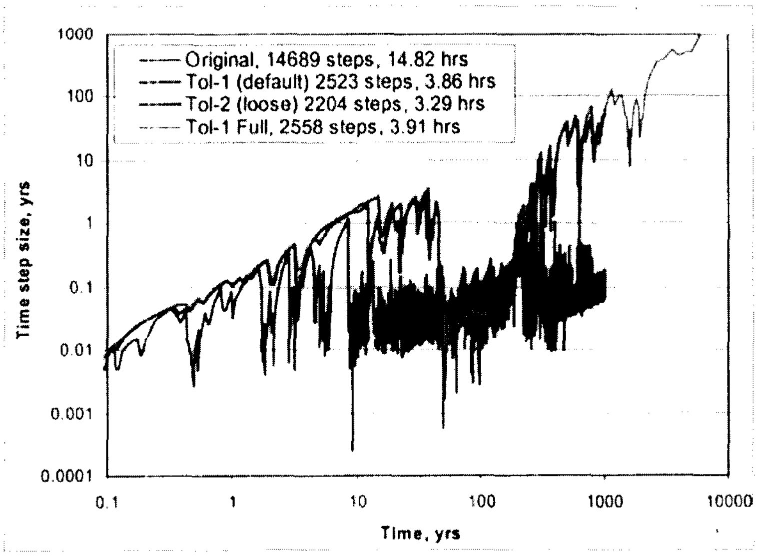
Spock ~rfedors/Metra/2D-UnstructDrift/*
./compare.xls and ./restart.xls

Nobody else was running on the SUN cluster, so cpu times are taken as clock time. CPU time is taken from end of "out" file, Total Metra Exec. =

./Original/*	input files from Alex run without modification except reduced end time to 1000 yrs (note tight tolerances). Run time = 14.82 hrs.
./Tol-1/*	changed TOLR and LIMIt inputs to default values. Run time = 3.86 hrs.
./Tol-2/*	loosened tolerances and step limits. Run time = 3.29 hours.
./Tol-1_full/*	tolerances between the tight (Original) and default (Tol-1) values.
./Tol-1restart/*	restarted ./Tol-1/* at 100 yrs to check on restart option; manipulated target times and added 3.15e9 to RSTART 0 3.15576e+9 Boundary conditions and sinks go by time + restart-time; output times go by time. Run time 1'48"

Large drop in time step size that lead to bogging down of simulations occur at 49, 256, 300, 620, 1600, 1910 yrs. *See worksheet "time steps" in ./compare.xls for plots*





Loosening the tolerances did significantly help in the computational clock time, but did the results change? Still there are some curious blips in the time stepping that periodically occur, which will be a subject for future efforts.

Original Setting As used by Alex, they seem to be very tight tolerances and limits

```
:TOLR    TOLP    TOLS     TOLT     TOLP2    TOLM     TOLA      TOLE     rtwotol  rmxtol    smxtol
Tolr      1.0    1.e-6    1.e-3    1.0      1.e-6    1.e-5     1.e-4    1.e-10   1.e-10    1.e-10
:
:Limit   dpmx        dsmx  dtmpmx     dpamx     dtmn     dtmx         dtfac
LIMIT   1.00E+05     0.08   6.0       1.00E+05 1.00E-10 1.00E+05     0.334
```

Tol-1 Settings

```
:TOLR          TOLP    TOLS     TOLT     TOLP2    TOLM     TOLA      TOLE     rtwotol  rmxtol    smxtol
Tolr            10.    1.e-4    1.e-3    10.      1.e-5    1.e-3     1.e-3    1.e-10   1.e-10    1.e-10
:
:Limit         dpmx          dsmx  dtmpmx     dpamx     dtmn      dtmx          dtfac
LIMIT          5.0E+04       0.08   10.        5.0E+04 1.00E-10 1.00E+05     0.334
```

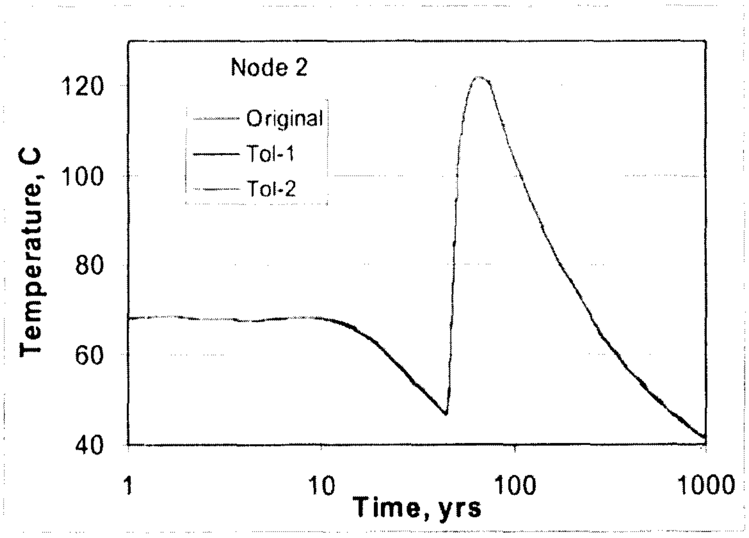
Tol-1 full Settings

```
:TOLR          TOLP    TOLS     TOLT     TOLP2    TOLM     TOLA      TOLE     rtwotol  rmxtol    smxtol
Tolr            10.    1.e-4    1.e-3    10.      1.e-5    1.e-3     1.e-3    1.e-10   1.e-10    1.e-10
:
:Limit         dpmx          dsmx  dtmpmx     dpamx     dtmn      dtmx          dtfac
LIMIT          5.0E+04       0.08   10.        5.0E+04 1.00E-10 1.00E+05     0.334
```

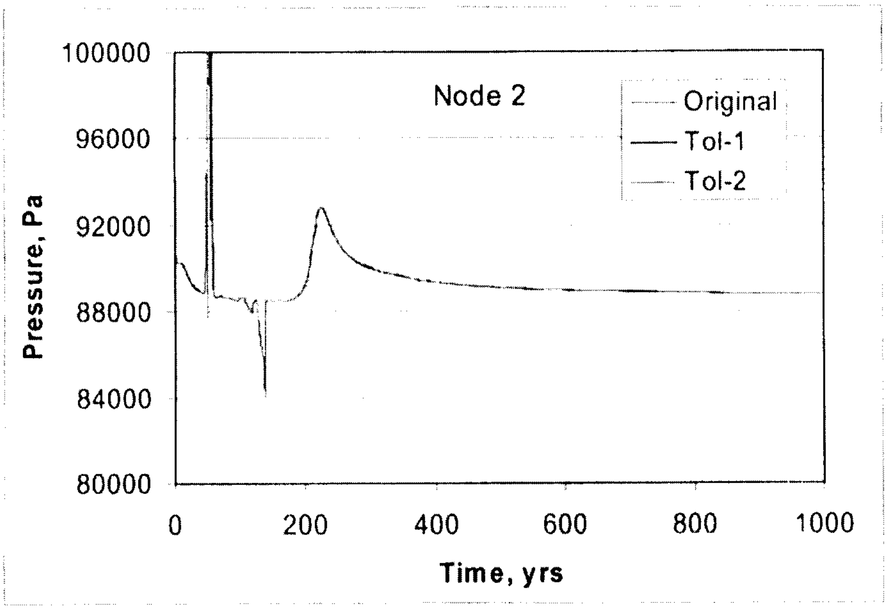
Tol-2 Settings

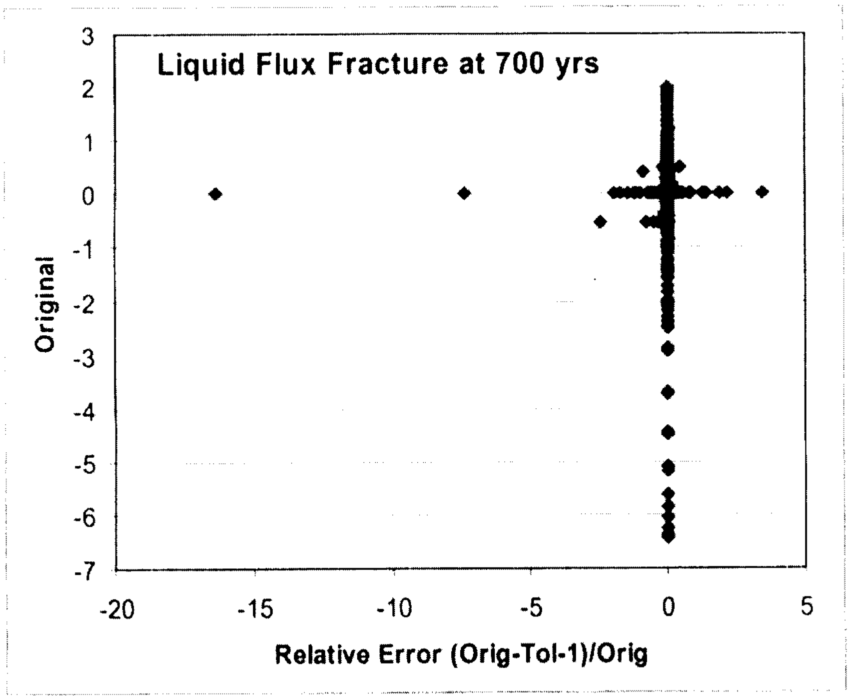
```
:TOLR    TOLP    TOLS     TOLT     TOLP2    TOLM     TOLA      TOLE     rtwotol  rmxtol    smxtol
Tolr      20.    2.e-4    4.e-3    20.      1.e-4    1.e-3     1.e-2    1.e-10   1.e-10    1.e-10
:
:Limit   dpmx        dsmx  dtmpmx     dpamx     dtmn      dtmx         dtfac
LIMIT   5.0E+04     0.10   10.       5.0E+04   1.00E-10 1.00E+05     0.334
```

.For a comparison of temperatures, pressures, and fluxes at node 2, see worksheets "drift_tmp Tol-1", "drift_press Tol-1", and "Compare Flux" in spock: ./comparison.xls



Temperature results (above) and pressure results (next page) indicate no visually recognizable difference in results over time for node 2 (which is located near the drift).



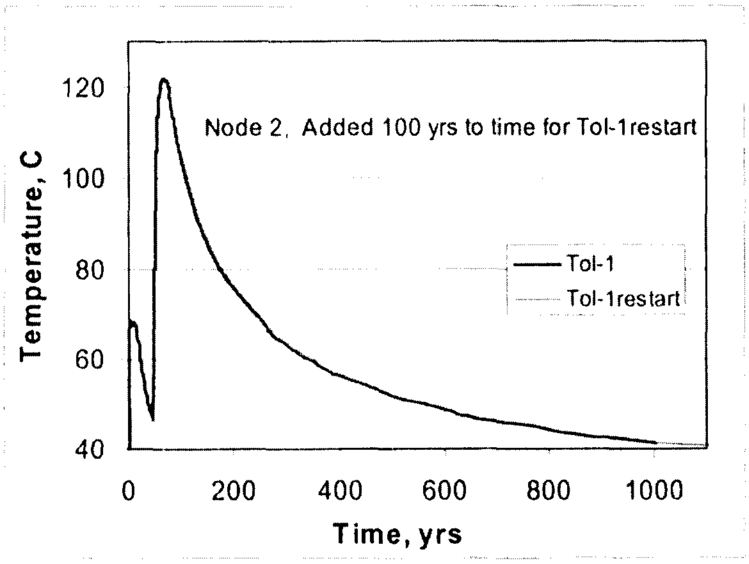


Only a couple outliers in the flux comparison for all the nodes in the grids; these outliers suggest only minor differences in results when tolerances are loosened.

Rather than waste time with the degradation model, I did a quick test to ensure that we knew how to restart Metra. The degradation modeling will be a large number of restarts, with properties of grid cells changing at each restart.

spock: ./restart.xls

The figure below for node 2 illustrates that the method described above works. The plot is from worksheet "drift_tmp Tol-1" in the spreadsheet restart.xls



RF 5/17/04

Analyses to Support In-Drift Heat Transfer Approach in Metra

Helping Chandrika Manepally and Alex Sun with the MULTIFLO modeling for the TEF intermediate milestone. The topic is a coupling in-drift and wallrock processes, including drift degradation.

All work is done in
bubo: E:\TEF_kti\Sensitivity-June2003\METRA_ModelingDegradation2004*
spock: ~/EdgeEffect/InDrift-March2004/* with results stored in ./Results_May2004/*

There are three ways to simulate heat transfer across air gaps in the drift using MULTIFLO: (i) direct process modeling by using 1D radiation module in MULTIFLO 2.0; (ii) use appropriate effective thermal conductivity for air cells (nodes) that accounts for convection and radiation; and (iii) link an in-drift algorithm or CFD code to the drift wall boundary conditions in MULTIFLO thus having MULTIFLO only directly calculate the wallrock processes.

The last approach cannot be done, linkage to MULTIFLO would require modifications to the code. While these changes were discussed with the code author and initially agreed on, they mysteriously got left out of the Software Requirements Description for MULTIFLO 2.0. Ditto for the effective thermal conductivity as a function of temperature or time. We can get around the constant effective thermal conductivity limitation by manually restarting the code when we want to change the value, but these necessarily coarse step changes are obviously is poor representation of the continuous variation expected. The restart approach is exactly how we are incorporating the drift degradation and cell/node property changes over time. Alex is using about 5 or 6 different periods as step changes to represent the continuously varying drift ceiling height and buildup of the rubble pile. It's too bad that "exploratory" code changes are not allowed with MULTIFLO for anyone else besides the code author, who is too busy to maintain the code adequately.

The in-drift heat transfer algorithm will be used to estimate temperatures a priori. These temperatures will be used to estimate the effective thermal conductivity of air cells that accounts for convection and radiation. This approach for estimating effective thermal conductivity that reflects convection and radiation for use in air cell/nodes of MULTIFLO will be performed for three scenarios

- no degradation (NBF, which stands for no backfill) [Case 2 in Fedors et al., 2003 2004]
- with degradation (BF, which stands for backfill) [Case 3 in Fedors et al., 2003 2004]
- with and without drip shield [Case 1 and Case 2 in Fedors et al., 2003, 2004]

The work uses results from our (George Adams, R Fedors, Steve Green) algorithm, run on spock.

The results are analyzed in Excel spreadsheets
bubo: ./degrade_May2004.xls (imported results from algorithm, plots of temperature)
./iterationreport_May2004.xls (BF and NBF)
./iterationreportCase-K1.59_May2004.xls
./iterationreportCase-K2.02_May2004.xls

The iterative approach is used in these spreadsheets, with initial and constant parameter values coming from the modified TPA run with the algorithm. The iterative approach is used because I wanted flexibility to change parameters without rerunning the code, and then have results of my calculations of effective properties automatically updated.

++++++++++++++++

RF 5/20/04

Because the radiation module in MULTIFLO 2.0 requires view factors, Alex and Chandrika simplified the problem by ignoring the drip shield; i.e., radiative heat transfer directly from the waste package to the drift wall. But we know that the waste packages temperature differ significantly when a drip shield is added.

The in-drift heat transfer algorithm will be used to estimate temperatures a priori with and without a drip shield. These temperatures will be used to estimate the effective thermal conductivity of air cells that accounts for convection and radiation with and without a drip shield.

Calculation of Temperature Profiles

The spreadsheet

Bubo: .\degrade_May2004

was developed by importing results from George's build5 code, which he provided as tpa50drift (Sci Ntbk #532e).

The results from these simulations (thermal.dat) are imported into a spreadsheet

Spock: ~/EdgeEffect/InDrift-March2004/tpa50drift/* code from George
Spock ~/EdgeEffect/InDrift-March2004/Results_May2004/* archive simulation results

To run tpa50drift, place the appropriate external files in the ./tpa50drift/data/ directory

The files to change are eqradius.dat (has drift and rubble thicknesses)

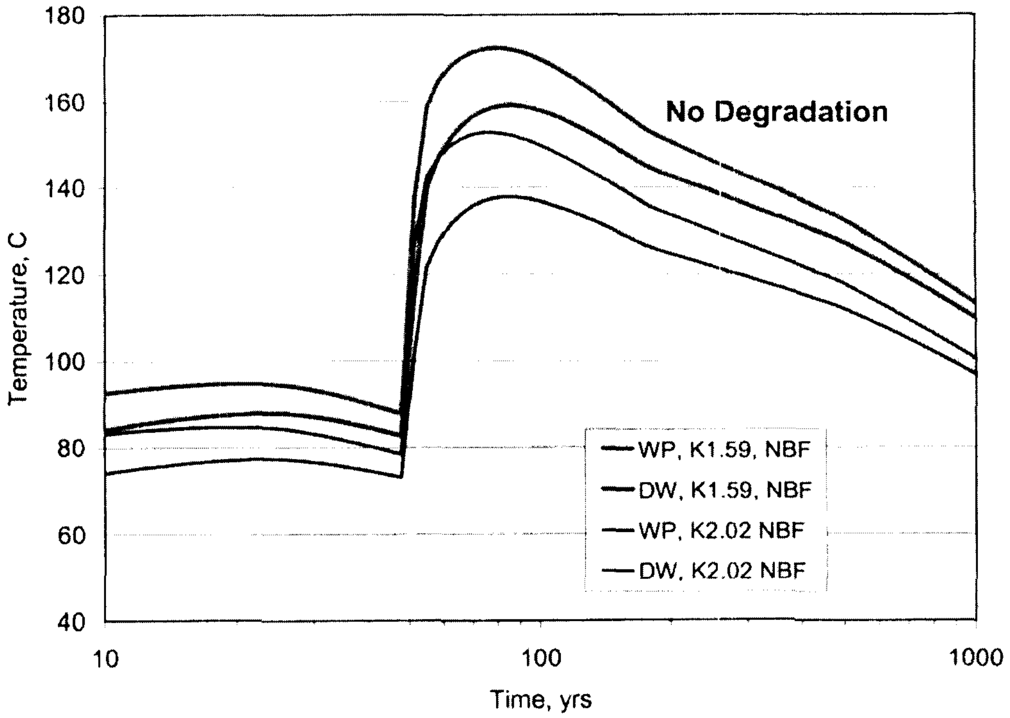
Set the environment variable TPA_TEST and TPA_DATA to the ~/tpa50pdrift directory

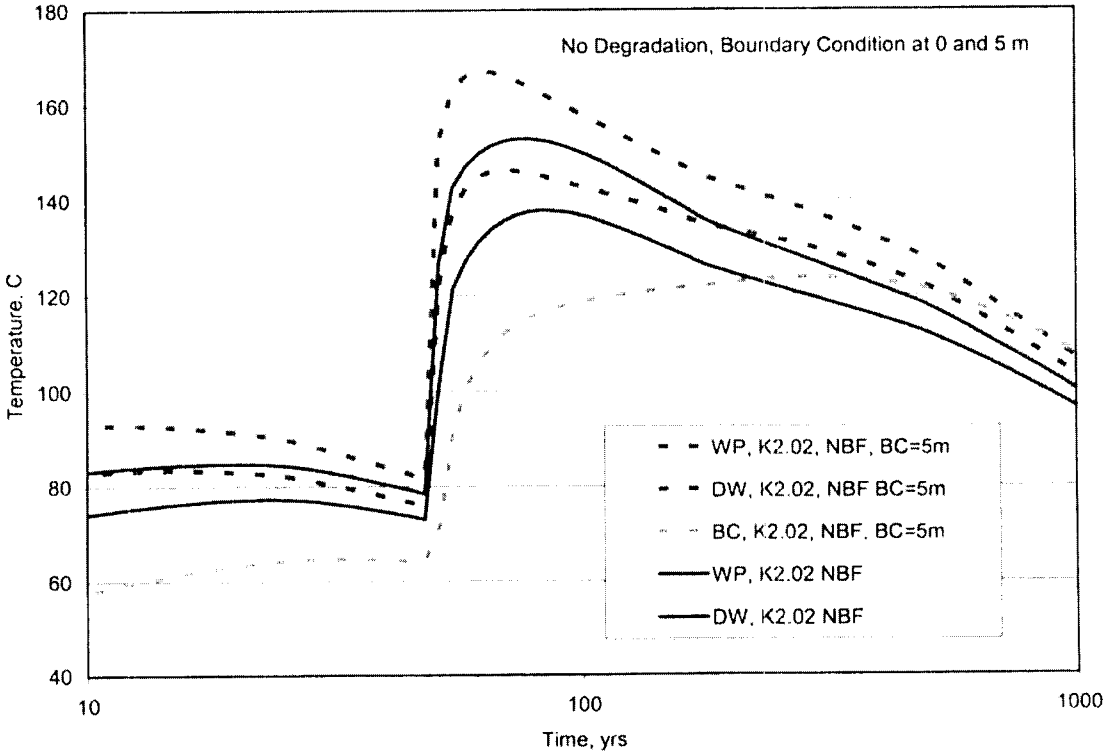
Edit the tpa.inp file to use the Model 1 thermal model, the correct host rock thermal conductivity, make sure the 1 realization (mean case) is used, and subarea 1

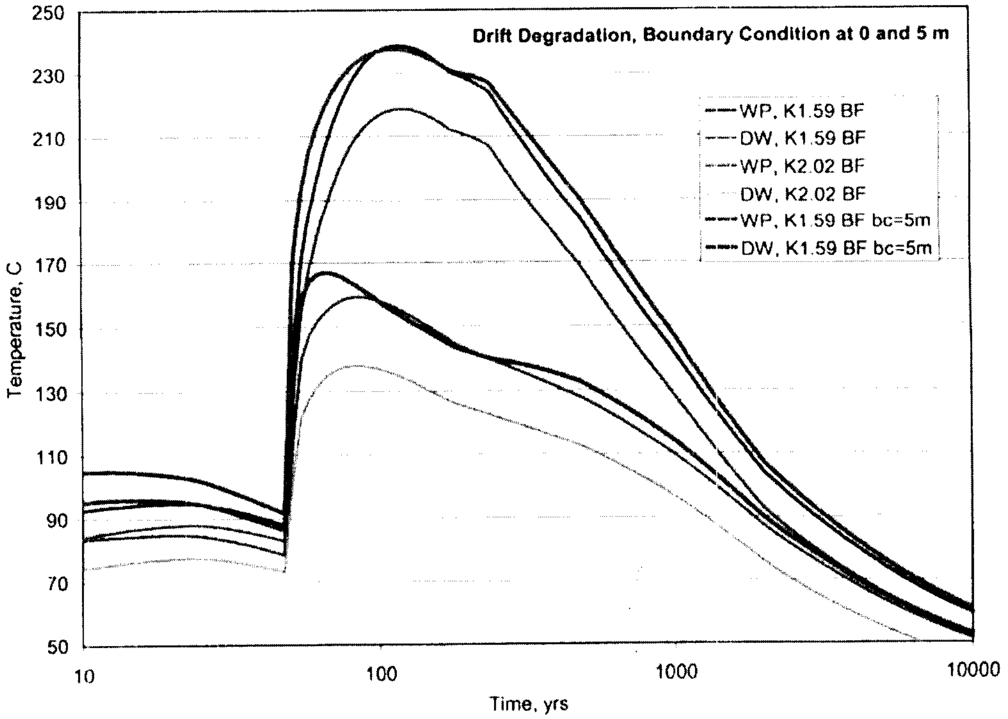
The results of the simulation are found in thermal.dat, which I save under appropriately named files in

Spock: ~/EdgeEffect/InDrift_March2004/Results_May2004/*

These output files were then imported into the spreadsheet degrade_May2004.xls with worksheets named according to backfill (BF) or nobackfill (NBF) and host rock thermal conductivity, and distance of boundary condition into the host rock (0 m is the drift wall).




No Degradation, Boundary Condition at 0 and 5 m
Temperature, C
Time, yrs
180
160
140
120
100
80
60
40
10
100
1000
WP, K2.02, NBF, BC=5m
DW, K2.02, NBF BC=5m
BC, K2.02, NBF, BC=5m
WP, K2.02 NBF
DW, K2.02 NBF


Drift Degradation, Boundary Condition at 0 and 5 m
Temperature, C
Time, yrs
250
230
210
190
170
150
130
110
90
70
50
10
100
1000
10000
WP, K1.59 BF
DW, K1.59 BF
WP, K2.02 BF
DW, K2.02 BF
WP, K1.59 BF bc=5m
DW, K1.59 BF bc=5m

lf 6/10/04

Calculation of Effective Thermal Conductivity of Air Cells

Bubo: E:\TEF-kti\Sensitivity-June2003\METRA_ModelingDegradation2004*
Spock: ~/EdgeEffect/InDrift-March2004/tpa50drift/* code from George
Spock ~/EdgeEffect/InDrift-March2004/Results_May2004/* archive simulation results

First I ran George's build5 code, which he provided as tpa50drift (Sci Ntbk #532e), as described in the previous section. The results from these simulations (thermal.dat) are imported into a spreadsheet
Bubo: .\degrade_May2004.xls
These results include degradation and no-drift degradation results for two thermal conductivity values for the host rock (1.59 and 2.03 W/m-K).

For the no degradation scenario, for use in comparing Metra radiation module results against Metra results obtained using effective thermal conductivity values for air gaps, the spreadsheets

Bubo: .\iterationreportCase1-K1.59_May2004.xls
Bubo: .\iterationreportCase1-K2.02_May2004.xls

The wet thermal conductivity of the lower lithophysal unit is 2.02 W/m-K per the MSTHM AMR Rev 00, and the mean case for the TPA 5.0 code is 1.59 W/m-K.

To obtain results for Metra modeling when drift degradation was occurring, I created
Bubo: .\iterationreport_May2004.xls using the K_{th}=1.59 W/m-K results

George started the original iteration spreadsheet when he was comparing iterative solutions to the in-drift heat transfer algorithm. I modified the spreadsheet to get temperatures at different times (note different worksheets for different times. If I remember correctly, George created the iteration spreadsheet to do a hand calculation. I added many worksheets to the original one, then created two other spreadsheets using my first modified iteration spreadsheet as a template. The results of each temperature estimate at each time are summarized in the worksheets:
"EffectiveK Summary BF" for the backfill scenario
"EffectiveK Summary NBF" for the no-backfill scenario

Once I have the temperatures, conductances, and other paramlerts , I back out an effective K to use in the Metra modeling for air cell that accounts for radiation and convection. I did these calculations over time so that I could pick representative and a range of effective thermal conductivity of air cells for them to use.

To calculate effective thermal conductivity of air cells that accounts for the radiative and convective heat transfer, use the following equation for a no-drip shield model with the temperatures calculated using a drip shield model.

$$Q = G * (T_{wp} - T_{dw})$$

where G can be redefined as $G=K_{eff} * C_i$ as in the conduction equation (and convection approximation) and where

$$C_i = \frac{2 f_c \, \pi\left(L_{wp} + 2\delta\right)}{\ln\left(\frac{D_{outer}}{D_{inner}}\right)}$$

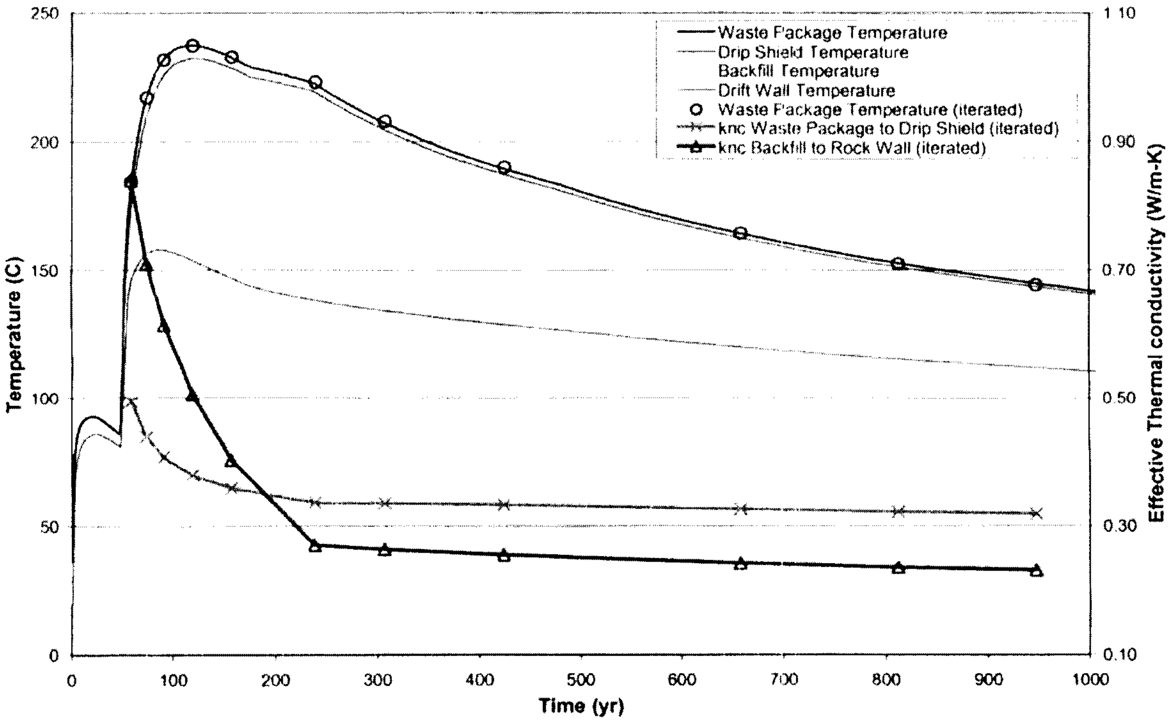
The different diameters are for waste package, drip shield, backfill, and drift wall. Thus there will be a Ci for each air gap; i.e., $C_{wp\text{-}dw}$, $C_{wp\text{-}ds}$, and $C_{ds/bf\text{-}dw}$. Using the appropriate C_i, K_{eff} is calculated as:

$$K_{eff} = \frac{Q}{C_i * \left(T_{wp} - T_{dw}\right)}$$

In the spreadsheet, I also put a description, more in terms of the terminology of the spreadsheet. The table on page #432, vol VIII, page 66 is an example from iterationreport_May.xls, worksheet "EffectiveK Summary BF" Note that the C_i term changes for each time.

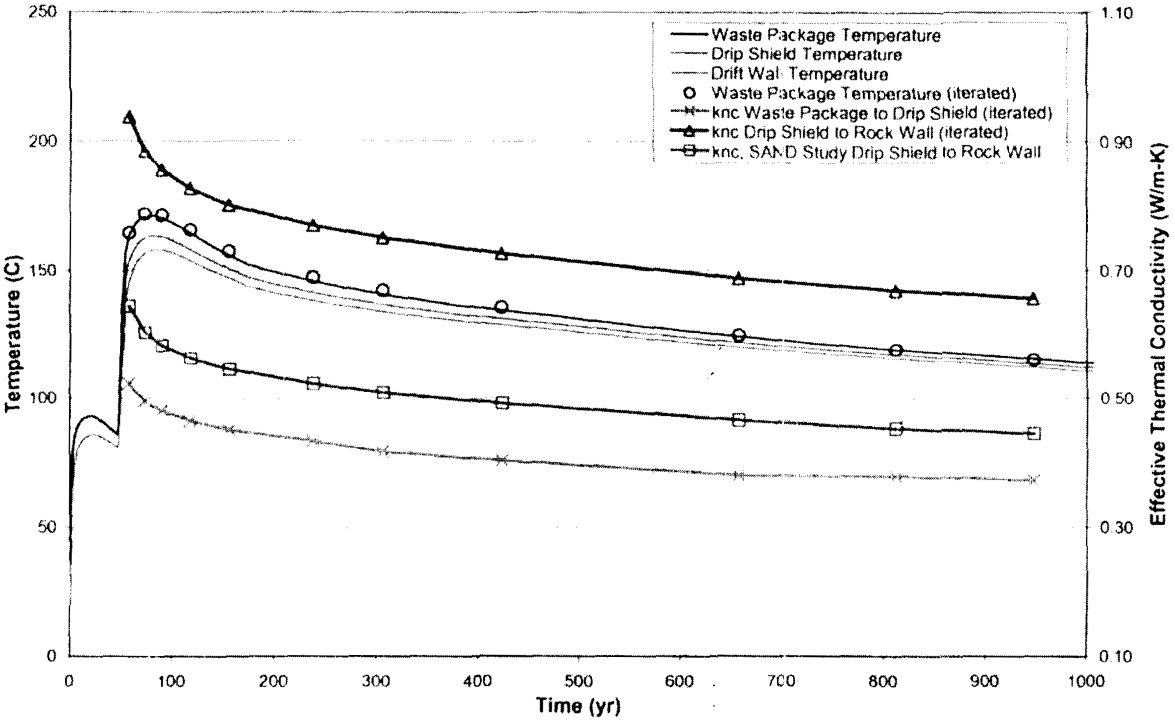
Just to see how the effective thermal conductivity for air changes over time, and in comparison with how temperature changes with time, here is a plot from worksheet "temp_keff_bf(0m)" in iterationreport_May2004.xls

Temperatures and Effective Thermal Conductivities, Natural Backfill

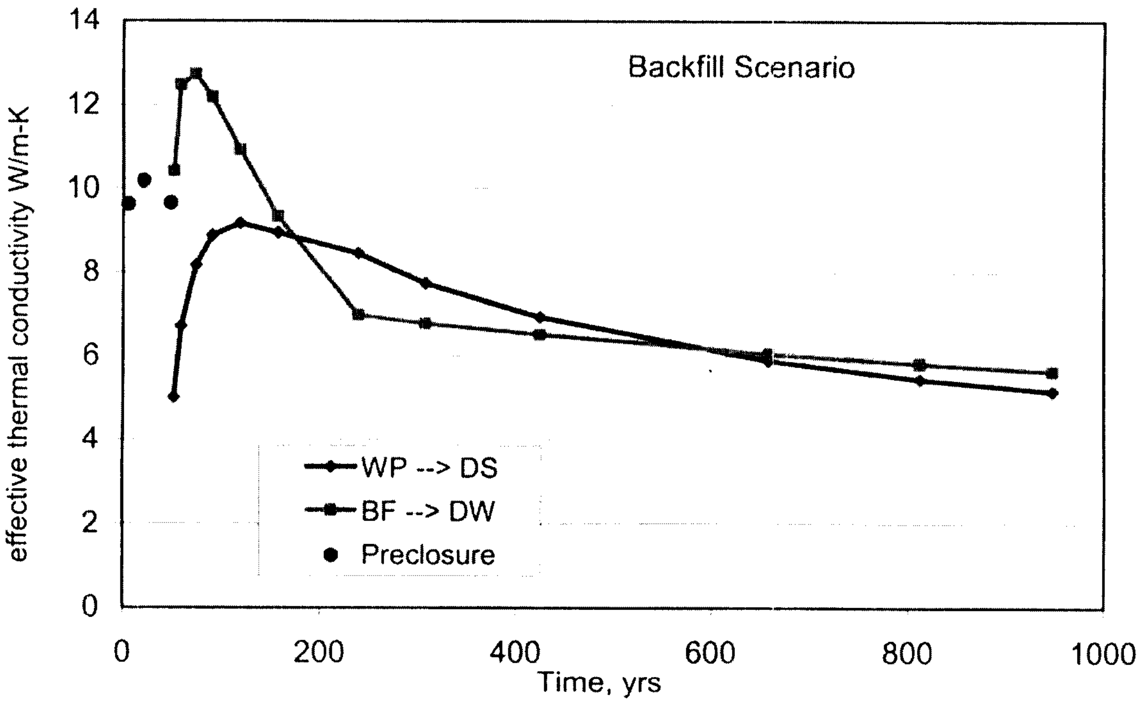


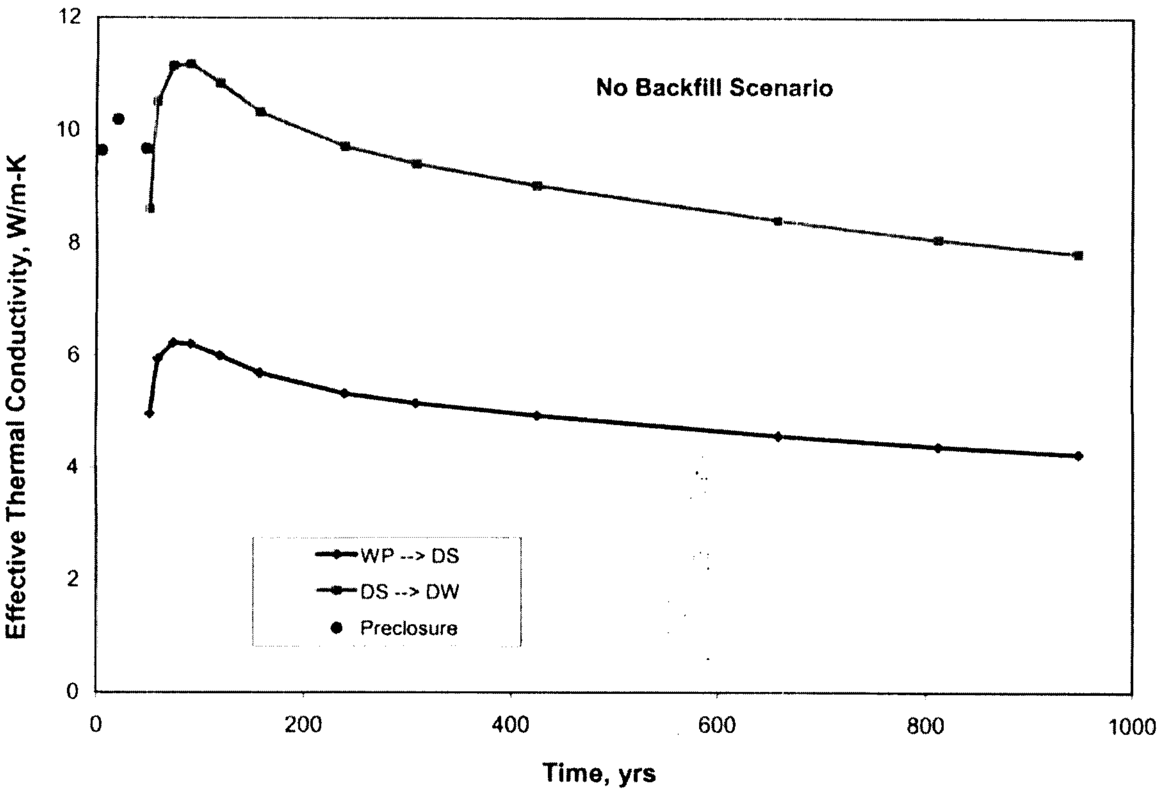
Similarly for the no-backfill case, with the " SAND" curve in the plot referring to the equations in a Sandia National Laboratories report SAND2002-4179. The calculations using equation 9 of the Sandia report are contained in the worksheet "SAND REPORT" of the spreadsheet iterationreport_May2004.xls. The equation 9 is based on general relationships supported by Sandia computational fluid dynamics modeling.

Temperatures and Effective Thermal Conductivities, No Backfill



The effective thermal conductivity for the no-backfill and natural rubble backfill cases using a host rock thermal conductivity of 1.59 W/m-K are, shown on the next page (page 65)


Backfill Scenario
effective thermal conductivity W/m-K
Time, yrs
0
2
4
6
8
10
12
14
0
200
400
600
800
1000
WP --> DS
BF --> DW
Preclosure


No Backfill Scenario
Effective Thermal Conductivity, W/m-K
Time, yrs
0
2
4
6
8
10
12
0
200
400
600
800
1000
WP --> DS
DS --> DW
Preclosure

Use NBF for preclousre period

Year	4.674	20.069	47.564	50.988	58.078	73.281	89.958	118.06
gcond_bf3				1.02E+03	131.5	50.377	32.217	21.576
Keff_3pd	1.472021	1.35148	1.25162	0.566311	0.494686	0.4385834	0.40724515	0.3791478
gconv_3pd	34.12459	31.33019	29.01523	29.53006	25.7952	22.869751	21.2356326	19.770506
Grad_3pd	189.1954	204.7607	194.9993	231.2814	324.4536	403.55585	442.584002	459.08423
Keff_3bw				0.97601	0.839711	0.7108549	0.6170602	0.5066029
gconv_3bw				41.7634	38.27202	36.682265	36.0010349	35.552728
Grad_3bw				400.1589	530.6693	620.53311	675.833482	731.80096
Temperature Waste Package (C)	85.91	94.22	87.42	138.11	184.41	217.22	231.79	237.42
Temperature Drip Shield (C)				125.30	175.761	211.35	227.25	233.96
Temperature Backfill (C)	77.026	87.675	82.717	122.0216	152.7245	161.69	161.96	157.16
Temperature Rock Wall (C)	8.88	6.54	4.71	114.46	147.4	157.88	159.00	155.00
ΔT WP-DS				12.81	8.65	5.87	4.54	3.46
ΔT BF-DW				7.56	5.32	3.81	2.96	2.16
Circumferential Fraction		0.75		**Conductance equation for convection, assume radiation is of same form**				
Waste Package Spacing(Lwp + 2delta) (m)		6.1392		$G= K_{eff} * [f_c * 2 \bullet pi * (L_{wp} + 2\delta)] / \ln(D_o/D_i)$				
Diameter Waste Package (m)		1.579		$G= K_{eff,} * C_i$				
Diameter Drip Shield Inner (m)		2.75		**C(WP-DS)**	**52.14459**			
Diameter Drip Shield Outer (m)		2.78		**C(DS-DW)**	**42.40132**			
Drip Shield Thickness (m)		0.015		**C(WP-DW)**	**23.18214**			
BF_Out_Dia				2.8014	2.9501	3.2463	3.5428	3.9928
Drift_Dia				5.5081	5.5655	5.6868	5.817	6.0299
Drift Diameter, original (m)		5.5						
C(BF-DW)				42.78994	45.57763	51.603027	58.3428248	70.178684
C(DS-BF)				3772.682	487.1393	186.5689	119.316709	79.908722
Grad + G conv for WP->DS	223.32	236.09	224.01	260.81	350.2488	426.4256	463.819635	478.85474
Grad + G conv for BF->DW				441.92	568.9413	657.21537	711.834517	767.35368
Keff for WP to DS	9.63	10.18	9.66	5.00	6.716876	8.177753	8.89487505	9.1832099
Keff for BF to DW				10.42	12.48291	12.735985	12.2008922	10.934284
Keff / L for WP to DS	8.23	8.70	8.25	4.27	5.736017	6.9835636	7.59596503	7.8421946
Keff / L for BF to DW				3.83	4.611855	5.2185966	5.36491611	5.3675737
Keff Backfill, check, G=Keff • Ci				0.270471	0.269943	0.2700182	0.27001248	0.2700081

Calculation of Effective Emissivity of Drift Wall

To calculate an effective emissivity to reflect the presence of a drip shield (when a drip shield is not explicitly modeled in MULTIFLO), take the temperatures from the in-drift algorithm with a drip shield (case 2), then use case 1 equation for radiation to back out an effective emissivity. This effective emissivity accounts not only for the presence of the drip shield (which increases waste package temperatures) but also for natural convection (which would decrease waste package temperatures, but is less important than the presence of the drip shield on radiation).

Starting with (from Steve Green's analysis, scientific notebook #536):

$$Q_{wp,r} = \frac{\sigma\left(T_{wp}^4 - T_{dw}^4\right) f_c \pi(L_{wp} + 2\delta)}{\frac{1}{D_{wp}\varepsilon_{wp}} + \frac{1}{D_{dw}}\frac{1-\varepsilon_{dw}}{\varepsilon_{dw}}} = G_{r1}\left(T_{wp} - T_{dw}\right)$$

σ is Stefan Boltzman constant, T is temperature, wp is waste package, dw is drift wall, f_c is fraction of heat transfer not going into invert, L is length of waste package, δ is waste package spacing D is diameter and ε is emissivity.

Rearrange to solve for emissivity of drift wall

$$\frac{1}{D_{wp}\varepsilon_{wp}} + \frac{1}{D_{dw}}\frac{1-\varepsilon_{dw}}{\varepsilon_{dw}} = \frac{\sigma\left(T_{wp}^4 - T_{dw}^4\right) f_c \pi(L_{wp} + 2\delta)}{Q_{wp}}$$

and

$$\frac{1-\varepsilon_{dw}}{\varepsilon_{dw}} = \left[\frac{\sigma\left(T_{wp}^4 - T_{dw}^4\right) f_c \pi(L_{wp} + 2\delta)}{Q_{wp}} - \frac{1}{D_{wp}\varepsilon_{wp}}\right] D_{dw}$$

Trial and error guesses are made for effective drift wall emissivity using the temperatures from the algorithm when the drip shield is present. The trial & error method is only needed for a few times, hence no need to code up a nonlinear solver.

This is setup in the spreadsheet:

bubo: .\iterationreportCase-K2.02_May2004.xls

Because the temperature profiles from the algorithm using K_{th}-=2.02 W/m-K better match thermohydrological results using METRA ....

WRONG!!

After seeing Alex's writeup on the radiation model in MULTIFLO, it is not clear that Metra provides reasonable results for radiation. The simplified model is further simplified by using an average emissivity of the waste package and drift wall. This single value of emissivity is intended to represent both the waste package and the drift wall. Except, the mental experiment whereby different emissivities are used for these two surfaces, then flip-flop the values used for each surface, should lead to different amounts of heat transfer. Using an average value negates this difference and would provide the same results no matter which surface has the higher emissivity value.

RF 6/21/04

Adjusting Timing of Rubble Pile Buildup on Drip Shield Based on MULTIFLO Simulations

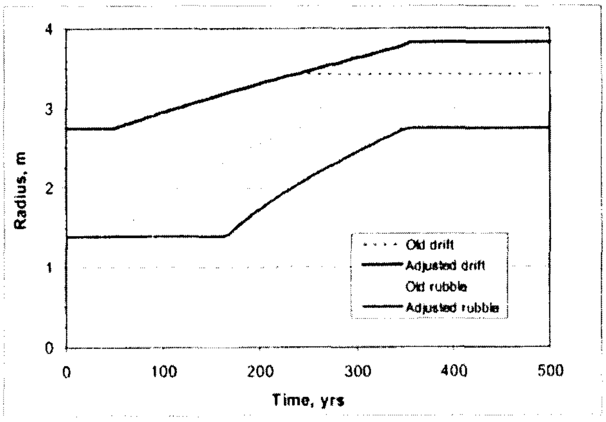
As a result of the Metra modeling that included drift degradation, we expanded analyses on the using the concept of the three-leg thermal network to better match the Metra results, which makes intuitive sense; i.e., the 3-leg thermal network accounts for rubble buildup on the side of the drip shield (limited by the nondegraded drift wall) occurring before rubble builds up on the top of the drip shield. The ceiling of the drift would degrade, thus an ever thickening pile of rubble would occur as the ceiling degraded. The sidewall of the drift would limit the thickness of the rubble pile laterally to the distance between the drip shield the original drift wall.

Until modifications could be made to the algorithm to directly calculate the rubble filling up the sides of the drip shield before beginning to cover the top of the drip shield, I shifted the rubble data to mimic the area-based calculation. The shifted approximation to rubble, building up on the sides of the drip shield first, appears to reasonably match the Metra modeling results.

Shifting of the rubble calculation and simulation results from the in-drift heat transfer algorithm are stored in:
    bubo: .\EquivalentRadiusDriftArea_May2004.xls
Summary of these results given to Chandrika:
    bubo: .\RubbleShiftedTemp.xls

The EquivalentRadiusDriftArea_May2004.xls spreadsheet provides the calculation used to shift the rubble. Basically the worksheets follow George's calculation in the spreadsheet EquivalentRadiusDriftArea.xls. Part of the shifting is the fitting of a curve, so that the slope of the rubble thickness time curve remains the same, but is time-shifted.

Based on the time at which the static load becomes zero, the area on the side of the drip shield is 8.2 (see worksheet Equivalent Height (mean)". Then the radii can be adjusted, see worksheet "HeightGeneratoriArea_Limit" (the plot included below includes shifted rubble)



Because I want to match the slope once the rubble starts covering the top of the drip shield, I shifted the data, fit the slope to an equation and then shifted the rubble thickness

Shift only the radius of the backfill, not the drift radius.
The shift accounts for volume of rubble building up on the side of the drip shield.

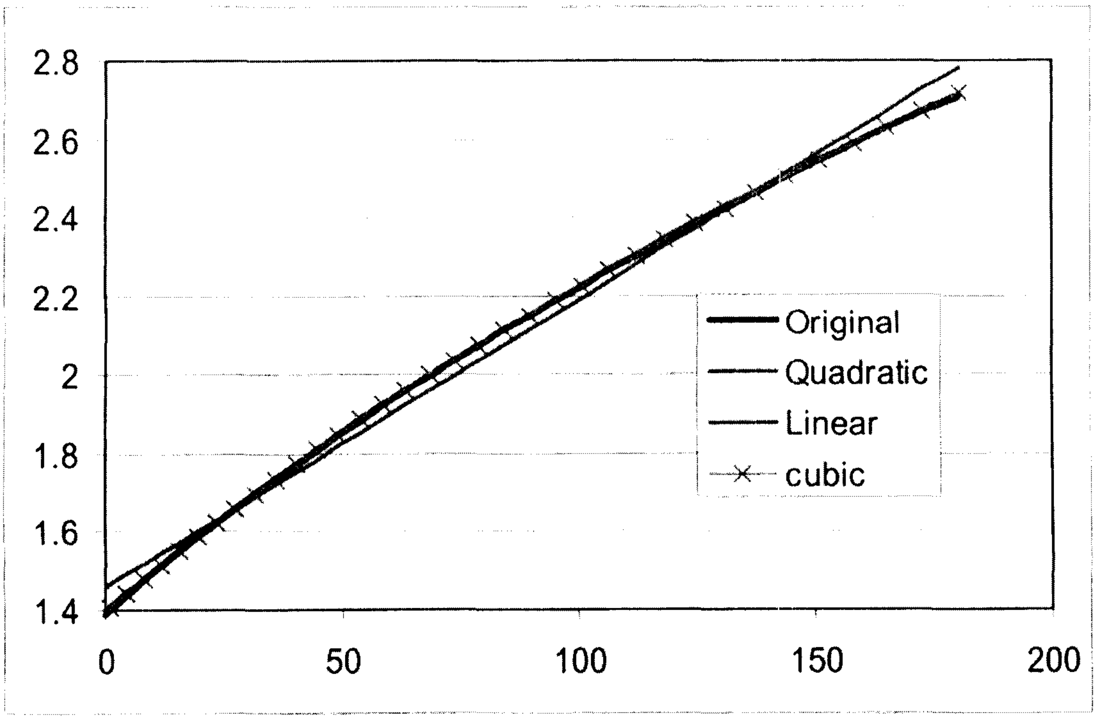
Sigma Plot 2000 Version 6.0 results using time shifted rubble thickness and a quadratic regression fit.
y = y0 +ax +bx^2

y0 =	1.40228
a =	0.00958348
b =	-1.31E-05

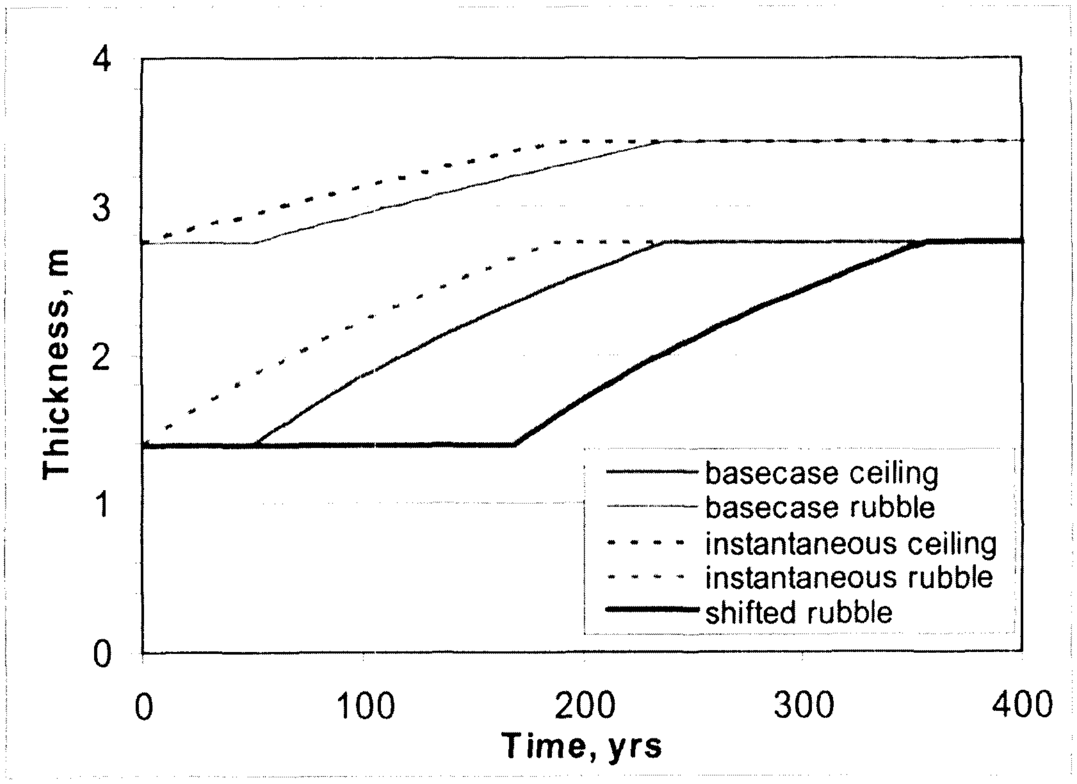
Sigma Plot 2000 Version 6.0 results using time shifted rubble thickness and a cubic regression fit.
y = y0 +ax +bx^2 +cx^3

y0 =	1.39255
a =	0.0103979
b =	-2.54E-05
c =	4.69E-08

I went with the cubic fit because it did better at early times.



The final shifted curve is included as a plot below and was taken from the "Basecase Shifted" worksheet



To help understand the organization of the spreadsheet, a summary page in the EquivalentRadiusDriftArea_May2004.xls spreadsheet summarizes the contents of the spreadsheet, and is included in the table below.

This spreadsheet started with George Adam's "EquivalentRadiusDriftArea.xls" spreadsheet, which had the MECHFAIL output (static load height, drift ceiling height, and area) and conversion to areas.

I modified his calculations so that the thickness of rubble did not include the rubble on the sides of the Drip Shield. In essence, the thickness of the rubble pile is zero until the static load height on top of the drip shield starts increasing. This was done because MULTIFLO simulations suggested that the temperatures did not start increasing (because of the rubble) until rubble was on top of the drip shield.

"**Mean Realization**" was not changed from George's version
"**Equivalent Height(mean)**" was modified, the columns I changed are highlighted
"**HeightGeneratorArea_Limit**" was modified, the columns and cells I changed are highlighted
"**Adjusted eqradius.dat**" was created to export comma-delimited ascii text file "eqradius.dat" for the in-drift fortran algorithm

Also added the following worksheets from the eqradius.xls spreadsheet, where I just shifted the rubble curve. Although this was okay for the rubble (it is the same curve as I calculated using areas in "Equivalent Height(mean)" and "HeightGeneratorArea_Limit"), the drift ceiling radius changes because of the threshold criteria of not increasing the drift radius after the rubble radius reaches the original drift radius.
"**Basecase_Shifted**" is the manual shifting of the rubble curve based on cubic regression of the intermediate rubble data
"**eqradius_degradation**" is George's data from the in-drift algorithm ./data directory for the basecase MECHFAIL output
"**eqradius_degradation_from_time0**" is George's data from the in-drift algorithm ./data directory for instantaneous backfilling at time=0 (preclosure, hence use "eqradius_emplaced_1_36" instead for instantaneous natural backfill).
"**eqradius_emplaced_1_36**" is George's data from the in-drift algorithm ./data directory for instantaneous backfilling

Results of In-Drift Heat Transfer Algorithm
"**K2.02-0.27bc0Cond_BF_ShiftRubb**" output from modified TPA code that has linkage of degradation and temperature
"**K2.02-0.2bc0Cond_BF_ShiftRubb**" output from modified TPA code that has linkage of degradation and temperature
"**K2.02-0.135bc0Cond_BF_ShiftRubb**" output from modified TPA code that has linkage of degradation and temperature
"**K1.59-0.27bc0Cond_BF_ShiftRubb**" output from modified TPA code that has linkage of degradation and temperature
"**K1.59-0.2bc0Cond_BF_ShiftRubb**" output from modified TPA code that has linkage of degradation and temperature
"**K1.59-0.135bc0Cond_BF_ShiftRubb**" output from modified TPA code that has linkage of degradation and temperature

KEY	
bc0	boundary condition at drift wall
bc5	boundary condition 5 m into wallrock
K2.02	thermal conductivity of wallrock
K2.02-0.27	thermal conductivity of wallrock and of rubble pile
Cond	used conduction-only model temperature results for outer boundary condition
TH	used thermohydrology model temperature results for outer boundary condition
BF	backfill, drift degradation
NBF	no backfill, no drift degradation

ShiftRubbl used rubble pile radius with shift to exclude rubble on sides of drip shield

RF 12/12/05

Figure. Temperature at waste package, drip shield, outside backfill surface, and drift wall when a host rock thermal conductivity of 2.02 W/m-K and effective thermal conductivity of rubble pile of 0.27 W/m-K are used.

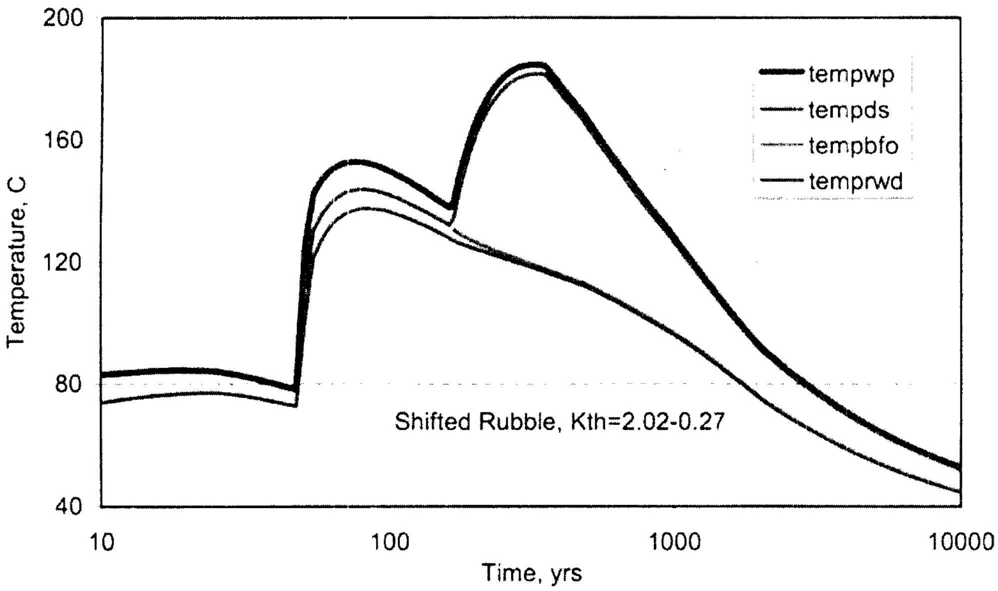


Figure. Temperature at waste package, drip shield, outside backfill surface, and drift wall when a host rock thermal conductivity of 1.59 W/m-K and effective thermal conductivity of rubble pile of 0.27 W/m-K are used.

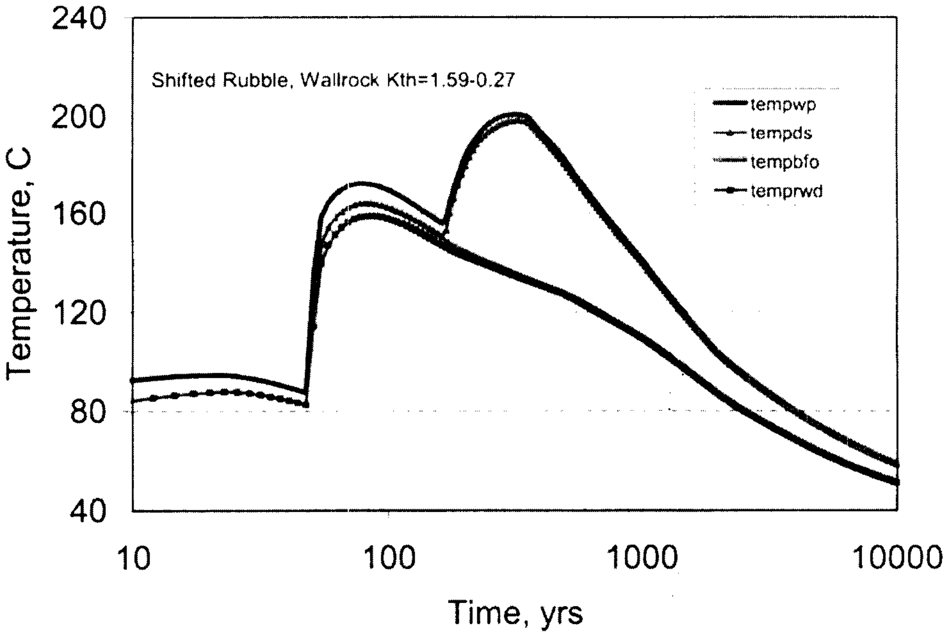


Figure below. Temperature at waste package, drip shield, outside backfill surface, and drift wall when a host rock thermal conductivity of 2.02 W/m-K and effective thermal conductivity of rubble pile of 0.2 W/m-K are used.

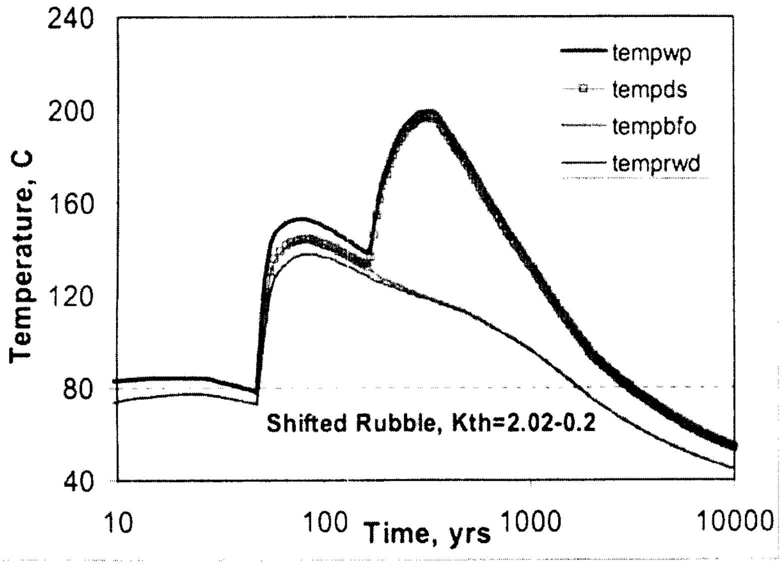
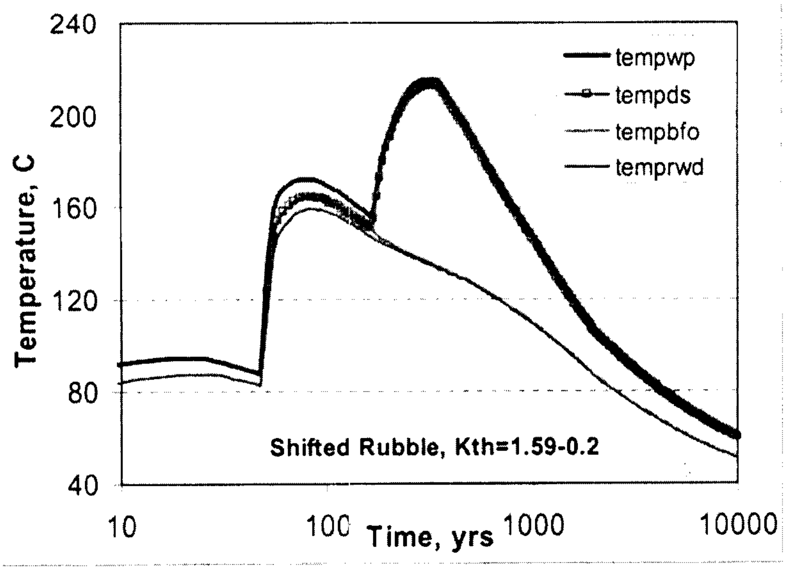


Figure below. Temperature at waste package, drip shield, outside backfill surface, and drift wall when a host rock thermal conductivity of 1.59 W/m-K and effective thermal conductivity of rubble pile of 0.2 W/m-K are used.



RF 4/15/05

Ventilation Failure Modeling

Although I could have put the ventilation failure modeling for preclosure into this scientific notebook volume (because of the use of Metra and the in-drift heat transfer algorithm), I instead decided to create a new volume. See Scientific Notebook #432, Volume XIII for information on the ventilation failure analyses being done for RDTME (now called the ENG2 ISI).

RF 12/12/05

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12/12/05 RF

Entries made into Scientific Notebook #432E Volume VIII have been made by Randall Fedors (Dec 12, 2005).

No original text or figures entered into this Scientific Notebook has been removed

RF 12/12/2005

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RL

4/10/2008

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