

SCIENTIFIC NOTEBOOK

612-11E

by

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INITIAL ENTRIES

Scientific Notebook: #612E

Issued to: R. Janetzke

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Account Number: 20.06002.01.354

Title: TPA 5.0 Code Development

Participants: R. Janetzke
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Objective:

This scientific notebook will document the work performed in the development of the TPA code.

Albert Lozano - Work done from March 2005 to April 21, 2005 follows.

SCR482 - New ash distribution model

I assisted Roland Benke in the acceptance test for this SCR. Razvan Nes provided me with a copy

of the mathematica code that implements the new model. The version used for this test was tpa500h. Many print statements were added to the test version of ashremob.f to compare with intermediate variables in the mathematica code.

Problems were found in ashremob.f. Both the mathematica code and the fortran code were compared with the reports. The mathematica code matches the report. The test version of ashremob.f was corrected until the results matched the mathematica code.

First change

```

        if (areaasheol(iashplumerealindex) .eq. 0.d0) then
            thicknesseolcm = 0.d0
        else
C asl SCR492 4-11-05 thicknesseolcm = 1.d2*masshlweol(iashplumerealindex)/
C   &                                     (areaasheol(iashplumerealindex) *
C   &                                     rhoasheol)
C asl masshlweol should be massasheol
            thicknesseolcm = 1.d2*massasheol(iashplumerealindex)/
            &                                     (areaasheol(iashplumerealindex) *
            &                                     rhoasheol)
        end if

```

Second change

```

C asl SCR482 4-11-05 massloadoutheavy should be massloadashheavy
C asl      abnmassldinth = massloadoutheavy * reductionfactor
            abnmassldinth = massloadashheavy * reductionfactor

```

Third change

```

Casl SCR 482 4-11-05 massloadoutlight should be massloadashlight
Casl      hlwgpm3intl(it) = wgtfactorinitial * concentfactorinit *
Casl &                                     massloadoutlight *
Casl &                                     resuspendiblefraction(it) *
Casl &                                     reductionfactor

            hlwgpm3intl(it) = wgtfactorinitial * concentfactorinit *
            &                                     massloadashlight *
            &                                     resuspendiblefraction(it) *
            &                                     reductionfactor

```

Fourth change

```

Casl SCR482 4-11-05 partmassloadeoli(it) should be abnmassldinth
Casl      hlwgpm3toth(it) = abnmassldinth +

```

```

Cas1 &          wgtfactorfluvial * partmassloadfluv(it) +
Cas1 &          wgtfactoreolian * partmassloadeoli(it)

      hlwmp3toth(it) = abnmassldinth +
&          wgtfactorfluvial * partmassloadfluv(it) +
&          wgtfactoreolian * abnmassldinth

```

Fifth change

```

Cas1 SCR482 4-11-05 partmassloadeoli should be abnmassldinth
Cas1      portioneolh = (partmassloadeoli(it) / hlwmp3toth(it))*
Cas1 &          wgtfactoreolian
      portioneolh = (abnmassldinth / hlwmp3toth(it))*
&          wgtfactoreolian

```

Sixth change

```

Cas1 SCR482 4-11-05 massloadoutlight should be massloadash light
Cas1      abnmassldintl = massloadoutlight * reductionfactor
      abnmassldintl = massloadashlight * reductionfactor

```

The acceptance test did not pass. The SCR was submitted to Roland for resolution

End of SCR482

SCR526 - Move indoor mass loading terms and offsite mass loading terms from equation for C2 to equation for C1

I implemented the changes as specified in SCR526.
The changes were implemented in dcags.f version q.

I assisted Razvan Ness in testing. Razvan wrote the equivalent code in Mathematica. I added print statements to the tpa code for testing. As part of the testing, I also modified the code so that only the inhalation values were used in determining the dose.

End of SCR526

SCR547 - Np solubility update.

I performed the acceptance test on this SCR.

The change consisted of changing the distribution of SolubilityNp[kg/m³] from logtriangular(1.2e-3, 3.4e-2, 2.4) to loguniform(1.1e-4, 5.9e-1).

End of SCR547

Albert Lozano - Work done from April 22, 2005 to June 21, 2005 follows.

SCR 561 - The stream tube information in *strmtube.dat* needs to be updated for the new repository footprint.

I tested this SCR by visually inspecting the p and q versions of *strmtube.dat*.

End of SCR 561

SCR 562

1) The following parameters need to be removed from *tpa.inp*:

- A) TiCorrosionRateVsFluorideSlope[]
- B) MinimumFluoride[mol/L]
- C) MaximumFluoride[mol/L]
- D) UseFluorideEnhancingFactor(0=no,1=yes)

These parameters need to be retained in *dsfailt.def*. The user can change the parameters in *dsfailt.def*, if necessary.

2) Observed that the name for the fluoride data file, *fluoride.dat* is both present in *dsfailt.def* and hardcoded in *dsfail.f*. If the user changes the fluoride data file in *dsfailt.def*, it has no effect (the changed name does not appear in *dsfailt.inp*).

3) There is a spelling error that appears in *dsfail.rtf*: "No failure of the drip *shiled* in:."

4) The thermal conductivity of the backfill in *tpa.inp* applies to both thermal model 1 and thermal model 2. This value incorporates the conduction through the backfill as well as other mechanisms such as convection. However, for thermal model 2, the convection through the backfill is calculated directly. Therefore, separate parameters need to be used for thermal models 1 and 2.

5) It is not clear how natural backfill degradation is turned off from *tpa.inp*.

I tested this SCR the results are:

1) Checked the *tpa.inp* file in the t version for removal of TiCorrosionRateVsFluorideSlope[], MinimumFluoride[mol/L], MaximumFluoride[mol/L], and UseFluorideEnhancingFactor(0=no,1=yes) from *tpa.inp* and *dsfail.f*.

Passed - All 4 parameters were removed from *tpa.inp*. **Passed** - All 4 parameters were removed from *dsfail.f*.

2) Modified *dsfail.f* to allow the user to change the name for the fluoride data file.

Passed - The modified version of *dsfail.f* obtains the name of the fluoride data file from *dsfail.def*.

3) Confirmed that the change from ThermalConductivityOfBackfill[W/(m-C)] to ThermalConductivityOfBackfillModelOne[W/(m-C)] was made and that the parameter ThermalConductivityOfBackfillModelTwo[W/(m-C)] was added. Also, placed these parameters near the parameter, SelectThermalModel(1,2) within *tpa.inp*.

Passed - Modification was made in *tpa.inp* and *nfenv.f*.

4) Corrected the spelling error in *exec.f* (changed shiled to shield). **Passed** - the spelling error was corrected.

5) Added a note in *tpa.inp* section Disruptive Scenario Flags to indicate that both SeismicDisruptiveScenarioFlag(yes=1,no=0) and DriftDegradationScenarioFlag(yes=1,no=0) must be set to no(0) in order to turn off natural backfill accumulation

Passed - The note was added to *tpa.inp*.

End of SCR 562

SCR 564

1. Should arrange the code so that each realization always has an intrusive event, and a simple flag (0,1) for extrusive event with default = 1 (include extrusive event). The current sampling of the 2 current parameters is confusing and not useful; no basis for probabilistic sampling of intrusive:extrusive. So, for VolcanismDisruptiveScenarioFlag = 1:

a) Always have an intrusive event, with groundwater release pathway

b) If ExtrusiveEventFlag = 1 [default], then do airborne release pathway, else only do intrusive event. There are no conditions where there is only an extrusive event without an intrusive event. All igneous events (i.e., VolcanismDisruptiveScenarioFlag = 1) have an intrusive event.

2. There is no longer any need for calculating area of the volcanic dike or any need for the volcanic dike width parameter. No need to calculate overlap of conduit and dike area.

3. In *exec.f*, number of WPs ejected is always reported for subarea 2. This should vary according to the subarea for the volcanic event.

4. The dike center should be sampled uniformly over the repository footprint

I tested this SCR the results are:

1. **Passed** - *RntoDetermineIfExtrusiveOrIntrusiveVolcanicEvent*, *FractionOfTimeVolcanicEventIsExtrusive*, and *WidthofVolcanicDike [m]* were deleted from *tpa.inp*.

```

**
** 4-5-05  css SCR564: remove current Extrusive parameters and replace
**          with ExtrusiveEventFlag(0=no,1=yes)
**uniform
**RntoDetermineIfExtrusiveOrIntrusiveVolcanicEvent
**0.0, 1.0
****
**constant
**FractionOfTimeVolcanicEventIsExtrusive
**0.999

```

```

**
**
** 4-20-05  css SCR564: WidthOfVolcanicDike no longer used - remove
**uniform
**WidthOfVolcanicDike [m]
**1.0, 10.0
**

```

Passed - ExtrusiveEventFlag (iflag,1) was added to *tpa.inp*.

```

**
** 4-5-05  css SCR564: remove current Extrusive parameters and replace
**          with ExtrusiveEventFlag(0=no,1=yes)
iflag
ExtrusiveEventFlag(0=no,1=yes)
1
**

```

Modify *volcano.f* so that ExtrusiveEventFlag is used in conditional statement checks instead of RntoDetermineIfExtrusiveOrIntrusiveVolcanicEvent.

```

c  css 04/05/05; SCR564: remove Extrusive parameters and add extrusive
c    event flag
c
cc    call clearchar( 60, name )
cc    name = 'RntoDetermineIfExtrusiveOrIntrusiveVolcanicEvent'
cc    iextint = ispquery( name )
cc
cc    call clearchar( 60, name )
cc    name = 'FractionOfTimeVolcanicEventIsExtrusive'
cc    ifractext = ispquery( name )

    call clearchar( 60, name )
    name = 'ExtrusiveEventFlag(0=no,1=yes)'
    iextrusive = ispquery( name )
c end change: SCR564
c
c  css 04/05/05; SCR564: remove Extrusive parameters and replace
c    with extrusive event flag
cc    if( pext .le. fext ) then
    if (extrusive .eq. 1) then
c end change: SCR564
    lExtrusive = .TRUE.
    else
    lExtrusive = .FALSE.
    end if

    if ( lExtrusive ) then
    wpentrained = valuesp( iwpentrained )
    else
    wpentrained = 0.0d0
    end if

```

2. Remove obsolete code from *volcano.f* that used the dike width to calculate dike area, and remove code that calculates where the conduit falls with respect to the dike. Remove the

parameter FractionOfTimeVolcanicEventIsExtrusive from *tpa.inp*.

```

c css 04/05/05; SCR564:  remove obsolete parameters & variables
ccc    dikeonlyarea
ccc    fext
ccc    iextint
ccc    ifractext
ccc    iwidth
ccc    pext
ccc    width
c end change:  SCR564

cc rwj 4-22-05 scr564
      integer iwpspace
      integer irnloc

c css 04/05/05; SCR 564:  remove Extrusive parameters and add
c      extrusive event flag; remove variables no longer used
cc      integer iextint
cc      integer ifractext

      integer extrusive
      integer iextrusive
c end change:  SCR 564

cc rwj 4-22-05 scr564
cc      call clearchar( 60, name )
cc      name = 'XLocationInRegionOfInterest[m] '
cc      ixloc = ispquery( name )
cc
cc      call clearchar( 60, name )
cc      name = 'YLocationInRegionOfInterest[m] '
cc      iyloc = ispquery( name )
c
c css 04/20/05; SCR564:  remove width of dike; area of dike no
c      longer used
cc      call clearchar( 60, name )
cc      name = 'WidthOfVolcanicDike[m] '
cc      iwidth = ispquery( name )
c end change:  SCR564

cc rwj 4-23-05; scr564;
      call clearchar( 60, name )
      name = 'WPSpacingAlongEmplacementDrift[m] '
      iwpspace = ispquery( name )
      wpspace = valuesp( iwpspace )

      call clearchar( 60, name )
      name = 'RNToDetermineCenterOfVolcanicDike[] '
      irnloc = ispquery( name )
cc end scr564;
cc rwj 4-23-05 scr564;
      totdriftlength = 0.0d0
      do idrift = 1, ndriffs

```

```

        driftlength = dsqrt(
&                (drxylout(1, idrift)-drxy2out(1, idrift))**2 +
&                (drxylout(2, idrift)-drxy2out(2, idrift))**2 )
        totdriftlength = totdriftlength + driftlength
    end do

    ikey=30231

endif

c
c css 04/05/05; SCR 564:  remove Extrusive parameters and add
c   extrusive event flag
cc   pext   = valuesp( iextint )
cc   fext   = valuesp( ifractext )
      extrusive = ivaluesp( iextrusive)
c end change:  SCR564

cc rwj 4-22-05 scr564;

      eventsubarea = ivaluesp( ieventsubarea )

cc   Check event subarea.
      if (eventsubarea .lt. 1 .or. eventsubarea .gt. nsa) then
          print *, ' ***>>> Error in volcano <<<*** '
          print *, ' eventsubarea .lt.1 .or. .gt. nsa'
          print *, ' eventsubarea = ', eventsubarea
          print *, ' nsa = ', nsa
          STOP
      endif

c
cc get aml as MTU per m2. (convert using acre/m2=2.47105e-4)
      amlperm2 = aml * 2.47105d-4
cc get area of conduit
      conduitarea = pi * diam**2 /4.d0
cc multiply aml*areaofcircle to get amtuejected.
      amtuejected = 0.0d0
      if (extrusive .eq. 1) amtuejected = amlperm2 * conduitarea
      amtuperwp = valuesp( imtuperwp)
cc End of scr564
cc rwj 4-23-05;scr564
cc   call gsarea( i, area )
cc   call gsamtu( i, amtupersa )
      wpentrained = 0.0d0
      if (i .eq. eventsubarea) then
          wpentrained = amtuejected / amtuperwp
      end if
cc End of scr564

c
c css 4/20/05; SCR564:  dike width not needed; dike area no
c   longer used
cccc   Find dike area in subarea
cc   call qlhitsa( xyp1, xyp2, i, iflaglhit, alengthinsa )
cc   if (iflaglhit .eq. 1) then
cc       dikeareainsa = alengthinsa * width
cc   else

```

```

cc          dikeareainsa = 0.0d0
cc          endif
c end change: SCR564

cc          If extrusive
c
c css 04/05/05; SCR564: delete Extrusive parameters and replace
c          with extrusive event flag
cc          if( pext .le. fext ) then
c
cc          if (extrusive .eq. 1) then
c end change: SCR564

c css 04/20/05; SCR564: dike area and overlap no longer used
c          just need to calculate amtuejected
cc          if (iflagchit .eq. 1) then
cc          amtuejected = amtupersa * conduitarea / area
cc          end if
cc
cccc       Find overlap between conduit and dike
cccc       Test for conduit in subarea
cc          if( iflagchit .eq. 1 ) then
cc          amtuejected = amtupersa * conduitarea / area
cc
cccc       Test for conduit completely contained in dike.
cc          if (width .ge. diam) then
cc
cccc       Conduit is inside dike
cc          overlaparea= pi*diam**2.d0/4.d0
cc          else
cc
cccc       Conduit exceeds dike width
cccc       Find portion (overlap) of dike inside conduit
cc          overlaparea = pi*diam**2.d0/4.d0 -
cc          &          diam**2.d0/2.d0*dacos(width/diam) +
cc          &          width/2.d0*dsqrt(diam**2.d0 - width**2.d0)
cc          endif
cc          else
cc          conduitarea = 0.d0
cc          overlaparea = 0.d0
cc          endif
cc          endif

cc
cc          dikeonlyarea = dikeareainsa - overlaparea
c end change: SCR564

cc rwj 4-22-05 scr564
cc amtufailed = amtu released due to intrusive failures in drift
cc wpfailedinsa = intrusive failures in drift
cc wpentrained = wp ejected if event is in this subarea, else 0.
cc failedfraction = intrusive plus extrusive failed fraction for this subarea.
Passed - Removed from tpa.inp
** 4-5-05 css SCR564: remove current Extrusive parameters and replace

```

```
**          with ExtrusiveEventFlag(0=no,1=yes)
**uniform
**RNtoDetermineIfExtrusiveOrIntrusiveVolcanicEvent
**0.0, 1.0
****
**constant
**FractionOfTimeVolcanicEventIsExtrusive
**0.999
**
```

End of SCR 564

Albert Lozano -Work done from June 22, 2005 to Aug 04, 2005 follows.

SCR 567

Developed the test test plan and performed the tests for SCR567
Testing is still in progress.

End of SCR 567

SCR 568

I implemented the changes to correct the problem described in the SCR

4. Affected Software Module(s), Description of Problem(s): *ashremob.f*, *tpa.inp*,
tpanames.dbs, and *remob_lut.dat*.

Implement code changes specified in Attachment C of SCR482.
The *ashremob.f* module makes use of files that are not available at run time (*gs_*.dat*).
Use *gnewdf.dat* file instead. Change *tpa* input file variable from
ReceptorAgeGroup(1=Nfnt,2Tod,3PTeen,4Teen,5Adlt,6AdltFGR11) to
Age&Dosimetry(1=Inf,2=Tod1,3=PTeen,4=Teen,5=Adlt,6=AdltFG11)

I implemented the changes described in attachment A.

Attachment A: List of code changes resulting from the acceptance review
of SCR482.

I implemented the changes described in attachment B

Attachment B: List of code modifications to use gsnewdf.dat in place of gs_*.dat files.

End of SCR 568

SCR 587

Development of test plan in progress.

End of SCR 587

SCR 588

Development of test plan in progress.

End of SCR 588

Entries into Scientific Notebook #612-11E for pages 1-12 have been made by Albert Lozano.

It should be noted that periodic printing of sections of this notebook may result in non-sequential page numbers even though there is no missing content. This may be caused by different printers having different fonts from the ones used for the original document.

No original text entered into this Scientific Notebook has been removed.

QRW for A. Lozano ^{QRW} ~~September 29, 2006.~~ 3/14/07

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

see attached checklist on Pg 15

JRW

3/14/07



GEOSCIENCES AND ENGINEERING DIVISION

SCIENTIFIC NOTEBOOK REVIEW CHECKLIST RECORD

Scientific Notebook No.: 612-116 Project Numbers: 06002.01.354

Accomplished

- QAW 1. Initial entries per QAP-001
- QAW 2. Dating of entries
- QAW 3. Corrections (crossed out, one line through w/initials/date) N/A
- QAW 4. No White out used
- QAW 5. Page number visible on copy or original notebook
- QAW 6. In process entries per QAP-001
- QAW 7. Figure information present N/A
- QAW 8. Text readable
- QAW 9. Copyrighted material is identified N/A
- QAW 10. Permanent ink or type only
- QAW 11. Signing of entries (not required on each page) not signed, but entries identified on each page.
- QAW 12. Electronic media in the scientific notebook properly labeled N/A
- QAW 13. NRC Supplementary Scientific Notebook Questions are addressed. see pg 16

Any discrepancies must be resolved before notebook closeout.

=====

I have reviewed this scientific notebook and find it in agreement with QAP-001.

[Signature]
Manager's Signature

3/14/07
Date

Attach this completed form to the last page of the notebook.