

SCIENTIFIC NOTEBOOK  
E580E  
GARY R. WALTER  
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Evaluation of the effect of the repository on physical/chemical conditions of groundwater in the saturated zone: Summary of review of reports.

February 27, 2003 G. Walter

This summarizes my findings regarding the effect of the YM repository on the physical and/or chemical properties of the saturated zone ground water beneath and downgradient of the Yucca Mountain repository. Based on my review of various DOE reports related to the modeling of radionuclide transport in the saturated zone, radionuclides are assumed to be transported in a "carrier plume" with the same physical and chemical characteristics as the ambient ground water in the saturated tuff and alluvium. Although the DOE acknowledges that "Thermal and chemical processes related to the emplacement of waste in the repository may alter hydrologic processes in the saturated zone" (Section 6.1.7.1 in Features, Events, and Processes in SZ Flow and Transport, ANL-NBS-MD-000002 REV 00), all of these effects are assumed to be handled in the total performance analysis modeling through the uncertainty in the  $K_d$  used to compute retardation.

In the documents that I have reviewed, I have not found a definitive answer to the question as to whether the thermal, hydrologic, or chemical changes created by the presence of the repository could alter the characteristics of the saturated zone in a way that would significantly affect the transport of radionuclides. Several interrelated processes could affect saturated zone radionuclide transport, such as: heating of the ground water due to conductive and advective heat transport from the unsaturated zone, changes in  $P_{CO_2}$  and  $P_{O_2}$  in the ground water due either to degassing of the saturated zone or gas transport in the unsaturated zone, changes in water percolation to the saturated zone, mixing of chemically-altered, unsaturated zone water with the saturated zone ground water, and creation of a buoyant plume that limits vertical mixing. Nearly all of these processes are related to heating of either the unsaturated or saturated zone near the repository.

The thermal and chemical processes in the unsaturated zone were extensively discussed in the Unsaturated Zone Flow and Transport Model Process Model Report, but primarily with respect to effect on the repository itself, the waste package, and transport through the unsaturated zone. For example, the effect of heating on the percolation rate from the unsaturated zone to the saturated zone was evaluated through the mountain-scale modeling and the predicted, transient increase in the mass loading rate to the saturated zone was incorporated into the TSPA model. The effect, if any, of the change in percolation rate and chemical composition of the unsaturated zone water on the flow and chemistry of ground water in the saturated zone is not evaluated.

As another example, the mountain-scale unsaturated zone modeling (performed using TOUGH) indicates that the temperature at the water table beneath the repository will reach 65 to 70 °C after 10,000 years with most of the temperature rise occurring between 1,000 and 10,000 years. Modeling performed as part of the near-field and altered zone evaluation (using NUFT)

indicated a temperature increase of 40 °C at the water table and the potential for formation of thermal convection cells within 10 kilometers of the repository.

Some of the temperature increases predicted by previous modeling could be due to the selection of the lower boundary conditions in the models and the computed temperature at the water table should be judged with caution. Nevertheless, if the temperature in the upper portion of the saturated zone was to increase by 30 to 40 °C, a thermal plume would be created. Such a thermal plume would affect vertical mixing processes beneath and downgradient of the repository, and also the rate of horizontal groundwater flow. The temperature increase could raise the pH in the ground water by degassing CO<sub>2</sub>. A change in pH could then affect sorption and colloidal transport processes. The extent to which any thermally-induced changes would affect far-field, radionuclide transport would, of course, depend on the downgradient extent of the thermal plume and the rate of recovery of the water chemistry to ambient conditions.

In addition to thermal effects, water reaching the saturated zone from the portion of the unsaturated zone thermally-affected by the repository will have an altered chemical composition. Although difficult to quantify from simply reading the CRWMS reports, percolation from the repository horizon may represent a significant portion of the groundwater flow in the shallow portions of the saturated, at least during portions of the repository heating and cooling history. I have not found any evaluation of the effect, if any, of this percolation on the chemistry of the saturated zone and the behavior of radionuclides.

In summary, a potential exists for the repository to alter the physical and chemical characteristics of ground water in the saturated zone beneath the repository and to an undetermined distance downgradient. As best as I can determine, these potential changes in ground water characteristics in the saturated zone have been assumed to have a negligible effect on radionuclide transport or has been assumed to have been subsumed in the uncertainty analysis of other parameters, and have not been quantitatively evaluated. The bottom line is that any effects of alterations in the physical or chemical properties of saturated zone groundwater due to the repository are considered to be negligible and far-field thermal-hydrologic effects are not currently considered in the TSPA (Yucca Mountain Scientific and Engineering Report Section 4.2.2.4). Some of the information needed to evaluate the significance of these changes could have been generated by the DOE as part of their unsaturated zone modeling and simply not reported because their focus was on the unsaturated zone rather than the saturated zone. Critically evaluating the significance of repository-induced changes to the characteristics of the ground water in the saturated zone would first involve performing some screening level calculations of the lateral extent of the thermal plume developed due to the repository. If the lateral extent of the plume is small with respect to the distance to 20 km boundary, then the effect of the plume on radionuclide transports may be small. If the thermal plume spreads over a significant area, then further evaluation of the repository impacts on saturated zone ground water flow and chemistry is warranted.

Suggested Actions:

1. Develop a simple thermal plume model to evaluate the potential extent of thermal effects.
  2. Has a geochemist give an opinion regarding effect of 30-40 °C temperature rise on pH and colloid behavior.
  3. Acquire TOUGH2 and input/output files used for the Mountain Scale Unsaturated Zone modeling.
  3. Acquire FEHM and input/output files for site-scale, saturated zone model.
  4. If indicated by 1 and/or 2, simulate thermal effects using TOUGH, FEHM, or MULTIFLO.
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March 3, 2003 G. Walter

Review of reports and documents related to fluid inclusions and geothermal upwelling at YM.

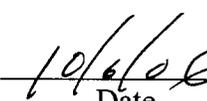
A few key issues to be resolved:

1. Does the homogenization temperature of the 2 phase inclusion represent formation temperatures? (Sandia report of vadose zone formation)
  2. Based on USGS presentation, the problem seems to focus on reconciling the apparent homogenization temperatures with the ages.
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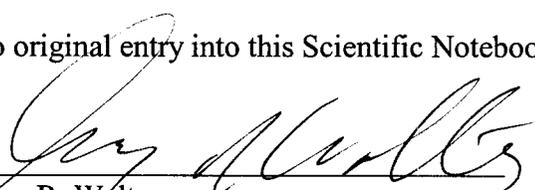
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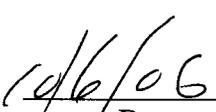
Entries into Scientific Notebook No. 580E for the period September 6, 2002 through March 6, 2003 have been made by:

  
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Gary R. Walter

  
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March 20, 2003 G. Walter

Based on further review of the controversy surrounding the origin of the vein-filling secondary minerals at Yucca Mtn, there seem to be some inconsistencies in the concept of slow and steady growth. Specifically, the Fabryka-Martin report on CI-36, fast-tracks, and pore water apparently under-saturated wrt calcite and silica; why do the apparently most recent calcites have high Mg (JS suggested derived from dolomites, but why a change, could it be wind direction); and the FIA temperatures.

June 24, 2003 G. Walter

The following pages contain a listing of the fortran program generate\_active\_frac\_table.f which was written to compute a "pck" file for Metra with active fracture properties (see scientific notebook 585)

```
      program generate_table
c this program was written to generate a table of active fracture
c water properties
c from metra
c written by g.r.walter June,2003
c language = fortran 77
c machine = solaris
C
c   fracpropfile = file name with fracture properties
c   vgm = van genuchten matrix m (mflo lambda)
c   vgf = van genuchten fracture m (mflo lambda)
c   gamma = active fracture Liu gamma
c   alphas = van genuchten matrix 1/bubbling pressure
c   alphaf = van genuchten fracture 1/bubbling pressure
c   swirm = matrixirreducible saturation
c   swrif = fracture irreducible saturation
c   satfactor = saturation multiplication factor used to
c             generate table of value
c   relpermwater = relative liquid permeability
c   cap_press = capillary pressure
c SUBROUTINES
c   comment - screens out comment lines starting with :
c             parameter(io_in=10,io_out=20,max_material=100)
c             parameter(zero=0.e+0,one=1.e+0,big_number=1.e+20,small_number=1e-3)
c             parameter(swextf=-1.e+7)
c
c             character*80 fracpropfile,outputfile,
material_name(max_material),dummy_char
c matrix properties
      real
vgm(max_material),gamma(max_material),alphas(max_material),swirm(max_material)
      real swext(max_material)
c fracture properties
      real vgf(max_material),alphaf(max_material),swrif(max_material)
c
c             write(*,*)'THIS PROGRAM IS USED TO GENERATE ACTIVE FRACTURE'
c             write(*,*)'PROPERTY TABLES FOR METRA'
c prompt for file name containing fracture parameters
c             write(*,*)'enter name of file containing input parameters'
c             read(*,'(a80)')fracpropfile
c
c prompt for outputfile name
c             write(*,*)'enter name of output file'
c             read(*,'(a80)')outputfile
c
June 24, 2003 G. Walter
c open fracpropfile
      open(unit=io_in,file=fracpropfile)
c
c open outoutfile
```

```

        open(unit=io_out,file=outputfile)
c declare a counter for number of materials to read
    mat_counter = 0
c start reading fracpropfile
    do i=1,max_material*3,2
c read a line with material name
    call comment(io_in,io_out,ierr)
    if(ierr.eq.1)go to 1000
c counter the number of materials defined (matrix + fracture = 1 material)
    mat_counter = mat_counter + 1
    read(io_in,'(a80)',end=1000,err=1000) dummy_char
    material_name(mat_counter) = dummy_char

        write(*,*)material_name(mat_counter)
c read a line with matrix properties
c irreducible saturation, v-g m (mflo lambda),alpha
    call comment(io_in,io_out,ierr)
    if(ierr.eq.1)go to 1000
    read(io_in,*)swirm(mat_counter),vgm(mat_counter),alphan(mat_counter),swext(mat_counter)
    write(*,*)'read matrix paramaters'
    write(*,*)'swirm = ',swirm(mat_counter),
    &      ' vgm = ',vgm(mat_counter),' alphan = ',alphan(mat_counter)

c read a line with fracture properties
    call comment(io_in,io_out,ierr)
    if(ierr.eq.1)go to 1000
c read > irreducible saturation, V-G exponent, V-G alpha, active fracture
exponent, saturation factor
c the saturation table will be generated by computing a series of saturation
c values (theta) starting with 0., then swirf, then theta(i) = theta(i-
1)*satfactor up to 1.0
    read(io_in,*)swirf(mat_counter),vgf(mat_counter),alphaf(mat_counter),gamma(mat_counter),satfactor
    write(*,*)'read fracture properties '
    write(*,*)'swirf = ',swirf(mat_counter)
    write(*,*)'vgf = ',vgf(mat_counter)
    write(*,*)'alphaf = ',alphaf(mat_counter)
    write(*,*)'gamma = ',gamma(mat_counter)
    write(*,*)'sfactor = ',satfactor

c generate an output line with V-G matrix properties for Metra
    write(io_out,2200)material_name(mat_counter)

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2200 format(8h: matrix,1x,a20)

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    mat = i
    write(io_out,*) mat , ' Van-Gen ',
    &
swirm(mat_counter),vgm(mat_counter),alphan(mat_counter),swext(mat_counter), '
0.0 0'

c generate an output line with keyword TABLE for fracture table
    write(io_out,2300)material_name(mat_counter)
2300 format(10h: fracture,1x,a20)

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```

        mat = i + 1
        write(io_out,2100)mat,swirf(mat_counter),vgf(mat_counter),swirf(mat_coun
ter),zero
c start generating table, loop until theta >= 1.

c set theta to swirf/satfactor
        theta = (swirf(mat_counter)+small_number)/satfactor
        iswitch = 0
        do j=1,1000
c      if(j.eq.1)then
        if(j.le.2)then
c make the first entry at zero saturation
c make the 2nd entry a residual saturation
        if(j.eq.1)then
c theta = 0
c compute capillary pressure at zero saturation from swirf - small-number
        se = (swirf(mat_counter) + small_number/2. -
swirf(mat_counter))/(one - swirf(mat_counter))
        cap_press =
capillarypressure(se,one,alphaf(mat_counter),gamma(mat_counter),vgf(mat_coun
ter))
                write(io_out,'(4(e12.5,1x))')zero,zero,one,cap_press
        else
c 2nd entry at residual saturation
c compute capillary pressure at zero saturation from swirf - small-number
        se = (swirf(mat_counter) + small_number/2. -
swirf(mat_counter))/(one - swirf(mat_counter))
        cap_press =
capillarypressure(se,one,alphaf(mat_counter),gamma(mat_counter),vgf(mat_coun
ter))
                write(io_out,'(4(e12.5,1x))')swirf(mat_counter),zero,one,cap_press
        endif
        else
        theta = theta*satfactor
        if(theta.ge.one)then
c set theta to one
        theta = one

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c set loop switchch
        iswitch = 1
        endif
c compute effective saturation
        se = (theta - swirf(mat_counter))/(one - swirf(mat_counter))
c compute relative permeability
        relpermwater = rel_perm(se,one,gamma(mat_counter),vgf(mat_counter))
c compute relative gas permeability
        relpermgas = one - relpermwater
c if liquid saturation > residual, force gas perm to 0.99999
        relpermgas = amin1(relpermgas,0.99999)
c compute capillary pressure
        cap_press =
capillarypressure(se,one,alphaf(mat_counter),gamma(mat_counter),vgf(mat_coun
ter))
c write next line of table
        write(io_out,'(4(e12.5,1x))')theta,relpermwater,relpermgas,cap_press
        endif
        if(iswitch.eq.1)go to 100

```

```

c endif of fracture table loop for this material
  enddo
100  write(io_out,2000)
2000 format(1h/)

c end of loop to read materials
  enddo
1000 write(*,*)'end of fracture properties file ',mat_counter-1,' materials
    &      processed'

c now, write the matrix-fracture property tables at the end of the file
c this is required by Metra
  mat_counter = mat_counter -1
  do i=1,mat_counter
c generate an output line for matrix-fracture transfer terms
  write(io_out,2400)material_name(i)
2400  format(17h: fracture-matrix ,a20)
  mat = i + mat_counter*2
c WARNING SWEXT HAS SOME MEANING IN THESE TABLES, SET TO 0.
  write(io_out,2100)mat,swirf(i),vgf(i),alphaf(i),zero
2100  format(' ',i4,1x,5hTable,1x,2(f7.3,1x),e10.3,1x,e10.3,1x,6h 0.0 0)
c generate matrix fracture table
c start generating table, loop until theta >= 1.

c set theta to swirm/satfactor
  theta = (swirf(i)+small_number)/satfactor
  iswitch = 0
  do j=1,1000
c   if(j.eq.1)then

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c make the first entry at zero saturation
c make the 2nd entry a residual saturation
  if(j.le.2)then
    if(j.eq.1)then
c theta = 0
c compute capillary pressure at zero saturation from swirm - small-number
  se = (swirf(i) + small_number/2. - swirf(i))/(one - swirf(i))
  cap_press = capillarypressure(se,one,alphaf(i),zero,vgf(i))
  cap_press = amin1(-swextf,cap_press)
  write(io_out,'(4(e12.5,1x))')zero,zero,one,cap_press
  else
c compute capillary pressure at zero saturation from swirm - small-number
  se = (swirf(i) + small_number/2. - swirf(i))/(one - swirf(i))
  cap_press = capillarypressure(se,one,alphaf(i),zero,vgf(i))
  cap_press = amin1(-swextf,cap_press)
  write(io_out,'(4(e12.5,1x))')swirf(i),zero,one,cap_press
  endif
  else
  theta = theta*satfactor
  if(theta.ge.one)then
c set theta to one
  theta = one
c set loop switch
  iswitch = 1
  endif

```

```

c compute effective saturation
  se = (theta - swirf(i))/(one - swirf(i))
c compute relative permeability based on FRACTURE properties
c this is done because METRA uses up-stream weighting based on
c fracture permeability for flow from fracture to matrix
  relpermwater = rel_perm(se,one,zero,vgf(i))
c make active fracture correction
  relpermwater = se**(one + gamma(i))*relpermwater
c compute relative gas permeability
  relpermgas = one - relpermwater
c force gas permeability to be LE 0.99999
  relpermgas = amin1(relpermgas,0.99999)
c compute capillary pressure
  cap_press = capillarypressure(se,one,alphaf(i),zero,vgf(i))
  cap_press = amin1(-swextf, cap_press)

c write next line of table
  write(io_out, '(4(e12.5,1x))') theta, relpermwater, relpermgas, cap_press
endif
if(iswitch.eq.1)go to 200
c endif of matrix-fracture table loop for this material
enddo
200  write(io_out,2000)
enddo

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  write(io_out,2000)

  stop
  end

  subroutine comment(inunit,io_out,ierr)
c this subroutine discards comment lines beginning with a :
  character*1 chrdum
  character*130 spoot
  ierr = 0
10  read(inunit,fmt='(a1)',end=1000,err=1000) chrdum
  if(chrdum.eq.':')then
    backspace inunit
    read(inunit,fmt='(a130)') spoot
    goto 10
  endif
  backspace inunit
  return
1000 write(*,*)'end of file'
  ierr = 1
  return
  end

  real function rel_perm(se,one,gamma,vg)
c compute relative liquid permeability
  rel_perm = se**((one + gamma)/2.)*(one - (one - se**((one -
gamma)/vg))**vg)**2.
  return
  end

```

```
real function capillarypressure(se,one,alpha,gamma,vg)
c compute capillary pressure
capillarypressure = one/alpha*(se**((gamma-one)/vg)-one)**(one - vg)
return
end
```

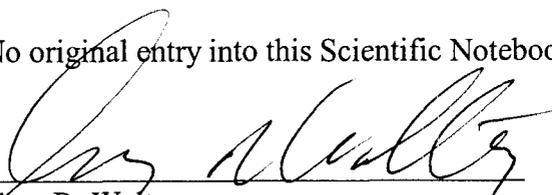
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Entries into Scientific Notebook No. 580E for the period March 7, 2003 through August 31, 2003 have been made by:

  
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Gary R. Walter

10/6/06  
Date

No original entry into this Scientific Notebook has been removed.

  
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Gary R. Walter

10/6/06  
Date